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DEFORMATION TWINNING

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CONTENTS

NOTATION

a	edge length of unit cell
$\mathbf{a}_i$	base vector of parent crystal
$\mathbf{a}^i$	reciprocal base vector
a, b, c, d	{111} planes of Thompson tetrahedron
A	coordinate system defined by base vectors $\mathbf{a}_i$
A	coefficient in expression for the elastic energy of a plate
A, B, C, D	vertices of Thompson tetrahedron
$\mathbf{b}_i$	base vector of twin crystal
$\mathbf{b}^i$	reciprocal base vector
$\mathbf{b}^{(I)}$	base vector of twin crystal with orientation relation I
$\mathbf{b}_T$	Burgers vector of twinning dislocation
$\mathbf{b}_A$	Burgers vector of dislocation in parent crystal
$\mathbf{b}_B$	Burgers vector of dislocation in twin crystal
B	coordinate system defined by base vectors $\mathbf{b}_i$
c	edge length of unit cell in tetragonal or hexagonal crystals
c^i	components of lattice vector joining adjacent $\mathbf{K}_1$ planes
c_{ij}	elastic stiffness constants
c	concentration of solute
C	correspondence matrix (parent to twin)
$\mathbf{C}^{-1}$	inverse correspondence matrix (twin to parent)
C^i_j	components of **C**
d	interplanar spacing of lattice planes parallel to $\mathbf{K}_1$
$\bar{d}$	spacing of rational facets resolved normal to irrational interface
d	mean grain diameter
g	unit vector parallel to $\boldsymbol{\eta}_2$
ΔG	free energy of homogeneously formed twin embryo
ΔG_c	critical free energy of twin embryo
G	metric tensor
G_{ij}	ijth component of $\mathbf{G}\,[=\mathbf{a}_i \cdot \mathbf{a}_j]$
$\mathbf{G}^{-1}$	reciprocal metric tensor
h	height of step in $\mathbf{K}_1$ interface
$(h_i)_T$	indices of plane **h** in twin (reciprocal lattice) coordinates
I	unit matrix
I, I'	cell factors
k	primitive reciprocal lattice vector normal to $\mathbf{K}_1$
k_m	solid–liquid distribution coefficient
$\mathbf{K}_1$	invariant plane of twinning shear (twinning or composition plane)
$\mathbf{K}_2$	undistorted (but rotated) plane (conjugate twinning plane)
l	unit vector parallel to $\boldsymbol{\eta}_1$
${}^A l^i$	ith contravariant component of **l** in co-ordinate system A
L	rotation matrix relating co-ordinate axes
L^i_j	ijth component of **L**
m	integer used to characterize shuffling in Bevis–Crocker theory
m	unit normal to $\mathbf{K}_1$
${}^A m_i$	ith covariant component of **m** in co-ordinate system A
m′	covariant components m_i of **m** represented as a row matrix
M	number of twinning dislocations in wall
n	unit normal to $\mathbf{K}_2$
N	number of twinning dislocations in pile-up
p	positive integer $\leqslant q$
P	plane of shear
q	number of $\mathbf{K}_1$ planes intersected by **w**
$\tilde{q}$	number of $\mathbf{K}_2$ planes intersected by **k**
r	positive integer $\leqslant q$
r_i	core radius of dislocation
R	long semi-axis of oblate spheroidal twin
R	radius of dislocation loop
s	magnitude of shear
S	simple shear tensor (or its matrix representation)
${}^A\mathbf{S}$	matrix representation of **S** in co-ordinate system A
S^i_j	ijth component of **S**
${}^A S^i_j$	ijth component of **S** in co-ordinate system A

$\mathbf{t}$	a non-lattice repeat vector
$\mathbf{u}$	lattice vector of a parent crystal or column matrix representation of the vector
u^i	ith contravarient component of $\mathbf{u}$
${}^{\mathrm{A}}\mathbf{u}$	column matrix representation of $\mathbf{u}$ in co-ordinate system A
${}^{\mathrm{A}}u^i$	ith contravariant component of $\mathbf{u}$ in co-ordinate system A
$[v^i]_{\mathrm{T}}$	components of $\mathbf{v}$ in twin-based co-ordinate system
v	volume of twin embryo
$\mathbf{v}$	lattice vector of a twin crystal or column matrix representation of the vector
v^i	ith contravarient component of $\mathbf{v}$
${}^{\mathrm{B}}\mathbf{v}$	column matrix representation of $\mathbf{v}$ in co-ordinate system B
${}^{\mathrm{B}}v^i$	ith contravariant component of $\mathbf{v}$ in co-ordinate system B
$\mathbf{w}$	primitive lattice vector parallel to $\boldsymbol{\eta}_2$
$\mathbf{W}$	correspondence matrix with integral components $[=m\mathbf{C}]$
ΔW	energy needed to form loop of twinning dislocation
ΔW_{c}	critical energy to nucleate twinning dislocation
x^i	contravariant components of a vector in an orthonormal basis
y	short semi-axis of oblate spheroidal twin
y_{c}	critical semi-thickness of homogeneously nucleated twin
$\mathbf{Y}$	matrix used in Bevis–Crocker theory
$\mathbf{z}$	vector defining a twin site
z^i	contravarient component of $\mathbf{z}$ in twin co-ordinate system B
$\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{\delta}$	face centres of Thompson tetrahedron
γ	axial ratio of tetragonal or hexagonal structures
δ^i_j	Kronecker delta ($=1$ when $i=j$, $=0$ when $i \neq j$)
$\Delta\mathbf{I}, \Delta^{\mathrm{II}}$	shuffle vectors
$\boldsymbol{\eta}_1$	direction of shear
$\boldsymbol{\eta}_2$	conjugate shear direction
μ	shear modulus
ν	Poisson's ratio
σ	surface free energy of $\mathbf{K}_1$ interface
σ'	surface free energy of step interface
σ^{f}	stacking fault energy
σ_{y}	yield or flow stress
σ_0	friction stress
Σ	reciprocal density of coincident lattice sites
τ	resolved shear stress on $\mathbf{K}_1$ in $\boldsymbol{\eta}_1$ direction

Notes: **Bold face type** is used for vectors (lower case) and second rank tensors (upper case), and for their matrix representations in particular co-ordinate systems. Column matrices of contravariant components always represent vectors whilst row matrices of covariant components represent plane normals and are distinguished by the notation $\mathbf{m}'$ for the transpose of a matrix $\mathbf{m}$. The transpose and inverse of $\mathbf{S}$ are written $\mathbf{S}'$ and $\mathbf{S}^{-1}$, respectively, and the Einstein summation convention is used. Further details may be found in Refs 23 and 20. When the usual convention for all equivalent sets of planes or directions is used to specify a crystallographic relation, the indices enclosed by { } and ⟨ ⟩ are always those of a particular variant so that permitted permutations of these indices will always give another self-consistent variant. The slightly unusual crystallographic notation ⟨uvw] used for tetragonal crystals is merely a reminder that to obtain equivalent vectors, u and v, but not w, may be permuted.

1. INTRODUCTION

The theory of deformation twinning merits attention both because of its intrinsic importance as a mode of plastic deformation in many crystalline solids and because of its close relationship to the theory of martensitic transformation. With the exception of one useful but necessarily very condensed Encyclopaedia article,[1] there has been no attempt to survey the whole of this rapidly developing field since 1973 when Mahajan and Williams[2] published a comprehensive review. Important earlier surveys include those of (R.W.) Cahn,[3,4] Hall,[5] Klassen-Neklyudova[6] and Partridge.[7] Deformation twins have long been identified in b.c.c., h.c.p. and lower symmetry metals and alloys,[1–7] and are now found

to be formed in many f.c.c. metals and alloys,[8–11] in ordered alloys[12] and other intermetallic compounds,[13] in elemental semiconductors[14] and compounds,[15] in other non-metallic compounds such as calcite and sodium nitrate,[16] and even in complex minerals[17] and crystalline polymers.[18]

At temperatures below those at which individual atoms are mobile, slip and twinning are the major deformation modes which enable a solid to change shape under the action of an applied stress. Experiments with single crystals have shown that some structures (e.g. f.c.c. metals) do not normally twin until appreciable plastic deformation by slip has been recorded, whilst in others (e.g. b.c.c. metals), twins often form in the elastic region of the stress vs strain curve before macroscopic yielding. Delayed twinning usually has a rather small effect on the actual stress vs strain curve, whereas immediate twinning is often characterized by very rapid formation of twinned regions, giving large load drops. Twinning of this latter type is also very sensitive to temperature of deformation and to strain rate, the relative contribution of twinning to the overall strain increases as the temperature is lowered or the strain rate increased. Very high strain rates, e.g. in shock-loaded or explosively deformed materials, often lead to twinning, and under such conditions, twins have been observed even in f.c.c. aluminium–magnesium alloys[11] which, according to conventional theory, should not twin because the stacking fault energy of aluminium is too high. Deformation by slip alone is frequently observed, but many investigators believe that twinning is always accompanied (or preceded) by some microslip, even though this slip may be difficult to detect.

Twinning is especially important in crystals of lower symmetry where the five independent slip systems required to satisfy the criterion for a general deformation may not be available. In this case, Taylor's "minimum total shear" hypothesis for specifying the active slip systems has to be expressed in terms of contributions to the overall deformation from both slip and twinning,[19] and is correspondingly more complex.

The classical definition of twinning[2–6,20] requires that the twin and parent (or matrix) *lattices* are related either by a reflection in some plane or by a rotation of 180° about some axis. In crystals of high symmetry, these orientations are frequently equivalent. Twin structures may form during nucleation and growth processes such as crystal growth from the vapour or liquid phases, phase transformation or recrystallization of the solid. In such cases, quite large and relatively perfect twins (i.e. containing only expected imperfections such as a reasonably low density of dislocation lines) may be produced. Another type of twinning ("transformation twinning") is found in the product structures of many martensitic transformations. Transformation twinning produces highly organized structures in which, as predicted by the crystallographic theories of martensite,[20] alternate twin lamellae of fixed thickness ratios form regular arrays. In many martensites, the twin boundaries in such an array are highly glissile, and their displacement under stress can be viewed as a highly ordered type of plastic (or in some cases pseudo-elastic) deformation.[20,21] In contrast, ordinary deformation twins usually form as individual thin plates embedded in the matrix or in contact with the free surface or a grain boundary. Deformation twins in the cubic metals, for which the twinning shear is large, are often very thin and this makes it difficult to ascertain the degree of perfection of the twin lattice.

Deformation twins form, in principle at least, by a homogeneous simple shear of the parent lattice, and this implies highly co-ordinated individual atom displacements, in contrast to the apparently chaotic processes of generation and growth of slip bands

during glide deformation. However, some recent theories of twinning require the twin to thicken by the random agglomeration of three- or four-layer twin faults which have been independently nucleated. These theories imply that deformation twins have imperfect structures containing many stacking faults. Most of the dislocations needed for slip are believed to be generated internally by double cross-slip or Frank–Read sources, and rather similar dislocation-type theories may be developed to describe deformation twinning in high symmetry structures when the shear takes place on a rational plane in a rational direction. However, it is more difficult to develop dislocation mechanisms for type I or type II deformation twinning when only the plane or the direction respectively is rational.

The present article is concerned only with deformation twinning and, to a lesser extent, with the related phenomenon of transformation twinning. The first part of the article describes in some detail the evolution of the formal crystallographic theory of deformation twinning, and its use to predict the observed twinning modes of many structures. The second part of the review is concerned with more physical aspects of deformation twinning such as mechanisms for the nucleation and growth of twins, experimental and theoretical investigations of twinning in real materials (especially the common metallic structures), and the effects of twinning on mechanical properties. A bridge between the crystallographic and physical theories is provided by studies of the atomic structure of twin interfaces, including computer simulations and high resolution electron microscopy, and of twinning dislocations and other defects.

The following topics are considered in some detail:

(1) the crystallographic theory of twinning and the choice of twinning mode,
(2) the twin interface and twinning dislocations,
(3) models for the nucleation and growth of twins, especially in b.c.c., f.c.c. and h.c.p. structures,
(4) the influence of material variables on twinning, and
(5) the accommodation of deformation twins and their role in crack nucleation.

2. CRYSTALLOGRAPHIC THEORY OF TWINNING

2.1. *Twinning Modes and Twinning Shears*

The central problem of the crystallographic theory is to understand the factors which influence the choice of twinning mode, and ultimately to predict which twinning mode or modes will operate in a given crystal structure. This problem is addressed here mainly for structures in which all atoms are equivalent, i.e. for ideally pure elements and ideally disordered solid solutions. (J.W.) Cahn[22] has emphasized that real materials are always impure, i.e. are always solid solutions with some short range order, so that "true" deformation twinning is impossible because the parent and sheared-parent structures will have different short-range order and hence different energies. This approach leads to the conclusion that all deformation twinning should strictly be regarded as a special type of stress-induced martensitic transformation, but whilst the reservation should be noted, experimental results indicate that in practice it is often unimportant, and most materials twin in the manner expected for ideal disorder.

In dealing with superlattice structures and intermetallic compounds, it is necessary to make the opposite assumption of perfect long-range order. An overview of the crystallography of the twinning modes expected in superlattice structures based on disordered f.c.c. and b.c.c.

solutions has recently been published,[12] so that only a brief discussion is included in the present review.

In the classical theory of deformation twinning, the original (parent) lattice is re-orientated by atom displacements which are equivalent to a simple shear of the lattice points, or of some integral fraction of these points. The invariant plane of this shear is called $\mathbf{K}_1$ and the shear direction η_1; the second undistorted (or conjugate) plane is $\mathbf{K}_2$, the plane containing η_1 and the normals to $\mathbf{K}_1$ and $\mathbf{K}_2$ is the plane of shear, here denoted by **P**, and the intersection of $\mathbf{K}_2$ and **P** is the conjugate shear direction η_2. The Bilby and Crocker sign convention (see Fig. 1) will be used for all specific modes of the form $(hkl)[uvw]$ and also for general indices $\{hkl\}\langle uvw\rangle$, where the indices always specify a particular variant. A particular *twinning mode* of the structure is defined when $\mathbf{K}_1$ and η_2 (or, equivalently, $\mathbf{K}_2$ and η_1) are fixed, but it is usual to specify all the crystallographic elements together with the scalar magnitude s of the shear. For a shear on the positive side of $\mathbf{K}_1$, the sign convention requires the angle between η_1 and η_2 to be obtuse in the parent crystal, the angles between η_1 and the positive normal to $\mathbf{K}_2$ and between η_2 and the positive normal to $\mathbf{K}_1$ to be acute, and the positive directions of η_1, η_2 and the positive normal to **P** to form a right-handed set. The *conjugate* or *reciprocal* mode then has the same **P** and s but $\mathbf{K}_1$ and $\mathbf{K}_2$, and η_1 and η_2 are interchanged. Twins are usually classified as type I ($\mathbf{K}_1$ and η_2 represent a rational plane and a rational direction of the parent lattice), type II ($\mathbf{K}_2$ and η_1 are rational) or compound (all four crystallographic elements are rational). In elementary treatments, this classification is based on the assumption that in order to reproduce the same lattice in a new orientation, some unit cell of the parent structure must be sheared into an equivalent unit cell of the twin. Such a unit cell may be defined by three non-coplanar vectors in $\mathbf{K}_1$ and $\mathbf{K}_2$, and the orientation of the new twin lattice relative to the original lattice is a reflection in $\mathbf{K}_1$ for a type I twin and as a rotation of 180° about η_1 for a type II twin. However, the important feature of twinning as a mode of deformation is the shape change resulting from the simple shear, so that a twin might be regarded as any reorientated region produced by a simple shear of the parent lattice. This more general definition, proposed by Bilby and Crocker,[23] leads to the prediction of additional possible modes, in which either three or four of the twinning elements may be irrational, and to non-classical orientation relations between twin and parent.

A homogeneous simple shear may be represented by the affine deformation

$$\mathbf{v} = \mathbf{S}\,\mathbf{u} \tag{1}$$

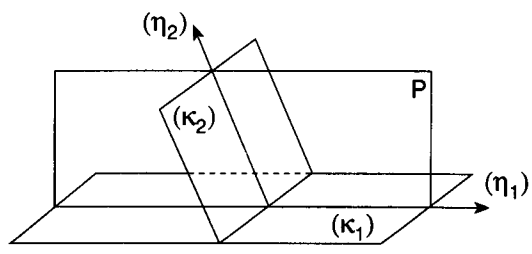

Fig. 1. The four twinning elements. The twinning and the conjugate (or reciprocal) twinning planes are $\mathbf{K}_1$ and $\mathbf{K}_2$ and the twinning and conjugate (or reciprocal) twinning directions are η_1 and η_2, respectively. The directions η_1 and η_2 and the normals to $\mathbf{K}_1$ and $\mathbf{K}_2$ are all contained in the plane of shear **P**.

where **u** and **v** are corresonding lattice vectors of the parent and twin, and **S** is a second rank tensor. If the vectors **u** and **v** are written as column matrices ${}^{A}\mathbf{u} \equiv [{}^{A}u^{i}]$, ${}^{A}\mathbf{v} \equiv [{}^{A}v^{i}]$ of their components in some co-ordinate system A, eq. (1) becomes a matrix equation in which ${}^{A}\mathbf{S} \equiv ({}^{A}S^{i}_{j})$ is a 3×3 matrix representation of the shear. Using the Einstein summation convention, this equation may be written in the alternative form

$$ {}^{A}v^{i} = {}^{A}S^{i}_{j}\,{}^{A}u^{j} \tag{2} $$

S has a particularly simple representation in an orthonormal co-ordinate system defined by the unit vector parallel to $\boldsymbol{\eta}_1$ and the unit normals to the $\mathbf{K}_1$ plane and the plane of shear; in this system all diagonal elements of ${}^{A}\mathbf{S}$ are unity and the only other non-zero element is ${}^{A}S^{1}_{2} = s$. In a general co-ordinate system,

$$ {}^{A}S^{i}_{j} = \delta^{i}_{j} + s\,{}^{A}l^{i}\,{}^{A}m_{j} \tag{3} $$

where δ^{i}_{j} is the Kronecker delta, ${}^{A}l^{i}$ are the contravariant (real space) components of a unit vector **l** parallel to $\boldsymbol{\eta}_1$ and ${}^{A}m_{i}$ are the covariant (reciprocal space) components of the unit normal to the $\mathbf{K}_1$ plane. Then if **u** is a lattice vector of the parent, its components will all be integers if the base vectors $\mathbf{a}_i$ of A define a primitive cell, and will be multiples of $\frac{1}{2}$ for a centred cell, whilst those of **v** will, in general, be irrational. However, since the vector **v** is a lattice vector of the twin lattice, it must have rational (integral or half-integral) components in a new basis B which is defined by the base vectors $\mathbf{b}_i$ of the twin lattice and is related to A by some rotation or reflection (improper rotation) **L**. This gives

$$ {}^{B}\mathbf{v} = \mathbf{L}\,{}^{A}S\,{}^{A}u = \mathbf{C}\,{}^{A}u \tag{4} $$

where **C** is called the correspondence matrix. Note that the condition that the parent and twin have the same specific volume ensures that **S**, **L** and **C** are all unimodular, i.e. have determinants of ± 1. The recent Bevis–Crocker approach to the theory of twinning makes extensive use of the properties of **C**. In tensor notation, eq. (4) becomes

$$ {}^{B}v^{i} = L^{i}_{k}\,{}^{A}S^{k}_{j}\,{}^{A}u^{j}. \tag{5} $$

For lattices or centrosymmetric structures, the two orientation relations mentioned above are the only distinct possibilities in the classical theory and twins of types I and II are often described simply as "reflection" (in $\mathbf{K}_1$) and "rotation" (about $\boldsymbol{\eta}_1$) twins respectively. Many metals form compound twins with only one orientation relationship, but this requires that the plane of shear **P** be a mirror plane. When this condition is not met, even compound twins have two possible orientation relations which have been called type I, compound and type II, compound twins respectively.[24] When the type I and type II orientations of a compound mode are equivalent, it may be described as having a "combined" orientation.[12]

When the structure does not have a centre of symmetry, there are two possible sets of atomic positions for each spatial orientation of the unit cell, leading to the four orientation relations of the classical theory of twinning (see below). In addition, the Bilby–Crocker theory allows other (non-classical) orientations as theoretical possibilities. A further complication

has become evident recently from work on the atomistic structure of twin interfaces. In some cases, the lattice sites of parent and twin may be related not by a simple shear but by a combination of a simple shear and a relative translation of the two lattices through a vector **t** which is not a repeat vector of either lattice. The pseudo symmetry elements of the combined parent and twin crystal are modified or destroyed at an atomic level by such a translation,[25–27] although this would not be evident in many measurements (e.g. selected area diffraction) which are independent of **t**.

In twinning, as in slip, some structures have a unique mode whilst others exhibit several modes which are not crystallographically equivalent. An operative slip mode is usually, but by no means invariably, characterized by the closest packed plane and direction of the structure; the operative twinning modes are similarly selected by a combination of easy atomic "shuffling" and minimum magnitude of the associated shear.

2.2. *Early Attempts to Predict Twinning Modes*

The simple crystallography of compound twins in structures of high symmetry led to a method of deducing the twinning elements by choosing a plane of mirror symmetry normal to $\mathbf{K}_1$ as the plane of shear, thus defining $\boldsymbol{\eta}_1$. A procedure of this kind has no obvious physical significance and also has the disadvantage of requiring an experimental determination of $\mathbf{K}_1$, whereas the aim of a theory should be to predict all of the twinning elements. The method does give the correct twinning elements for many of the twins observed in metals[5] but examples are known for which the basic assumption is incorrect, and the method becomes unwieldy or incorrect in cases where some of the elements are irrational. A more systematic theory was developed by Kiho[28,29] and by Jaswon and Dove[30–32] who assumed that the twinning elements may be selected by minimizing the magnitude of the shear. Since these theories have been reviewed previously,[20] only an outline description is given here.

For single lattice structures with only one atom in the primitive unit cell, Jaswon and Dove showed how to calculate the minimum twinning shear consistent with the condition that **S** carries all atoms into their correct final positions. Although this assumption may be incorrect because of an additional lattice translation **t**, the crystallographic elements of a mode are independent of **t**, so that only the shear components of the total relative displacements will affect the calculation of the mode of minimum shear. Of course, it is quite possible that the operative mode is determined by the energy, and hence by the atomic structure, of the interface, rather than simply by the value of s, but the assumption of minimum shear with no shuffles leads, in fact, to the correct prediction of the actual twinning modes of almost all the metallic single lattice structures.

When there are two atoms in the primitive unit cell (double lattice structures) some shuffling is unavoidable except in certain special modes. Jaswon and Dove analysed the possible shuffles by associating a "motif unit" of two atoms with each lattice point; during the shear, the motif unit is considered as rigid and each atom is thus given the same displacement as its lattice point, which is conveniently regarded as situated at the centre of symmetry, i.e. the mid-point of the atom pair. The simplest modes then arise from the condition that, apart again from a possible relative translation **t**, either all or one-half of the lattice points are correctly carried into twin positions by the shear. For type I twins, this leads to two basic "double lattice" ("structure") shuffles, the X′ and Y

mechanisms, and one suggested "double lattice" (combined "lattice" and "structure") shuffle, the X mechanism (see Ref. 20 for details). Essentially similar procedures may be used for type II twins in single and double lattice structures.[32]

The Jaswon and Dove division of the net atomic displacements into shear plus shuffles was also followed by Bilby and Crocker[23] in their later, more comprehensive treatment, but this division can, with equal validity, be made in other ways. In particular, if the atoms are regarded as embedded in a continuum which is sheared homogeneously to give the twin, the two atoms of a motif pair will undergo different shear displacements, and the shuffles to complete the structural change will correspondingly be different from those in the Jaswon–Dove treatment. The conditions under which there are no required shuffles are also slightly different for these two treatments (see below).

The suggestion that the magnitude of the twinning shear is an important factor in determining the operative twinning mode or modes was also made by Kiho[28,29] whose first paper predated that of Jaswon and Dove. He considered specifically the atom movements at an idealized parent–twin interface, and assumed that each atom moves to the nearest available twin site, and that the vector sum of the shuffles is zero. The shuffle mechanisms which he described included the X and Y mechanisms, together with another mechanism to explain the anomalous twins in titanium. Kiho also suggested that in choosing between a twinning mode and its conjugate, the mode for which the Burgers vector of a twinning dislocation in the interface is least should be preferred. This is equivalent to a statement that the preferred mode of a conjugate pair should be that for which the spacing of the lattice $\mathbf{K}_1$ planes is least.

2.3. *Analysis of Shears and Shuffles: The Bilby–Crocker Theory*

The available experimental results undoubtedly show for structures with a basis that shuffles may be as important as the magnitude of the shear in controlling the operative twinning modes. The theory of Bilby and Crocker[23] included a more rigorous treatment of the orientation relations and of the division of the atomic displacements into shear and shuffles. In particular, the analysis of the shuffles is the most complete currently available, so that although this theory has also been extensively reviewed,[20] it is useful to re-consider some of its salient features.

Since a parent crystal and its twin remain in contact at the interface plane during the formation of the twin, the relation between the structures must be such that this plane is invariant in any deformation carrying one lattice into the other. This is automatically accomplished in the shear description, but the orientation relations between the two lattices are not specified in terms of a shear but as proper or improper rotations. Consideration of the operations of this type which will leave the $\mathbf{K}_1$ plane unaltered leads at once to the four orientation relations of the classical theory, namely:

(I) reflection in $\mathbf{K}_1$,
(II) rotation of 180° about $\boldsymbol{\eta}_1$,
(III) reflection in the plane normal to $\boldsymbol{\eta}_1$, and
(IV) rotation of 180° about the direction normal to $\mathbf{K}_1$. (6)

As already mentioned, it is also possible to have orientations which do not correspond to any of the relations I–IV, but in which the lattices (or suitable superlattices) are nevertheless

connected by a simple shear. Non-classical twins may possibly form as a result of "double twinning",[33] but a more systematic general theory developed by Bevis and Crocker[34,35] is outlined in Section 2.4. However, there is currently no very convincing experimental evidence for the occurrence of non-classical twinning modes, so that in this section the classical orientation relations are assumed to be valid. The orientation relations I–IV, and the associated division into type I and type II twins, follow necessarily from the more general shear definition if the assumption is made that there exists a cell of the parent which is sheared into an equivalent cell of the twin.

The orientation relations of eq. (6) may be written as relations between the base vectors $\mathbf{a}_i$ and $\mathbf{b}_i$:

$$\mathbf{b}_i^{(\mathrm{I})} = \mathbf{a}_i - 2(\mathbf{a}_i \cdot \mathbf{m})\mathbf{m},$$

$$\mathbf{b}_i^{(\mathrm{II})} = 2(\mathbf{a}_i \cdot \mathbf{l})\mathbf{l} - \mathbf{a}_i,$$

$$\mathbf{b}_i^{(\mathrm{III})} = \mathbf{a}_i - 2(\mathbf{a}_i \cdot \mathbf{l})\mathbf{l}, \text{ and}$$

$$\mathbf{b}_i^{(\mathrm{IV})} = 2(\mathbf{a}_i \cdot \mathbf{m})\mathbf{m} - \mathbf{a}_i. \tag{7}$$

Since $\mathbf{b}_i^{(\mathrm{I})} = -\mathbf{b}_i^{(\mathrm{IV})}$ and $\mathbf{b}_i^{(\mathrm{II})} = -\mathbf{b}_i^{(\mathrm{III})}$, the lattices given by orientations I and IV are identical, as are those given by II and III. When the atomic positions are considered, however, the two orientations in each pair are seen to be equivalent only for structures which have a centre of symmetry. It is thus sufficient to consider only $\mathbf{b}_i^{(\mathrm{I})}$ and $\mathbf{b}_i^{(\mathrm{II})}$ when there are no more than two (identical) atoms per primitive unit cell (single or double lattice structures), but the other two relations may be needed for more complex structures.

It may readily be shown that twin orientations I and II (and III and IV) are related by a reflection in the plane of shear, **P**. Let any parent vector have components x^i in an orthonormal basis defined by **l**, **m** and the unit normal to the plane of shear, **l**Λ**m**. Then for orientation I, the twin vector has components $[x^1, -x^2, x^3]$ and for orientation II, it has components $[x^1, -x^2, -x^3]$. There is no distinction between orientations I and II if the two twin vectors are crystallographically equivalent, i.e. if the plane of shear is a mirror plane. Clearly, since orientations IV and II have position vectors which are the negatives of I and II, respectively, these two orientations are also equivalent when **P** is a mirror plane.

In their development, Bilby and Crocker prove that if **u** is a lattice vector of the parent structure, then for orientations I and II, the rational lattice vector $({}^{\mathrm{A}}u^i + {}^{\mathrm{B}}v^i)\mathbf{a}_i$ must lie in the plane $\mathbf{K}_1$.* For orientation I, this represents any vector in $\mathbf{K}_1$ whereas for orientation II it must be parallel to $\boldsymbol{\eta}_1$. Similarly for orientations II and IV, the rational vector $({}^{\mathrm{A}}u^i - {}^{\mathrm{B}}v^i)\mathbf{a}_i$ lies in the interface and is parallel to $\boldsymbol{\eta}_1$ for orientation III. Moreover, the rational vector $({}^{\mathrm{A}}u^i - {}^{\mathrm{B}}v^i)\mathbf{a}_i$ is parallel to $\boldsymbol{\eta}_2$ for orientation I and represents any vector in $\mathbf{K}_2$ for orientation II, and the same results hold for $({}^{\mathrm{A}}u^i + {}^{\mathrm{B}}v^i)\mathbf{a}_i$ with orientations IV and III, respectively. These results thus prove that if the classical orientation relations are valid, $\mathbf{K}_1$ and $\boldsymbol{\eta}_2$ must be rational for orientations I and IV (type I twinning) and $\boldsymbol{\eta}_1$ and $\mathbf{K}_2$ must be rational for orientations II and III (type II twinning). It follows that the usual assumption that a unit cell of the parent

*In Bilby and Crocker's equations, $(x^i - y^i)$ is equivalent to $({}^{\mathrm{A}}u^i + {}^{\mathrm{B}}v^i)$ and $(x^i + y^i)$ is equivalent to $({}^{\mathrm{A}}u^i - {}^{\mathrm{B}}v^i)$; the apparent change of sign arises because of the effective definition $\mathbf{y} = -\mathbf{Sx}$ instead of $\mathbf{v} = \mathbf{Su}$. More details of the Bilby–Crocker theory are given in a previous description[20] which uses the sign convention of the present review.

is sheared into an equivalent cell of the twin is valid if the twin has a classical orientation relation with its parent.

In eqs (2), (3) and (5), an upper prefix identifying the coordinate system in which the components of a vector or tensor are defined has been used but in order to simplify the equations in the remainder of this review, this prefix will now be omitted unless it is required to avoid ambiguity. Thus a unit vector in the η_2 direction may be written simply as $\mathbf{g} \equiv g^i\mathbf{a}_i$. From eq. (3), it is apparent that a twinning mode is fully specified by s, $\mathbf{l}$ and $\mathbf{m}$, but as noted in the introduction, it is also fully determined by $\mathbf{K}_1$ and η_2 (or by $\mathbf{K}_2$ and η_1). Thus if $\mathbf{K}_1$ and η_2 are known, the shear direction η_1 is given by

$$s\mathbf{l} = 2[\mathbf{m} - (\mathbf{g} \cdot \mathbf{m})^{-1}\mathbf{g}] \tag{8}$$

and the magnitude of the twinning shear is given by:

$$s^2 = 4[(g^i m_i)^{-2} - 1]. \tag{9}$$

Consider next whether or not all the parent lattice points are carried to twin lattice sites by the shear. Let $\mathbf{w} = w^i\mathbf{a}^i$ be a primitive lattice vector in the η_2 direction, and let its projection along the normal to the $\mathbf{K}_1$ plane have magnitude

$$\mathbf{w} \cdot \mathbf{m} = w^i m_i = qd \tag{10}$$

where q is a positive integer giving the number of lattice $\mathbf{K}_1$ planes of spacing d traversed by this vector. Whatever the structure of the interface, it reaches an equivalent position after moving forward a distance qd, so that the atom displacements are repeated in each successive group of q planes, and only one such group need be considered.

Let any lattice point in the nearest $\mathbf{K}_1$ plane to that through the origin be $c^i\mathbf{a}_i$ (i.e. $c^i m_i = d$). Then all the parent sites within the q planes of interest are represented by $pc^i\mathbf{a}_i$, where p is a positive integer such that $p \leqslant q$. After the homogeneous shear, the positions of these sites will become $pc^i\mathbf{a}_i + spd\mathbf{l}$, and this may be written:

$$[pc^i - (2p/q)u^i]\mathbf{a}_i + 2pd\mathbf{m}. \tag{11}$$

Now consider the positions of the twin lattice sites. The parent site defined by $\mathbf{w}$ becomes a twin site at $\mathbf{z} = z^i\mathbf{b}_i$ relative to the same origin, where

$$-z^i m_i = qd. \tag{12}$$

Since the bases A and B define similar unit cells, all other twin sites relative to this site are given by $rc^i\mathbf{b}_i$, where $r \leqslant q$ if we confine our attention to the sites in the q planes of interest. Note that the twin site defined by a particular value of r lies in the same $\mathbf{K}_1$ plane as the parent site defined by a value of p provided $p + r = q$. Thus all the twin lattice sites in these q planes are specified by the vectors

$$(z^i + rc^i)\mathbf{b}_i. \tag{13}$$

The lattice shuffles must relate the twin lattice sites to the parent lattice sites. Assume, as seems reasonable for type I twinning, that all sites in a given $\mathbf{K}_1$ plane (i.e. having a fixed value

of p) shuffle in the same way, and describe these shuffles by the vectors Δ^{I}, obtained by subtracting (11) from (13). However, for orientation I

$$c^i\mathbf{b}_i = c^i_{ai} - 2d\mathbf{m}$$

and

$$z^i\mathbf{b}_i = z^i\mathbf{a}_i + 2qd\mathbf{m}$$

so that after subtracting,

$$\Delta^{\mathrm{I}} = [(r-p)c^i + (2p/q)w^i + z^i]\mathbf{a}_i + 2d(q-r-p)\mathbf{m}. \tag{14}$$

For a given parent site, the parameters z_i and r representing the twin site may be regarded as disposable; that is, any pair of parent and twin sites may be related by the vector Δ^{I}. In general, the shuffles will probably be chosen so that $|\Delta^{\mathrm{I}}|$ is as small as possible. If $q = 1$ or 2, it is always possible to choose the parameters so that $\Delta^{\mathrm{I}} = 0$ for all sites. For $q = 1$, $p = 1$ and $r = 0$, $z_i = -w_i = -c_i$. For any value of q, the same choice of r and z_i will ensure that the sites on the plane $p = q$ do not have to shuffle, as is physically obvious. Now consider $q = 2$ and the sites on the plane defined by $p = 1$. The shuffle vectors for this plane are now all zero if $r = 1$ and $w_i = -z_i$. More generally, if q is even, the lattice points in the plane $p = q/2$, as well as those in the plane $p = q$, are sheared directly to their twin positions, as may be seen by choosing $r = p$ and $z_i = -w_i$.

A similar, slightly more complex treatment can be given for the lattice shuffle vectors Δ^{II} of a type II mode.[20] Lattice shuffling in type II twinning depends upon a parameter $\bar{q}$ which is equal to the number of $\mathbf{K}_2$ lattice planes traversed by a primitive lattice vector in the $\boldsymbol{\eta}_1$ direction. No shuffles are required for $\bar{q} = 1$ or 2, and equations similar to those given above for Δ^{I} may be developed for Δ^{II} on the assumption that all lattice sites in any $\mathbf{K}_2$ plane shuffle in the same way.

Any structure with a basis of more than one atom per primitive unit cell must normally require relative translations of the atoms ("structure shuffles") during a twinning operation. In the case of relatively simple, centrosymmetric, double-lattice structures, such shuffles may readily be classified and combined where necessary with any lattice shuffles which may be required in a particular twinning mode. This description will not be repeated here since it has essentially not been developed further since the work of Kiho, Jaswon and Dove, and Bilby and Crocker, previously reviewed.[20]

2.4. *Classical and Non-Classical Twins: The Bevis–Crocker Theory*

The Bilby–Crocker theory applies to twins which satisfy the classical orientation relations; the more general definition was first addressed by Crocker[33] who considered the possibility of "double twinning" in which a combination of two simple shears plus a rigid body rotation acts simultaneously to produce an equivalent simple shear. The two component shears and the resultant deformation must all have a principal strain equal to zero, and this restricts the combinations to be considered to those in which the two twinning directions and the normals to the two $\mathbf{K}_1$ planes are all coplanar. The two planes of shear are thus coincident, and the problem is essentially two-dimensional. Consideration of the various possible combinations of type I and type II twins shows that the plane of shear must be rational, and furthermore

all eight twinning elements of the two component twinning modes must also be rational, so that only compound modes may be combined together in this way.

The combined effect of the three component deformations is to produce an equivalent simple shear with the same rational plane of shear, so that this also represents a compound twinning mode if it satisfies one of the usual types of twin orientation relation. However, it is also possible for all four elements of the equivalent shear mode to be irrational, and this is thus an example of the more general type of twinning shear which is defined[23] as any simple shear which restores the lattice or a superlattice in a new orientation. The possible existence of "twins" with four irrational twinning elements is a remarkable result of the theory of double twinning. The assumptions of this theory nevertheless appear to be rather artificial and it seems preferable to generalize the classical theory of deformation twinning by beginning directly with the proposed general definition. The relevant theory for lattices (i.e. excluding detailed consideration of atomic shuffles) was first given by Bevis and Crocker.[34,35]

The original tensor development is transferred here to matrix notation; it utilizes certain properties of the correspondence matrix **C** defined in eq. (4). An expression for the magnitude of the shear which depends only on the correspondence matrix and the metric tensor **G** with components $G_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$ ($\mathbf{G} = \mathbf{I}$, where **I** is the unit matrix with components δ_{ij}, in an orthonormal coordinate system) may be obtained[36] from the trace of the matrix product $\mathbf{C}' \mathbf{G} \mathbf{C} \mathbf{G}^{-1}$; this relation is

$$s^2 = \mathrm{tr}(\mathbf{C}' \mathbf{G} \mathbf{C} \mathbf{G}^{-1}) - 3. \tag{15}$$

The theory is developed to show there is a restriction on the correspondence matrix

$$\mathrm{tr}(\mathbf{C}' \mathbf{G} \mathbf{C} \mathbf{G}^{-1}) = \mathrm{tr}\{(\mathbf{C}^{-1})' \mathbf{G}^{-1} \mathbf{C}^{-1} \mathbf{G}\}. \tag{16}$$

Once the correspondence is specified, it fixes not only the magnitude s but also the direction **l** of the shear and the normal **m** to the $\mathbf{K}_1$ plane, both defined here as unit vectors. For example, the equation

$$Y_{11} m_2^2 - 2 Y_{12} m_1 m_2 + Y_{22} m_1^2 = 0 \tag{17}$$

where

$$\mathbf{Y} = \mathbf{G} - \mathbf{C}' \mathbf{G} \mathbf{C} \tag{18}$$

is a quadratic in the ratio m_2/m_1 and there are two similar equations for the ratios m_3/m_2 and m_1/m_3; if **C** is known, the three equations give two possible solutions for the components of **m**. The three components of **l** may be determined directly from **m** and s, or may be derived from three similar quadratic equations derived from the components of $\mathbf{Y}^{-1}$.

Bevis and Crocker show that if the twinning mode is of type I, the matrix **C** must be of the form

$$\mathbf{C} = \mathbf{L} \mathbf{S} = -\mathbf{I} + 2 \mathbf{g} \mathbf{m}'/(\mathbf{m}' \mathbf{g}) \tag{19}$$

and the correspondence matrix for type II twinning is similarly

$$\mathbf{C} = -\mathbf{I} + 2\,\mathbf{l}\,\mathbf{n}'/(\mathbf{n}'\mathbf{l}) \tag{20}$$

The two correspondence matrices just derived are independent of the metric tensors $\mathbf{G}$ and $\mathbf{G}^{-1}$ and so give rise to classical twins in all lattices; they have the property that $\mathbf{C} = \mathbf{C}^{-1}$ so that eq. (16) is automatically satisfied. They also have the property that $\mathrm{tr}\,\mathbf{C} = -1$ and this is a useful necessary, although not sufficient, condition for $\mathbf{C}$ to represent a deformation twin of classical type.

2.5. *Operative Twinning Modes in Single Lattice Structures*

The theory of the preceding section will now be applied to the prediction of the most likely twinning modes in particular structures, assuming these modes to be governed by the magnitude of the lattice shear and the complexity and magnitude of the shuffles. Equation (9) may be rewritten as

$$s^2 = 4\frac{|\mathbf{w}|^2}{(\mathbf{w}\cdot\mathbf{m})^2} - 1. \tag{21}$$

Now writing $s \leqslant s_{\max}$, where $s_{\max}$ is any chosen maximum shear, and using eq. (10), gives

$$|\mathbf{w}|^2 \leqslant q^2 d^2\{(s_{\max}^2/4) + 1\} \tag{22}$$

which is a condition on the interplanar spacing d of a set of possible $\mathbf{K}_1$ planes and the shortest lattice vector $\mathbf{w}$ between two such planes qd apart. The inequality (22) reduces to $d^2 \geqslant |b|^2/(s_{\max}^2 + 4)$ for $q = 2$, and to $d^2 \geqslant |b|^2/4(s_{\max}^2 + 4)$ for $q = 4$, if $|\mathbf{w}|$ is replaced by $|\mathbf{b}|$. This may sometimes be convenient, but the inequality then becomes a necessary condition only (i.e. it may not be a sufficient condition) for the minimum shear on the planes of spacing d to be less than $s_{\max}$. There is no need to investigate separately the conditions for type II twinning, since the possible type I modes with $\mathbf{K}_1$ rational will automatically give the type II modes with $\mathbf{K}_2$ rational.

The inequality (22) is independent of any co-ordinate system, but in using it, care must be taken if a superlattice cell of higher symmetry is used instead of a primitive unit cell. Thus if the $\mathbf{K}_1$ planes are represented by the vector $\mathbf{k} = k_i\mathbf{a}^i$ in a primitive reciprocal lattice basis with metric $\mathbf{G}^{-1}$, the components k_i are integers with no common factor (as also are w^i). The condition (22) may thus be written

$$(G_{ij}w^iw^j)(G^{ij}k_ik_j) \geqslant (w^ik_i)^2\{(s_{\max}^2/4) + 1\}. \tag{23}$$

However, if a larger (centred) unit cell is used, and k_i and w^i are still given integral values, we have to introduce the cell factors[20] I, I' and the inequality becomes:

$$(I')^2(G_{ij}w^iw^j)(G^{ij}k_ik_j) \geqslant I^2(w^ik_i)^2\{(s_{\max}^2/4) + 1\}. \tag{24}$$

It is frequently more convenient to refer the twinning elements to a centred cell, and thus to use (24). For single lattice structures, the normally observed twinning mode has the lowest

shear consistent with the absence of shuffles. This applies in particular to the normal $\{112\}\langle 1\bar{1}\bar{1}\rangle$ mode for b.c.c. twinning and to the $\{111\}\langle 11\bar{2}\rangle$ mode for f.c.c. twinning. In almost all single lattice structures, the operative mode and its conjugate are crystallographically equivalent, and the shear is very much smaller than that of any rival "no-shuffle" mode. This is not true for mercury which is considered separately below.

In double lattice structures, more than one twinning mode may be active during deformation, but almost all of the many experimental observations of deformation twinning in cubic and tetragonal single lattice structures indicate that only the minimum shear modes are operative. However, there are isolated reports of additional twinning modes, for example in b.c.c. iron–beryllium alloys[37–39] and in b.c.t. iron–nickel–carbon martensites.[24,38] Thus, it is appropriate to consider briefly the application of the Bevis and Crocker general theory to the prediction of other possible modes, including non-classical modes, in single lattice structures.

Following the Jawson–Dove approach, eq. (15) may be rewritten as an inequality in order to list all correspondences for which the twinning shear is less than or equal to some chosen value $s_{\max}$. In particular, this gives for the cubic system

$$\mathrm{tr}(\mathbf{C}'\,\mathbf{C}) \leqslant s_{\max}^2 + 3. \tag{25}$$

The columns of $\mathbf{C}$ are the components of the vectors specifying the cell into which the reference cell defined by $\mathbf{a}_i$ is deformed by $\mathbf{S}$. The lattice is not reproduced if any of the components of $\mathbf{C}$ are irrational. When $\mathbf{a}_i$ define a primitive unit cell, the point lattices of parent and twin are identical if the columns of $\mathbf{C}$ represent lattice vectors. However, if the base vectors define a base-centred cell, it is additionally necessary that the sum of the first two columns of $\mathbf{C}$ must be twice a lattice vector, for a body-centred cell the sum of all three columns of $\mathbf{C}$ must be twice a lattice vector, and for a face-centred cell the sum of any two columns must be twice a lattice vector. When the elements of $\mathbf{C}$ are rational but do not satisfy these conditions, the point lattice produced by $\mathbf{S}$ differs from the parent lattice but has a superlattice in common, so that a twin may be produced by combining the shear with a shuffling of some fraction of the lattice sites. If some elements of $\mathbf{C}$ are fractions, a matrix $\mathbf{W} = m\,\mathbf{C}$ with only integral elements may be defined, and the inequality (25) becomes

$$\mathrm{tr}(\mathbf{W}'\,\mathbf{W}) \leqslant m^2(s_{\max}^2 + 3). \tag{26}$$

Using a trial and error procedure, Bevis and Crocker list 10 correspondences for cubic systems in which $m = 1, s_{\max}^2 = 9$, 19 correspondences for $m = 2, s_{\max}^2 = 3.5$, and 31 correspondences for which $m = 4, s_{\max}^2 = 2.5$. For primitive lattices, the fraction of the lattice points sheared direct to twin positions is $1/m$, but it may be $2/m$, $1/m$ or $1/2m$ for centred lattices.

New unimodular matrices may be derived from any given $\mathbf{C}$ by interchanging rows or columns, or changing their signs. In the cubic system, these operations simply lead to equivalent variants of $\mathbf{C}$, but in systems of lower symmetry, many non-equivalent variants may be derived from each cubic correspondence. However, some of these do not represent possible twins because the restriction of eq. (16) involves lattice parameters in non-cubic systems. Bevis and Crocker show that the possible correspondence matrices may be divided into seven different classes and there are various predicted relations between the individual twinning elements. Forty-two of the 60 correspondence matrices mentioned above represent conventional or classic modes and 18 represent non-conventional modes.

A uni-modular lattice correspondence **C** leading to twinning elements $\mathbf{K}_1\ \mathbf{K}_2\ \boldsymbol{\eta}_1\ \boldsymbol{\eta}_2\ s$ will also have an associated conjugate mode obtained by interchanging $\mathbf{K}_1$ and $\mathbf{K}_2$ and $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$. For cubic lattices, the pair of additional modes obtained by interchanging the indices of $\mathbf{K}_1$ and $\boldsymbol{\eta}_1$ and of $\mathbf{K}_2$ and $\boldsymbol{\eta}_2$ and reversing the sign of either the old or the new $\mathbf{K}_2$ and $\boldsymbol{\eta}_1$ also has the same shear magnitude although the amount of shuffling required will be different if the lattice is centred. Bevis and Crocker[35] used the 60 correspondence matrices as input data to derive the twinning elements of the corresponding modes for cubic lattices and gave examples from all seven classes of correspondence. They published a table showing a selection of their results in the form of 26 different sets of indices derived from the various matrices **C** and $\mathbf{C}^{-1}$, each giving rise, in the absence of crystallographic degeneracy, to up to four different twinning modes by applying the above permutations of indices. Of the 26 basic modes, 13 are both conventional and compound whilst the other 13 are non-conventional, and 11 of these have four irrational twinning indices of the form $x \pm y^{\frac{1}{2}}$ where x and y are integers. Many of the $\mathbf{K}_1$ planes in the compound modes are mirror planes so that the shear would reproduce the parent lattice in the same orientation and this operation could thus not be described as twinning. However, in such cases the $\mathbf{K}_2$ plane is generally not a mirror plane so that the conjugate shear represents a possible twinning mode. The plane of shear is always rational for the non-conventional modes, and this is a general feature of cubic lattices; the orientation relation may be described as a rotation about the normal to this plane of shear.

To investigate the possible twinning modes in the six non-cubic crystal systems, Bevis and Crocker first considered the modes which arise from variants of the unit correspondence matrix. The unit matrix itself leads, of course, to zero shear in all systems but nine of its variants obtained by interchanging rows, interchanging columns and changing the signs of rows and columns satisfy the restriction (16) and so may lead to twins in some crystal systems. These nine correspondence matrices are all symmetric and three of them are diagonal; they all satisfy the condition $\mathbf{C} = \mathbf{C}^{-1}$ and so represent conventional twinning modes with at least two rational elements. The nine independent modes of the triclinic system reduce to four modes in the monoclinic system, to three modes in the orthorhombic system, to a single mode (excluding shears which restore the original lattice) in the hexagonal system, to single modes in the tetragonal and rhombohedral systems, and of course to no modes in the cubic system.

The procedure was repeated for a slightly more complex correspondence which has 20 variants leading to twinning in triclinic systems, reducing to 8, 6, 3, 2 and 1 independent modes in the monoclinic, orthorhombic, tetragonal, hexagonal and cubic systems, respectively. Most of these modes are non-conventional with four irrational elements.

The twinning modes predicted for the f.c.c. and b.c.c. structures by the no-shuffle, minimum shear hypothesis are derived from the correspondence matrices **C** and **C′**, respectively, where

$$\mathbf{C} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & \bar{1} & 1 \\ \bar{2} & 2 & \bar{2} \\ 1 & 1 & \bar{1} \\ \bar{2} & \bar{2} & 2 \end{pmatrix}. \tag{27}$$

Shears of magnitude $2^{-\frac{1}{2}}$ on the $\{111\}$ plane lead to twins in the simple cubic, f.c.c. and b.c.c. structures but the fractions of parent lattice sites which are sheared directly to twin positions

are respectively $\frac{1}{2}$, 1 and $\frac{1}{4}$, whereas for a twinning shear of the same magnitude on the {112} plane, these fractions are $\frac{1}{2}$, $\frac{1}{4}$ and 1. Several other examples of f.c.c. or b.c.c. modes which involve no shuffles are found among the cubic modes listed by Bevis and Crocker, but these are all conventional type modes, and non-conventional modes with zero shuffles are only possible if shear magnitudes outside the above limits are allowed.

All reported instances of twinning in f.c.c. structures have the expected {111} habit plane but in an experimental study of twinning in iron–beryllium alloys and iron–nickel–carbon martensites, Richman and Conrad[37] and Richman[38] found evidence for b.c.c. twins with rational {013} and irrational "{089}" and "{127}" habits. However, the iron–beryllium alloys were ordered and they twinned copiously on the {112} planes whilst the untempered martensites should have been b.c.t. rather than b.c.c. and in addition presumably contained a fine structure of {112} transformation twins. These factors combined with the small size of most of the anomalous twins makes the experimental determination of the anomalous modes very difficult, and Green and Cohen[39] were unable to find evidence of the anomalous modes reported by Richman. Table 1 lists all the predicted b.c.c. "no-shuffle" modes with $s \leqslant 2$ and the modes in which one-half of the lattice points shuffle with $s \leqslant 1$. The {013} habit is seen to be a possible no-shuffle mode, albeit with a rather large shear, but the other two of Richman's reported modes are not among those predicted.

Further experiments on twinning in cubic iron–nickel and tetragonal iron–nickel–carbon martensites were reported by Rowlands *et al.*[24] who found some b.c.c. deformation twins with the {5, 8, 11} habit of Table 1. Although all four sets of indices are rational, so that the mode is compound, the orientation relationship is of type II, probably because of a minimum shuffle criterion. With a type II orientation relation, only one-half of the atoms have to shuffle whereas five-sixths of the atoms would have to shuffle to restore the structure in a type I relation. Since the $\{\bar{1}01\}$ plane is a mirror plane, the reciprocal mode is not a true twinning mode in b.c.c.; a shuffle of half the atoms results in an unchanged orientation of the original structure. Rowlands *et al.*[40] in a further investigation reported that deformation twins of other than {112} type are extremely rare, but they found some fine (possibly transformation) twins with a {145} habit which is the conjugate mode to the {013} mode reported by Richman. In contrast, Fearon and Bevis[41] in a later publication, reported only {112} transformation twins in a cubic iron–nickel alloy.

Rowlands *et al.* also tentatively identified two tetragonal derivatives of the "{5, 8, 11}" mode in the carbon-containing martensite, both of which correspond to conventional type II modes. They point out, however, that non-conventional derivatives of this mode are also possible and there seems no reason why these should not occur in suitable circumstances. Although only one-half of the atoms are sheared to the correct positions, this mode has a smaller shear than the usually observed b.c.c. mode (see Table 1). A possible reason for its occurrence in martensites is that in the cubic structure the {5, 8, 11} twin can propagate undeviated across a {112} twin boundary, and hence across the set of fine parallel {112} twins which are produced by the transformation mechanism. Bevis and Vitek[42] suggested that a possible reason for the observation of some fine {145} twins in martensite is that a determining factor is the interfacial energy of the coherent $\mathbf{K}_1$ habit plane, rather than the magnitude of the shear, since atomistic calculations indicate that the {145} habit has the next lowest interfacial energy after {112}.

The present position seems to be that the anomalous twinning modes have been identified in the b.c.t. structure with no more certainty than in b.c.c. and the overwhelming majority of observations on both deformation and transformation twins in b.c.t. martensites show only

Table 1. Predicted and Observed Twinning Modes in Single Lattice Structures

Structure	$\mathbf{K}_1$ { }	$\mathbf{K}_2$ { }	$\boldsymbol{\eta}_1$ ⟨ ⟩	$\boldsymbol{\eta}_2$ ⟨ ⟩	s	$\mathbf{P}$ { }	References to some supporting experimental studies
f.c.c.	111	$11\bar{1}$	$11\bar{2}$	112	$2^{-\frac{1}{2}}$	$1\bar{1}0$	Cu,[8,103] Ag and Cu alloys,[9,144,159,162,163] Ni,[10,169,170] Al alloys[11, 205] and Co–Fe alloys[19,158,243,259]
b.c.c.	112	$\bar{1}\bar{1}2$	$\bar{1}\bar{1}1$	111	$2^{-\frac{1}{2}}$	$1\bar{1}0$	Fe and its alloys,[147,153,154,206,207,223,226,227,229,285–290] Nb and its alloys,[151,224,225] Mo–Re alloys[104–106,150,256] and Mo[228]
(no shuffle)	147	$\bar{1}01$	$\bar{3}\bar{1}1$	111	$3^{\frac{1}{2}}/2^{\frac{1}{2}}$	$\bar{1}2\bar{1}$	
	112	110	$11\bar{1}$	001	$2^{\frac{1}{2}}$	$1\bar{1}0$	
	013	$4\bar{1}5$	$5\bar{3}1$	$\bar{1}11$	$7^{\frac{1}{2}}/2^{\frac{1}{2}}$	$\bar{2}\bar{3}1$	Fe–Be alloys[37,38]
b.c.c.	112	$33\bar{2}$	$11\bar{1}$	113	$2^{\frac{1}{2}}/4$	$1\bar{1}0$	
($\frac{1}{2}$ atoms	5,8,11	$\bar{1}01$	$\bar{5}\bar{1}3$	111	$6^{\frac{1}{2}}/4$	$\bar{1}2\bar{1}$	Fe–Ni and Fe–Ni–C martensites[24]
shuffle	145	$34\bar{1}$	$11\bar{1}$	$\bar{1}39$	$7/58^{\frac{1}{2}}$	$3\bar{2}1$	Fe–Ni alloy[40]
	013	$0\bar{1}1$	031	011	1	$\bar{1}00$	
f.c.t.	011	$0\bar{1}1$	$0\bar{1}1$	011	$\gamma^{-1}-\gamma$	$\bar{1}00$	
	111	$11\bar{1}$	$11\bar{2}$	112	$(2\gamma^2-1)/2^{\frac{1}{2}}\gamma$	$1\bar{1}0$	
b.c.t.	011	$0\bar{1}1$	$0\bar{1}1$	011	$\gamma^{-1}-\gamma$	$1\bar{1}0$	
(no shuffle)	112	$\bar{1}\bar{1}2$	$\bar{1}\bar{1}1$	111	$(2-\gamma^2)/2^{\frac{1}{2}}\gamma$çê	$1\bar{1}0$	
	121	a	b	111	$(2-5\gamma^2+5\gamma^4)^{\frac{1}{2}}/2\gamma$	d	
b.c.t.	e	$\bar{1}01$	$\bar{5}13$	f	$(26-29\gamma^2+9\gamma^4)^{\frac{1}{2}}/4\gamma$	g	
($\frac{1}{2}$ atoms shuffle)	h	$\bar{1}10$	$\bar{5}3\bar{1}$	111	$(4+2\gamma^2)^{\frac{1}{2}}/4$	$11\bar{2}$	
f.c. rhombohedral	011	100	100	011	$8^{\frac{1}{2}}c/(1+2c)^{\frac{1}{2}}(1-c)^{\frac{1}{2}}$	$0\bar{1}1$	
	j	$\bar{1}11$	$\bar{1}21$	k	$\dfrac{(2+8c+22c^2)^{\frac{1}{2}}}{2(1-c)^{\frac{1}{2}}(1+2c)^{\frac{1}{2}}}$	m	Hg[43–45]

Notes: The two f.c.t. modes are linked to their equivalent b.c.t. modes. All b.c.c. no shuffle modes with $s \leqslant 2$ and half-shuffle modes with $s \leqslant 1$ are included, but not all the derived b.c.t. modes are listed. γ is the axial ratio of the appropriate tetragonal lattice ($\simeq 1.035$ for b.c.t. martensite), and c ($\simeq -1/7$ for Hg) is the cosine of the rhombohedral interaxial angle. The irrational indices a, b and d-m are:

a $= \gamma^2-2, 3\gamma^2, 2-3\gamma^2$; b $= -1-\gamma^2, 3\gamma^2-1, 3-5\gamma^2$; d $= 2\gamma^2-1, 1-\gamma^2, -\gamma^2$; e $= 14-9\gamma^2, 8, 26-15\gamma^2$; f $= 5-3\gamma^2, 1+\gamma^2, 5-3\gamma^2$; g $= -1, 5-3\gamma^2, -1$; h $= 6-\gamma^2, 10+\gamma^2, 8\gamma^2$; j $= -1-5c, -1-c, 1-3c$; k $= -1-7c, -2-6c, 1-c$; m $= 1+c, -2c, 1+5c$.

*Predicted minimum-shear, no-shuffle modes which have not been observed.

the dominant twinning mode to have the same elements as the b.c.c. {112} mode and a shear $s = 2^{\frac{1}{2}}(a/c) - 2^{-\frac{1}{2}}(c/a)$. This mode is derived from the correspondence (27); it is also the same mode as that deduced for the f.c.t. structure. Any b.c.t. structure may, of course, alternatively be regarded as f.c.t. with $a_{\text{fct}} = 2^{\frac{1}{2}}a_{\text{bct}}$ and when this change is made the {112} plane of the b.c.t. structure becomes the {101} plane of the f.c.t. structure, with similar changes of the other twinning elements as shown in Table 1. When face-centred indices are used, this twinning mode arises from four of the variants of the unit correspondence matrix and when the axial ratio is made equal to unity so that the structure is f.c.c., the shear becomes zero and the twinning mode ceases to exist. When the structure becomes b.c.c., on the other hand, the shear is not zero but $2^{-\frac{1}{2}}$ and the usual b.c.c. crystallography applies. There are equivalent relations between the b.c.t. {011} mode and the f.c.c. {111} mode, and these are also shown in Table 1. In general, it is convenient to choose the unit cell of a centred tetragonal structure so that the axial ratio differs as little as possible from unity. Thus ferrous martensites with interstitial solutes are described as b.c.t. and have twinning shears of approximately $2^{-\frac{1}{2}}$ since the {011} b.c.t. low shear mode apparently does not operate, whereas indium and its alloys are described as f.c.t. and have very small twinning shears.

Twinning in solid mercury which has a rhombohedral structure is notable, as the only other known example of a single lattice structure in which the no-shuffle, minimum shear mode is not the operative twinning mode. In contrast to the other single lattice structures, the predicted lowest shear mode and its conjugate are not crystallographically equivalent for the rhombohedral structure, so that there are two possible $\mathbf{K}_1$ planes, namely (001) and (110) for shears of lowest magnitude. Early observations suggested that only the (110) plane is operative, but later results[43–45] show that the true mode is of type II with an irrational habit plane close to $(\bar{1}\bar{3}5)$. The elements of this mode are given in Table 1; it involves no shuffles and has the second smallest shear, which is nevertheless appreciably larger than the shear of the (001)–(110) conjugate pair (0.63 and 0.46 respectively for mercury). The conjugate type I mode is seen from Table 1 to have a $(\bar{1}11)$ $\mathbf{K}_1$ plane, but apparently does not occur. Crocker speculates that this may be because the slip plane is also (111) and points out that the same reason was previously advanced for the non-appearance of the (001) mode at a time when both the slip plane and the twinning plane had been incorrectly determined. It is also interesting to note that the observed mode has the same correspondence (27) as the f.c.c. and b.c.c. modes whilst the unobserved minimum shear modes are derived from variants of the unit correspondence matrix.

2.6. *Twinning in Superlattices*

The twinning modes of the pure components which have single lattice structures are normally also found for essentially disordered solid solutions based on these single lattice solvents. However, if long-range ordering produces a perfect or imperfect superlattice structure, the ordinary twinning mode may become a pseudo mode which will give incorrect ordering in the sheared lattice. A true twin would then require atoms to change places in addition to the shear, but such "interchange shuffles" are clearly not possible at the temperatures and strain rates of deformation twinning.[12] For superlattice structures which retain cubic symmetry, all variants of the normal mode become pseudo-modes of the superlattice, and the true modes of lowest shear without shuffles have $s = 2^{\frac{1}{2}}$ or $8^{\frac{1}{2}}$. These true modes are listed in Table 2, but only the $L1_2$ mode actually seems to occur. The B2 mode, which is also included among the possible b.c.c. modes of Table 1, has the same shear as the $L1_2$ mode but has not been observed. Some B2 alloys are known to form pseudo twins in

Table 2. Possible true twinning modes in cubic superlattices[12]

Mode no.	S	$\mathbf{K}_1$	$\mathbf{K}_2$	$\boldsymbol{\eta}_1$	$\boldsymbol{\eta}_2$	s^2	True twin in	Some supporting experimental results
(a) *Modes without shuffles*								
1.3	(110)	$(1\bar{1}1)$	(001)	$[\bar{1}12]$	$[1\bar{1}0]$	2	$L1_2$	Cu_3Au[49,50] and $Ni_3(Al,Ti)$[51,52]
1.3^T	(110)	$(\bar{1}12)$	$(\bar{1}10)$	$[\bar{1}1\bar{1}]$	[001]	2	B2	Ti–Ni and Ti–Fe–Ni alloys[48]
1.9	$(\bar{1}\bar{1}0)$	$(\bar{1}12)$	(001)	$[1\bar{1}1]$	$[\bar{1}10]$	8	B2, B32, $D0_3$, $L1_2$	$Fe_3Al(D0_3)$[47]
1.9^T	$(\bar{1}\bar{1}0)$	$(1\bar{1}1)$	$(1\bar{1}0)$	$[1\bar{1}\bar{2}]$	[001]	8	B2, B32, $D0_3$, $L1_2$	
(b) *Modes with* 50% *(non-interchange) shuffles*								
2.3^T	(110)	$(1\bar{1}\bar{4})$	$(1\bar{1}0)$	$[2\bar{2}1]$	$[00\bar{1}]$	$\frac{1}{2}$	B2	Ti–Ni and Ti–Fe–Ni alloys[48]
1.2	(001)	$(1\bar{2}0)$	(100)	[210]	$[0\bar{1}0]$	1	B2, $L1_2$	
2.5	(001)	$(\bar{1}30)$	(110)	[310]	$[\bar{1}10]$	1	B2, B32, $D0_3$	
1.3	(110)	$(1\bar{1}1)$	(001)	$[\bar{1}12]$	$[1\bar{1}0]$	2	B2, B32, $D0_3$	
1.3^T	(110)	$(\bar{1}12)$	$(\bar{1}10)$	$[\bar{1}1\bar{1}]$	[001]	2	$L1_2$	

preference to the higher shear, true mode, whilst in others an alternative twinning mode of lower shear in which 50% of the atoms undergo non-interchange shuffles has been found experimentally.

The pseudo mode in B2 is formally a martensitic transformation from the simple cubic structure with space group $Pm\bar{3}m$ to an orthorhombic structure of space group Cmmm. The product structure is sometimes erroneously stated to be tetragonal because two of the axes of the orthorhombic cell are equal in the idealized case of no change of lattice parameters on ordering. Relaxation of the parameters will lead, in principle, to three unequal axes but this may be difficult to detect. Since the pseudo mode and the true mode of lowest shear have the same $\mathbf{K}_1$ plane, it is thus essential to obtain experimental evidence of either the symmetry of the product or the magnitude of the shape deformation in order to establish which mode is operating. For a two-phase α + B2 structure in alloys of approximate composition Fe_3Be, Green and Cohen[39] showed that there is indeed the anticipated change of symmetry in the very small, coherent B2 regions within the much larger twins, and they linked this observation with the pseudo-elastic behaviour of these alloys.

Iron–beryllium alloys with compositions near Fe_3Be were formerly reported to form a DO_3 superlattice on ordering. Several authors have stated that deformation twinning is impossible in this structure, but Fig. 2 and Table 2 show that *geometric* twinning without shuffles may readily be defined. However, the very large shear makes this twinning mode very improbable in practice, and there are no reported observations of deformation twinning in either the DO_3 or the B32 structures. Rather similar but less complete results have been found for iron–aluminium alloys variously reported to have either the B2 or the DO_3 structure. Cahn and Coll[46] found that alloys with less than 50% long range order form pseudo twins, but that twinning was suppressed in more highly ordered alloys. Guedo and Rieu[47] obtained evidence for twinning and detwinning in alloys with the B2 structure and super-elastic effects in alloys with the DO_3 structure, but it is uncertain whether or not this latter effect is due to pseudo-twinning.

As an alternative to a pseudo mode or a high shear mode, it is possible that a twin might form in a superlattice by a mode which requires non-interchange shuffles. The first evidence

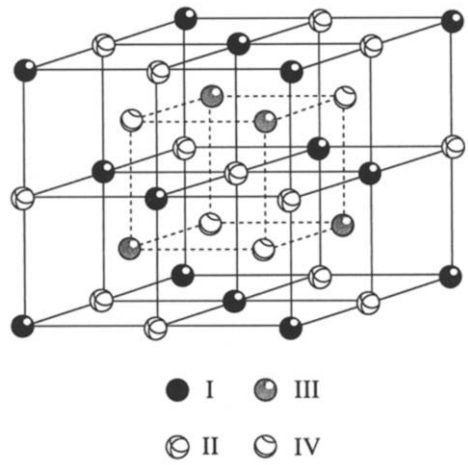

Fig. 2. Atomic site occupancy for B2, B32 and DO_3 cubic superlattices. B atoms occupy sites I and II in the B2 structure, I and III in the B32 structure and I in the DO_3 structure (after Christian and Laughlin[12]).

for such a mode was given by Goo *et al.*[48] for titanium–nickel and titanium–iron–nickel alloys with the B2 structure. The mode, which involves shuffles of half the atoms ($q = 4$ in both the b.c.c. and simple cubic lattices), has the same shear magnitude as the disordered b.c.c. mode but $\mathbf{K}_1 = \{114\}$ and $\boldsymbol{\eta}_1 = \langle 22\bar{1} \rangle$; the full indices are shown in Table 2. This table also gives the other possible modes with 50% shuffles, all of which have higher shear magnitudes. The shuffles involved are relatively simple and have been discussed by Goo *et al.* and by Christian and Laughlin.[12] Assuming that all atoms are displaced by the shear (i.e. the motif units are *not* treated as rigid), the atoms which must shuffle are alternately A and B on successive planes of shear and are contained in alternate $\mathbf{K}_2$ planes normal to the plane of shear. Goo *et al.* suggested that these atoms are all displaced in the same direction (see Fig. 3(c-i)); alternative possibilities in which the atoms move in opposite directions in successive $\mathbf{K}_2$ shuffle planes or in successive rows of one shuffle plane are shown in Fig. 3(c-ii) and 3(c-iii).

In contrast to B2, pseudo-twinning has not been reported in $L1_2$ structures, but there is evidence for the true mode of Table 2 in Cu_3Au alloys[49,50] and in microtwins in $Ni_3(Al, Ti)$ γ' phases.[51,52] In their work on Cu_3Au, Chakraborty and Starke[50] found that the true mode was observed only in alloys with nearly complete long-range order, whilst disordered or partially ordered alloys formed twins with the usual f.c.c. mode. The f.c.c. type twinning was also observed in highly ordered alloys tested in compression to relatively high strains, which would have reduced the initial long-range order. In this case, the twins formed only at applied shear stresses an order of magnitude larger than those required to produce true twins of the ordered structure.

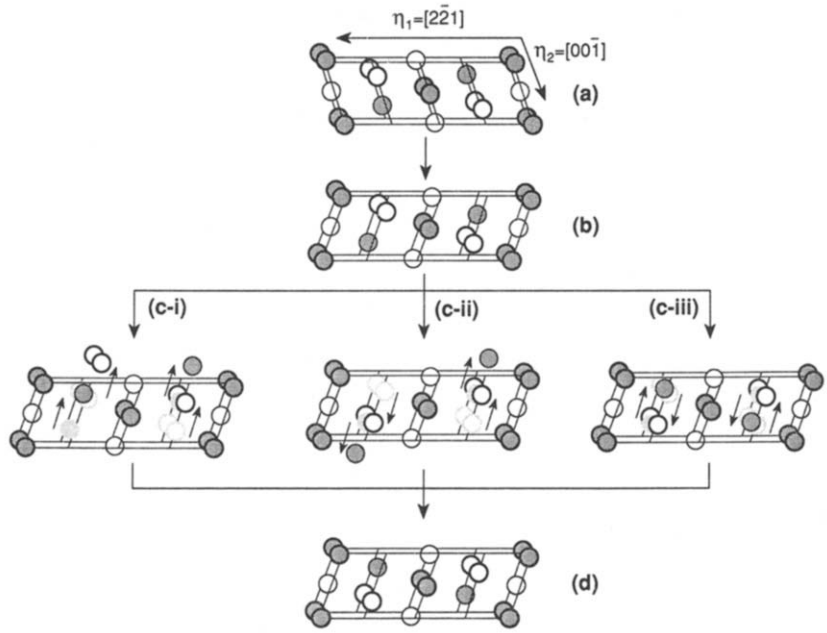

Fig. 3. Schematic illustration of the {114} shuffle mode in the B2 structure. B and A atoms are shown by shaded and open symbols, respectively. (a) Parent structure; (b) sheared structure; (c) (i), (ii) and (iii) alternative possible shuffles; (d) combined orientation twin (after Christian and Laughlin[12]).

For non-cubic superlattices of the f.c.c. structure, the variants of the usual f.c.c. mode may be divided into six pairs, each comprising a mode and its conjugate and having one of the six cubic {110} planes as the plane of shear. Four of the superlattices listed by Richards and Cahn[53] are tetragonal, with either two or, in the case of Ni_4Mo, four f.c.c. mode pairs which give true twins in the superlattice. There are 5, 3, 3 and 3 possible true mode pairs for the orthorhombic (Pt_2Mo), the two (predicted but unobserved) monoclinic superlattices and the rhombohedral ($L1_1$) superlattice, respectively. Experimental results have been reported for the $L1_0$, Pt_2Mo, DO_{22} and D1a structures.

The most complete investigation of twinning in the tetragonal $L1_0$ structure is that of Shechtman *et al.*[54] for a Ti–Al alloy. The specific variants of the $\{111\}\langle 11\bar{2}\rangle$ cubic twin which formed during deformation were identified and shown to correspond to the true modes of the superlattice, and the shear magnitude was also measured. There are several experimental investigations of the CuAu I superlattice with the $L1_0$ structure, among which we may mention that by Pashley *et al.*[55] who concluded that {111} twinning is an important deformation mechanism and speculated that the structure may be changed in some of the twins.

Hansson and Barnes[56] and Pashley *et al.* pointed out that the structure produced by pseudo twinning of $L1_0$ has a single set of {111} cubic planes which are alternately occupied by atoms of each species, so that this structure is effectively that of the $L1_1$ (CuPt) superlattice. The reverse is also true; the pseudo mode of $L1_1$ yields the $L1_0$ structure. Unfortunately, there are no experimental results on twinning in $L1_1$.

Except at high temperatures, twinning is frequently the major deformation mechanism in alloys with the tetragonal DO_{22} structure, and it has been studied extensively in Ni_3V[57–59] and in Al_3Ti.[60,61] The deformation always utilizes only the four true modes (two mode pairs) derived from disordered f.c.c. modes.

Finally, twinning has been established, but not fully investigated in the D1a structure of Ni_4Mo[62] and in certain nickel–molybdenum–chromium alloys with the orthorhombic Pt_2Mo structure.[63] The true twins in Ni_4Mo are type I–type II in each conjugate pair, whereas in the Ni_3Pt structure, one mode pair gives true twins with combined orientations and four pairs give type I–type II orientations. In both structures, it seems probable that true twins are formed but the detailed crystallography was not established.

2.7. *Twinning Modes in Hexagonal Close-Packed Structures*

The most important double lattice structure is the h.c.p. structure with axial ratios (γ) differing by varying amounts from the ideal value of $(8/3)^{\frac{1}{2}} = 1.633$, which corresponds to the close-packing of spherical atoms. The metals cadmium and zinc with the rather high axial ratios of 1.886 and 1.856, form a separate sub-group, whilst the remaining metals have axial ratios ranging from slightly smaller than 1.633 (cobalt and magnesium) down to 1.568 (beryllium). All the metals twin on $\{10\bar{1}2\}$, but most of the low axial ratio metals also have several other active modes. Additional $\mathbf{K}_1$ planes reported for titanium, for example, are $\{10\bar{1}1\}$, $\{11\bar{2}1\}$, $\{11\bar{2}2\}$, $\{11\bar{2}3\}$ and $\{11\bar{2}4\}$, and additional modes for magnesium include $\{10\bar{1}1\}$, $\{30\bar{3}4\}$, $\{10\bar{1}3\}$ and $\{10\bar{1}4\}$. Some of these "anomalous" twinning modes are well established; in others, the identification of habit plane traces as twins is open to some doubt. Experimental determination of all the elements of a mode is not possible unless the shear is measured, and this is rather difficult.

Early work showed that the full description of the $\{10\bar{1}2\}$ mode is

$$\mathbf{K}_1 = \{10\bar{1}2\}; \quad \mathbf{K}_2 = \{\bar{1}012\}; \quad \boldsymbol{\eta}_1 = \langle 10\bar{1}\bar{1}\rangle; \quad \boldsymbol{\eta}_2 = \langle \bar{1}01\bar{1}\rangle.$$

$$\text{Plane of shear} = \{1\bar{2}10\}; \quad s = (\gamma^2 - 3)/3^{\frac{1}{2}}\gamma \tag{28}$$

This is one of the two hexagonal modes derived from variants of the unit correspondence matrix applied to the orthohexagonal basis. A systematic investigation of the low shear, simple shuffle modes for the ideal axial ratio, shows that there are eleven such modes with $s < 1$ and $q \leqslant 4$, whilst Crocker and Bevis[64] listed fifteen possible modes satisfying these restrictions for the axial ratio ($\gamma = 1.587$) of titanium. For all likely values of γ, the $\{10\bar{1}2\}$ mode gives the lowest shear, and there can be little doubt that this is an important factor in the universal observation of this mode. However, there is also presumably a lower limit to the shear magnitude which can be effectively utilized in twinning; for $\{10\bar{1}2\}$ twins, for example, s becomes zero when $\gamma = 3^{\frac{1}{2}}$ and the shear direction reverses as γ passes through this value by varying the composition in, for example, magnesium–cadmium alloys. Experiments show that no $\{10\bar{1}2\}$ twins form near the critical composition.[65]

A projection of the h.c.p. structure on to the plane of shear is shown in Fig. 4, from which it follows that $\{10\bar{1}2\}$ is a $q = 4$ mode. The structure is formed by the stacking of two planes of shear of type $\{1\bar{2}10\}$ in different relative positions, half of the atoms of each lattice being contained in each plane. The motif unit thus lies in the plane of shear, which is a mirror plane of the h.c.p. structure, so that all four orientation relations of eq. (7) are equivalent, and there is no distinction between a type I and a type II twin. As in the f.c.c. and b.c.c. modes, this mode is crystallographically equivalent to its own conjugate.

Some schematic shuffle mechanisms for double lattice modes with $q = 4$ are shown in Fig. 5, and comparison with Fig. 4 shows that the probable shuffle mechanism is a degenerate case of Fig. 5(e) or 5(f), these two mechanisms being identical when the motif unit lies in the plane of shear. The additional atom movements in the shuffles are thus all parallel to $\boldsymbol{\eta}_1$ or normal to $\mathbf{K}_1$ if the motif unit is regarded as rigid, or parallel to $\boldsymbol{\eta}_1$ or $\boldsymbol{\eta}_2'$ if the shear is applied homogeneously to all the atom sites. The twinning mode is favoured not only by the low shear, but also by the very simple shuffle mechanism, shown also in Fig. 6(b). Figure 6(b) is drawn for twinning in titanium, where $\boldsymbol{\eta}_1 = \langle \bar{1}011\rangle$, and Fig. 4 corresponds to zinc or cadmium (i.e. $\gamma^2 > 3$) so that $\boldsymbol{\eta}_1 = \langle 10\bar{1}\bar{1}\rangle$.

The predicted twinning mode with the next lowest shear for $q \leqslant 4$ has a $\mathbf{K}_1$ plane of type $\{22\bar{4}1\}$, and has not been observed in any h.c.p. metal. The third smallest shear is a $q = 4$,

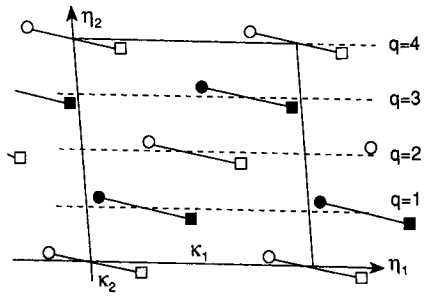

Fig. 4. Projection of h.c.p. structure parallel to $\{1\bar{2}10\}$. Open and full circles represent atoms on one set of lattice sites on two successive $\{1\bar{2}10\}$ planes. Open and filled squares represent atoms on the other set of lattice sites in the same two $\{1\bar{2}10\}$ planes.

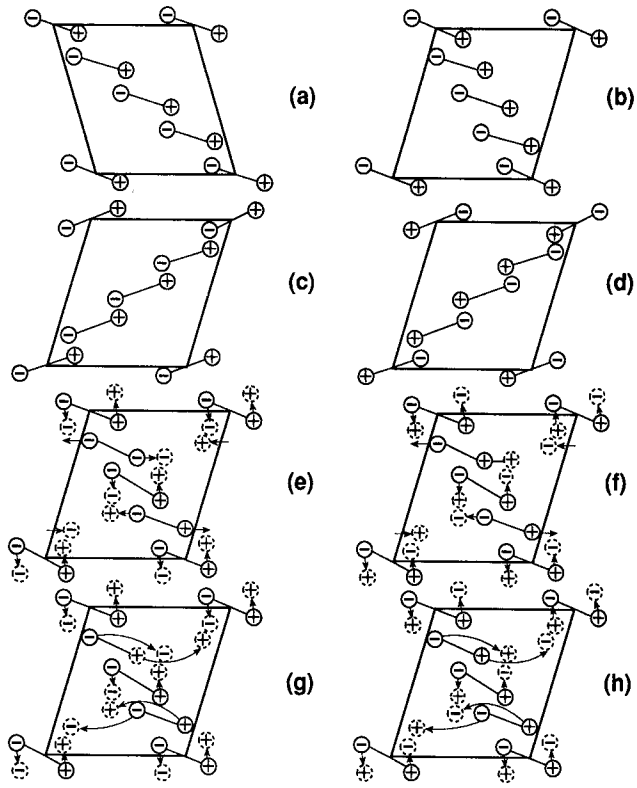

Fig. 5. Possible shuffling mechanisms in the twinning of a double lattice structure when $q = 4$. (a) Parent structure; (b) sheared parent; (c) type I twin; (d) type II twin; (e) possible type I shuffle; (f) possible type II shuffle; (g) alternative type I shuffle; (h) alternative type II shuffle.

type I twin with $\mathbf{K}_1 = \{10\bar{1}1\}$, $\boldsymbol{\eta}_2 = \langle 41\bar{5}3\rangle$, and $\mathbf{K}_2$ and $\boldsymbol{\eta}_1$ irrational. This mode is important in the theory of martensite crystallography since it specifies the relationships between the two product lattices in some h.c.p. phases produced by transformation from high-temperature b.c.c. phases. Such a transformation occurs, for example, in pure titanium and zirconium and in many of their alloys and the h.c.p. plates are then often finely twinned on a single set of $\{10\bar{1}1\}$ planes. The reasonable assumption that the two product orientations have crystallographically equivalent correspondences with the parent lattice then fixes the $\boldsymbol{\eta}_1$ direction and hence the equivalent twin mode (or its conjugate; both have been observed). A possible mechanism for deformation of the h.c.p. product involves the displacement of the $\{10\bar{1}1\}$ transformation twin boundaries, as in other martensitic structures,[20] and these twins may then be regarded as deformation twins, albeit of a rather unusual type.

Conventional deformation twinning on $\{10\bar{1}1\}$ has been reported in magnesium and in titanium above about 400°C but there was initially confusion between genuine $\{10\bar{1}1\}$ $\mathbf{K}_1$ planes and habits described as $\{30\bar{3}4\}$ but which are probably associated with double, or secondary, twinning. Reed-Hill[66] suggested a $\{10\bar{1}1\}$ low shear deformation mode, quite different from the $q = 4$ transformation twinning mode. This new mode is compound, and is the reciprocal of a $\{10\bar{1}3\}$ twinning mode previously noted by Reed-Hill and Robertson;[67] it has $\mathbf{K}_1 = \{10\bar{1}1\}$, $\mathbf{K}_2 = \{10\bar{1}\bar{3}\}$, $\boldsymbol{\eta}_1 = \langle 10\bar{1}\bar{2}\rangle$, $\boldsymbol{\eta}_2 = \langle 30\bar{3}2\rangle$, $s = (4\gamma^2 - 9)/4(3)^{\frac{1}{2}}\gamma$, $q = 8$. The magnitude of the shear is 0.138 for magnesium, which is appreciably smaller than that for the $q = 4$ mode. Although only one quarter of the lattice points are carried to their correct

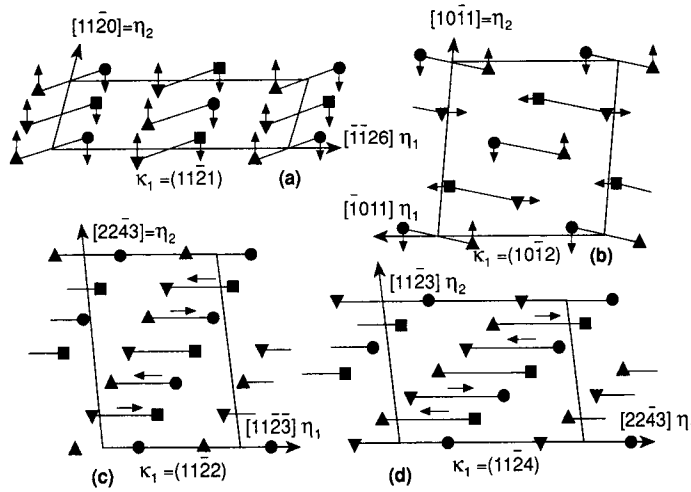

Fig. 6. Atomic shuffles associated with (a) $\{11\bar{2}1\}$, (b) $\{10\bar{1}2\}$, (c) $\{11\bar{2}2\}$ and (d) $\{11\bar{2}4\}$ twinning shears in titanium. The $\mathbf{K}_1$ plane and the directions η_1 and η_2 are labeled in each case and the motif pairs of atoms at each Bravais lattice point are indicated. The atoms associated with the two interpenetrating lattices comprising the h.c.p. structure are indicated by circles and squares (first lattice) and upright and inverted triangles (second lattice). In (a), (c) and (d), the atoms lie in four adjacent $\{1\bar{1}00\}$ planes, circles in the plane of the figure and squares, upright and inverted triangles at distances $\sqrt{3}a/2$, $\sqrt{3}a/6$ and $2\sqrt{3}a/3$ below the plane of the figure. In (b) the atoms lie in only two adjacent $\{1\bar{2}10\}$ planes with circles and upright triangles in the plane of the figure and squares and inverted triangles in the next plane at a distance of $a/2$ below it. The shuffles, if assumed formally to precede the shear, are indicated by arrows, and in (c) and (d), motif pairs of atoms move together. Shuffle components normal to the plane of the figure are required in (c) and (d); these are not shown and depend on whether the orientation relationship is of type I or type II (after Crocker and Bevis[64]).

twin positions by the shear, the atomic shuffles are simplified since the plane of shear $\{1\bar{2}10\}$ is a mirror plane which contains the motif unit, as in the $\{10\bar{1}2\}$ twins already discussed. An alternative compound mode was suggested by Hall,[5] using the plane of shear projection method, but the shear ($s \sim 1.07$) is improbably large.

The observed $\{10\bar{1}3\}$ twins in magnesium could in principle represent a type I twin with two irrational elements and $q = 4$, but although the shear for this mode is reasonably small, the reciprocal of the $\{10\bar{1}1\}$, $q = 8$ mode seems more probable. (A $q = 11$ mode which has also been suggested has improbably complex shuttles.) Experimental observations on magnesium indicate, however, that both $\{10\bar{1}3\}$ and $\{10\bar{1}1\}$ twins are often components of double twins rather than single twins. Reed-Hill[66] found that a twin plate or band appeared to form by double, or secondary, twinning on $\{10\bar{1}3\}$ and $\{10\bar{1}2\}$ over most of its length, except at the tips where there was single $\{10\bar{1}3\}$ twinning. The tips are thus separated from the rest of the twin by internal $\{10\bar{1}2\}$ interfaces, which presumably move outward as the twin grows. Similar observations were made for (smaller) twins with habits near $\{10\bar{1}1\}$ in agreement with a suggestion[68,69] that observed $\{30\bar{3}4\}$ twins in magnesium are actually double twins of $\{10\bar{1}1\} + \{10\bar{1}2\}$ type.

The predicted twinning elements of the equivalent simple shear mode for the $\{10\bar{1}3\} + \{10\bar{1}2\}$ simultaneous double twinning are all irrational, but experimental results fit theoretical predictions[34] quite well. The measured angle between the basal plane and the habit plane, for example is 29°, compared with a predicted value of 32° for the $\{10\bar{1}3\}$ twin alone and 26°34′ for the double twin on the assumption that the latter has a simple shear relation to

the matrix produced by simultaneous operation of the two twinning shears. The small discrepancy of $2\frac{1}{2}^\circ$ was attributed by Crocker to accommodation effects and he also showed that the expected orientation relations and shear (0.258) of the double twinned region are in good agreement with experiment. However, in retrospect, the alternative possibility that a previously formed $\{10\bar{1}3\}$ twin retwins on a $\{10\bar{1}2\}$ plane over most of its volume seems more probable and agrees better with the observed morphology. The secondary twinning would slightly rotate the habit to 32°17′ from the basal plane, in equally good agreement with experiment.

Two sets of indices were originally suggested tentatively for single $\{30\bar{3}4\}$ twins; those given by Reed-Hill and Robertson[67] have $q = 10$, and those by Couling and Roberts[69] have $q = 4$, but also have a very large shear. Since there is no mode with $q \leqslant 6$ and $s < 1$, it seems highly probable that these bands are actually double twins and the combination $\{10\bar{1}1\} + \{10\bar{1}2\}$ is clearly indicated. However, although the experimental orientations are reasonably consistent with the theory, the measured habit planes deviate by about 15° from that predicted on the assumption of simultaneous double twinning. This discrepancy is reduced to ~6° if a $\{10\bar{1}1\}$ twin is assumed to form first and then to retwin on $\{10\bar{1}2\}$, thus supporting the secondary twinning hypothesis. The small remaining differences between theoretical predictions and experimental results may simply reflect the experimental difficulties with such small twins.

The remaining observed h.c.p. modes are $\{11\bar{2}1\}$ and $\{10\bar{1}4\}$ which both have $q \leqslant 4$ and $s \leqslant 1$, and $\{11\bar{2}2\}$, $\{11\bar{2}4\}$ and $\{11\bar{2}3\}$ which are all unpredicted within these ranges of q and s. The $\{10\bar{1}4\}$ observations are rather doubtful, but the other modes, and especially $\{11\bar{2}1\}$, are important in the deformation of several h.c.p. metals. Note that $\{11\bar{2}1\}$ is the only mode listed in Table 3 with $q = 2$, i.e. it is the only h.c.p. mode in which all the lattice points are carried to their correct positions by the shear so that *lattice* shuffles are not required. Experimental values for the shear in rhenium[70] and zirconium[71–73] generally agree with the predicted value of ~0.6, but some confusion was caused by an earlier measurement[74] of ~0.2 which implied a very high value for q. It now seems probable that undetected accommodation effects were responsible for the reported low value of s.

The plane of shear for the $\{11\bar{2}1\}$ mode is a mirror glide plane $\{1\bar{1}00\}$ so that the two orientation relations I and II are in principal different but may be related by a simple translation of $\frac{1}{2}\mathbf{c}$. The shuffles required to produce a type I twin are shown in Fig. 6(a); they all involve equal and opposite displacements of the atoms in a motif pair through a small distance ($\sim 0.2a$) perpendicular to the K_1 plane (assuming the motif unit to be translated rigidly by the shear) as in the Y mechanism of Jaswon and Dove.[31] Crocker and Bevis[64] suggested that the simplicity and small magnitudes of the shuffles account for the dominance of this mode (together with the smaller shear $\{10\bar{1}2\}$ mode) in the observed deformation behaviour of titanium.

An interesting feature of the $\{11\bar{2}1\}$ mode is that it provides one of the few examples in which $\mathbf{K}_2$ and $\boldsymbol{\eta}_2$ correspond to an observed slip plane and slip direction, respectively. Since a twin boundary may be regarded formally as a high angle tilt boundary formed by a dense array of lattice dislocations of edge type, it could, in principle, be created by the accumulation of a large number of slip dislocations in a local region which then re-arrange to form a twin with a consequent lowering of energy.[75] Comparing with the low angle case (polygonization), the dislocations must have a lattice Burgers vector in the $\boldsymbol{\eta}_2$ direction and their glide plane must be $\mathbf{K}_2$. According to this model, the twinning mode would be determined by the known deformation properties in glide. A knowledge of these elements does not uniquely define the mode, but an additional assumption about the fraction of lattice sites carried directly into

their correct twin positions, or equivalently about the spacing of the dislocations in the tilt boundary, is sufficient to fix all the variables.

Bullough's formal theory[75] is closely related to the theory of martensite crystallography. Figure 7 shows hypothetical stages in the formation of a twin. The combination of the lattice invariant deformation, which is a simple shear on $\mathbf{K}_2$ in the direction $\boldsymbol{\eta}_2$, with the lattice deformation, which is a rotation about the direction in $\mathbf{K}_2$ normal to $\boldsymbol{\eta}_2$, produces the shape deformation, which is a simple shear on $\mathbf{K}_1$ in the direction of $\boldsymbol{\eta}_1$. The more complex case of martensite differs formally in having a lattice deformation which is not simply a rotation and the dislocations needed to ensure compatibility of lattice and shape deformations are then not pure edges. In the application to twinning, however, the dislocation content of the tilt boundary is so high that it loses physical significance; if all the lattice points are related by the twinning shear, there is one lattice dislocation on each $\mathbf{K}_2$ lattice plane intersecting the twin interface. This very high dislocation content may alternatively be regarded as zero, since an equally valid description of the final situation is that the shape and lattice deformations are identical and there is no lattice invariant deformation. Bullough's theory shows the relevance of the alternative description if the twin really does form by accumulating slip dislocations.

Since $\mathbf{K}_2$ and $\boldsymbol{\eta}_2$ hardly ever correspond to slip modes, this approach cannot be generally valid, but it might apply to one possible mode in the diamond structure (see below) and also to the interesting case of hexagonal graphite which forms $\{11\bar{2}1\}$ twins with a much lower theoretical shear (0.367) than titanium because of its high axial ratio ($\gamma = 2.725$). Freise and Kelly[76] found that deformation of graphite frequently produced bend planes (tilt boundaries) of varying angle in addition to genuine twins, thus lending some support to the Bullough model. On the other hand, it does not seem possible to assign much more than formal significance to the dislocation model of the completed twin boundary, since the dislocations

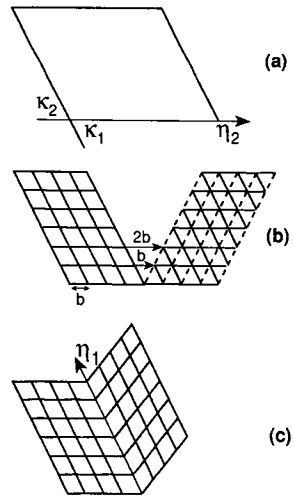

Fig. 7. Schematic illustration of Bullough's theory of twinning. (a) Original parent lattice. (b) Part of the parent lattice is given a homogeneous lattice invariant shear on the $\mathbf{K}_2$ plane (horizontal in the figure); this requires a lattice dislocation of Burgers vector $\mathbf{b}$ to glide through each lattice $\mathbf{K}_2$ plane, as shown. The full lines outline the original unit cells and the dashed lines alternative, equivalent cells in the sheared region. (c) Combination of the lattice invariant shear with a rotation about the normal to the plane of shear now produces the twin. The total shape deformation is a shear on the $\mathbf{K}_1$ plane in the $\boldsymbol{\eta}_1$ direction (after Bullough[75]).

must lose their individual identities. Freise and Kelly used the Read–Shockley formula for grain boundary energy to deduce that the "dislocations" in the boundary will dissociate into partial dislocations, there being one partial on each atomic $\mathbf{K}_2$ plane instead of one lattice dislocation on each lattice $\mathbf{K}_2$ plane. This formal description means only that a twin of this type may have an interface in which all the atomic positions match. Statements which are sometimes made that in this type of twinning the shear is on the $\mathbf{K}_2$ plane rather than the $\mathbf{K}_1$ plane focus attention on the dislocation aggregation mode, but are rather confusing because a proper distinction is not being made between the different kinds of deformation shown in Fig. 5.

There are no other observed h.c.p. modes for which $s < 1$ and $q \leqslant 4$ but it is well established that $\{11\bar{2}2\}$ and $\{11\bar{2}4\}$ twins occur in some metals. In fact, if $q = 6$, these two planes are conjugate twinning planes of a single mode, as first pointed out by Kiho,[28,29] and the shear is only ~ 0.22 for titanium and zirconium, although it would exceed 0.5 if this mode were operative in cadmium or zinc. With $q = 6$, the shuffles are necessarily rather complex, but are considerably simplified in each case because there is a motif unit in the composition plane. Type I and type II twins are possible in principle but since the plane of shear is the mirror glide plane $\{1\bar{1}00\}$, the two orientations differ only by a relative translation which in this case may be regarded as parallel to $\boldsymbol{\eta}_1$. This introduces additional symmetry; for example, the atoms in a reflection twin are also related to the parent atoms by a two-fold screw rotation about $\boldsymbol{\eta}_1$. The atomic structure of the various possible h.c.p. twin interfaces and the corresponding twinning dislocations are discussed in Section 3; a possible set of shuffles for the $\{11\bar{2}2\}$ type I twin is shown in Fig. 6(c) and for the conjugate $\{11\bar{2}4\}$ in Fig. 6(d).

Table 3. Predicted and Observed Twinning Modes in h.c.p. Structures

$\mathbf{K}_1$ { }	$\mathbf{K}_2$ { }	$\boldsymbol{\eta}_1$ ⟨ ⟩	$\boldsymbol{\eta}_2$ ⟨ ⟩	s	q	References to some supporting experimental studies
$10\bar{1}2$	$\bar{1}012$	$10\bar{1}\bar{1}$	$\bar{1}01\bar{1}$	$(\gamma^2-3)/3^{\frac{1}{2}}\gamma$	4	Mg,[66,68,69,307] Ti,[307] Co,[187] Zr,[181] Zn,[306,307] and Be[307]
$22\bar{4}1$	0001	1,1,$\bar{2}$,$\bar{1}$2	$11\bar{2}0$	$1/2\gamma$	4	
$10\bar{1}1$	$10\bar{1}\bar{3}$	$10\bar{1}2$	$30\bar{3}2$	$(4\gamma^2-9)/4(3)^{\frac{1}{2}}\gamma$	8	Mg[66,68,69] and Ti[180,181]
$10\bar{1}1$	i	i	$41\bar{5}3$	$(4\gamma^4-17\gamma^2+21)^{\frac{1}{2}}/2(3)^{\frac{1}{2}}\gamma$	4	
$20\bar{2}1$	0001	$10\bar{1}\bar{4}$	$10\bar{1}0$	$3^{\frac{1}{2}}/2\gamma$	4	
$11\bar{2}1$	0001	$11\bar{2}\bar{6}$	$11\bar{2}0$	γ^{-1}	2	Re,[70] Ti,[305,307] Zr,[71–73,304] Co[187] and graphite[76]
$10\bar{1}\bar{3}$	$10\bar{1}1$	$30\bar{3}2$	$10\bar{1}2$	$(4\gamma^2-9)/4(3)^{\frac{1}{2}}\gamma$	8	Mg[66]
$10\bar{1}3$	i	i	$21\bar{1}\bar{3}$	$(4\gamma^4-17\gamma^2+21)^{\frac{1}{2}}/2(3)^{\frac{1}{2}}\gamma$	4	
i	i	i	i	$(4\gamma^4-21\gamma^2+36)^{\frac{1}{2}}/4(3)^{\frac{1}{2}}\gamma$		Mg[66]
({$10\bar{1}3$} 'double twinning')						
$13\bar{4}0$	$\bar{1}100$	$7\bar{5}\bar{2}0$	$11\bar{2}0$	$3^{-\frac{1}{2}}$	4	
$13\bar{4}1$	$\bar{1}101$	i	$11\bar{2}0$	$(4\gamma^2+3)^{\frac{1}{2}}/2(3)^{\frac{1}{2}}\gamma$	4	
$13\bar{4}2$	$\bar{1}102$	i	$11\bar{2}0$	$(4\gamma^2+3)^{\frac{1}{2}}/2(3)^{\frac{1}{2}}\gamma$	4	
$22\bar{4}3$	0001	$11\bar{2}\bar{4}$	$11\bar{2}0$	$3/2\gamma$	4	
$10\bar{1}4$	$10\bar{1}0$	$20\bar{2}1$	0001	$\gamma/3^{\frac{1}{2}}$	4	
$11\bar{2}2$	$11\bar{2}\bar{4}$	$11\bar{2}\bar{3}$	$22\bar{4}3$	$2(\gamma^2-2)/3\gamma$	6	Ti[180,181,307] and Zr[181]
$11\bar{2}\bar{4}$	$11\bar{2}2$	$22\bar{4}3$	$11\bar{2}\bar{3}$	$2(\gamma^2-2)/3\gamma$	6	
$30\bar{3}4$	—	—	—			
$11\bar{2}3$	—	—	—			

Notes: i denotes an irrational plane or direction. As explained in the text, some of the reported modes have not been confirmed and appear doubtful. For greater clarity, each mode and its conjugate are listed separately. The table includes the eleven predicted modes which have $s \leqslant 1$ and $q \leqslant 4$ for the ideal axial ratio, and also the more probable $q = 8$ modes for $\{10\bar{1}1\}$ and $\{10\bar{1}3\}$ and the $q = 6$ modes for $\{11\bar{2}2\}$ and $\{11\bar{2}4\}$.

An alternative mode with a $\{11\bar{2}2\}$ habit[28] has $\mathbf{K}_2 = \{11\bar{2}\bar{2}\}$, $\boldsymbol{\eta}_1 = \langle 11\bar{2}\bar{3}\rangle$, $\boldsymbol{\eta}_2 = \langle 11\bar{2}3\rangle$, $s = \gamma - \gamma^{-1}$ and $q = 4$; this is the second hexagonal mode obtained from variants of the unit correspondence matrix applied to the orthohexagonal basis, and like the $\{10\bar{1}2\}$ mode, it has the $\mathbf{K}_1$ and $\mathbf{K}_2$ planes and the $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$ directions crystallographically equivalent. The shear s slightly exceeds unity for $\gamma = 1.63$, but it is less than unity for the axial ratios of titanium and zirconium. Although fewer atoms would be required to shuffle than in the $q = 6$ mode, experimental work (e.g. Rapperport and Hartley[77]) shows that the $q = 6$ mode is preferred, presumably because of the much smaller shear.

There remains, finally, the observation of $\{11\bar{2}3\}$ twins. Hall[5] found a possible mode with $q = 2$, but this has a very large shear of ~ 1.9. The lowest shear for this mode with $q \leqslant 8$ occurs with $q = 7$; another mode suggested by Kiho has $q = 5$ and $s \sim 0.5$. Both of these modes would require very complex shuffles. At present there is thus no good description of $\{30\bar{3}4\}$ and $\{11\bar{2}3\}$ twinning, and it is possible that the habit plane markings of these types represent rather complex double twinning modes.

Table 3 gives a selection of observed and predicted twinning modes for the various h.c.p. metals. It does not include the high shear $\{11\bar{2}\bar{2}\}$ mode mentioned above for which $q = 4$ and three other unobserved $q = 4$ modes in the Crocker and Bevis list are also omitted. These have $\mathbf{K}_1$ planes of types $\{2,8,\bar{1}\bar{0},7\}$ (a compound mode) and $\{10\bar{1}2\}$ and $\{10\bar{1}\bar{1}\}$ (type 1 modes).

2.8. *Twinning in Other Double Lattice Structures*

The metals arsenic, bismuth and antimony are double lattice structures which may be compared to the face-centred rhombohedral structure of mercury since each consists of two interpenetrating face-centred rhombohedral lattices, the origin of the second being displaced along the $\langle 111\rangle$ direction with respect to the origin of the first. The observed twinning mode is not, however, equivalent to the operative mercury mode but corresponds instead to the minimum shear mode predicted but not observed for mercury. Experimental observations show that the operative $\mathbf{K}_1$ plane is always $\{110\}$ and the conjugate mode with a $\{001\}$ habit is not observed. Crocker showed that with a proper choice of motif unit, the rotation (type II) twin involves much smaller atomic shuffles than the alternatives, and it is presumably preferred for this reason.

The least shear hypothesis also explains the observed twinning modes in the white tin structure, which may be regarded as two interpenetrating b.c.t. lattices with the origin of the second lattice at $[\frac{1}{2}0\frac{1}{4}]$ with respect to the origin of the first. Because of the low axial ratio of the structure (~ 0.55) the mode previously given for martensite (and equivalently for indium) no longer gives the smallest shear. The minimum shear mode is

$$\mathbf{K}_1 = \{101\} \quad \mathbf{K}_2 = \{\bar{3}01\} \quad \boldsymbol{\eta}_1 = \langle\bar{1}01\rangle \quad \boldsymbol{\eta}_2 = \langle 103\rangle$$

$$s = \tfrac{1}{2}(9\gamma^2 + \gamma^{-2} - 6)^{\frac{1}{2}} \quad q = 4. \tag{29}$$

Both $\{101\}$ and the conjugate $\{\bar{3}01\}$ are observed as $\mathbf{K}_1$ planes, the latter being more frequent. Both possibilities involve quite small and simple shuffles since the motif unit may be chosen to lie in the plane of shear; these represent the degenerate case in which Fig. 5(e) is equivalent to Fig. 5(f). The preferred plane is that for which the shuffles normal to the $\mathbf{K}_1$ plane are smaller than those parallel to the $\boldsymbol{\eta}_1$ direction.

The elements carbon (as in diamond), silicon, germanium and grey tin all have the diamond structure in which each atom has four tetrahedrally arranged neighbours around it. The structure is equivalent to two inter-penetrating face-centred cubic lattices, the origin of the second being at $\frac{1}{4}\frac{1}{4}\frac{1}{4}$. By analogy with the f.c.c. structure, the twin of least shear for $q = 2$ has both $\mathbf{K}_1$ and $\mathbf{K}_2$ planes of type $\{111\}$, and this is the commonly observed mode in silicon, germanium and diamond. Jaswon and Dove pointed out, that the following $q = 4$ mode is possible in the diamond structure

$$\mathbf{K}_1 = \{111\}, \quad \mathbf{K}_2 = \{11\bar{3}\}, \quad \boldsymbol{\eta}_1 = \langle \bar{1}\bar{1}2\rangle, \quad \boldsymbol{\eta}_2 = \langle 332\rangle$$

$$s = 8^{-\frac{1}{2}} \quad q = 4. \tag{30}$$

This has quite acceptable shuffles, and one-half of the shear of the $q = 2$ mode.

No observation appears to have been made of the $\{113\}$ twins which would be conjugate to the above mode, but Churchman *et al.*[78] reported a $\{123\}$ twinning mode. Bullough[75] showed that the mode could be predicted by using the parent slip system for $\mathbf{K}_2$ and $\boldsymbol{\eta}_2$, and not allowing atomic shuffles. Unfortunately, the accompanying shear is improbably large, and later work makes it appear rather doubtful that $\{123\}$ twins do in fact exist in this structure.

The last double lattice structure to be discussed is that of α-uranium which is of considerable interest not only because of its industrial importance but also because it twins on several systems and provided the first known example of a metallic structure in which type II twins form with irrational $\mathbf{K}_1$ planes. Alpha-uranium has a crystal structure made up from two inter-penetrating base-centred orthorhombic cells, with origins separated by a vector $[0, -0.31, 0.5]$. The structure may be regarded as derived from the h.c.p. structure, and the first theoretical analysis by Frank[79] showed that one prominent mode with an irrational $\mathbf{K}_1$ plane equal to "$\{172\}$" approximately, and its conjugate with $\mathbf{K}_1 = \{112\}$, which is also an observed mode, may be regarded as the orthorhombic equivalent of h.c.p. $\{10\bar{1}2\}$ twins. There is another possible orthorhombic mode which also degenerates into $\{10\bar{1}2\}$, but this has a larger shear and is not observed. The most frequently occurring twins in α-uranium have $\mathbf{K}_1 = \{130\}$, and Frank pointed out that the corresponding h.c.p. plane is a $\{11\bar{2}0\}$ mirror plane. The above three modes were all discovered in a classic experimental study by (R.W.) Cahn[80] who also found another twin with $\mathbf{K}_1 = \{121\}$. Cahn correctly identified the twinning elements of the $\{130\}$ (compound), $\{112\}$ (type I) and "$\{172\}$" (type II) modes and also proposed that the $\{121\}$ habit represents a type I mode with $\boldsymbol{\eta}_2 = \langle 311\rangle$.

Most of the α-uranium twinning modes were explained by Jaswon and Dove who also predicted a minimum shear, $q = 4$, mode with $\mathbf{K}_1 = \{111\}$ for the type I twin and $\boldsymbol{\eta}_1 = \langle 512\rangle$ for the type II twin. This pair of modes may be regarded as the orthorhombic equivalents of the possible h.c.p. type I mode with $\mathbf{K}_1 = \{10\bar{1}1\}$ and $\boldsymbol{\eta}_2 = \langle 41\bar{5}3\rangle$ and the conjugate type II mode. The type II twins with irrational habit plane near "$\{176\}$" were discovered in later work by Lloyd and Chiswik[81] who did not, however, detect the $\{112\}$ and $\{121\}$ twins found by Cahn. The Jaswon and Dove theory is unable to distinguish between the observed and unobserved predictions, but a more systematic analysis of the shuffle mechanisms by Crocker[82] suggests that the most frequently observed twinning mode, which is compound with $\mathbf{K}_1 = \{130\}$, is preferred because of its simple shuffle mechanism ($q = 2$). No significance appears to be attached to the fact that the mode is compound; there are actually four possible twinning modes with a lower shear than the $\{130\}$ mode, including another compound mode, but these all have $q = 4$. It is not clear, however, why the reciprocal to the $\{130\}$ mode, which would have a $\{110\}$ composition plane, is not observed.

Table 4. Predicted and Observed Twinning Modes in Double Lattice Structures

Structure	$\mathbf{K}_1$ { }	$\mathbf{K}_2$ { }	$\boldsymbol{\eta}_1$ ⟨ ⟩	$\boldsymbol{\eta}_2$ ⟨ ⟩	s	q	References to supporting experimental studies
Rhombohedral	110	001	001	110	0.27–0.125	1	As, Bi, Sb[364]
b.c. tetragonal	101	$\bar{3}01$	$\bar{1}01$	103	0.113	4	Sn[308]
Diamond	111	$11\bar{1}$	$11\bar{2}$	112	$2^{-\frac{1}{2}}$	2	Si[279] and GaAs[15,178,220,221]
	111	$\bar{1}\bar{1}3$	$\bar{1}\bar{1}2$	332	$8^{-\frac{1}{2}}$	4	
α-uranium	'176'	111	512	—	0.214	4	[81]
	112	'172'	312	—	0.227	4	[80]
	'172'	112	—	312	0.227	4	[80]
	$1\bar{3}0$	110	310	$1\bar{1}0$	0.299	2	[80]
	121	'$1\bar{4}1$'	'$3\bar{2}1$'	311	0.329	6	[80]

Notes: Irrational planes or directions are shown as approximately rational indices in quotation marks. Numerical values of the shear are given to avoid complexity. Only observed modes are listed.

The type I twin of lowest shear has a {111} composition plane, and its reciprocal type II twin an irrational, approximately '{176}', plane. The shuffles in both cases would be quite large, and only the type II twin has been found. The shuffles for the mode of next lowest shear are simpler, explaining the more frequent occurrence of both the type I, {112}, and the type II, approximately '{172}', twins. The type II twin has the simpler shuffles, and is observed more frequently than the type I twin. The other two possible modes with $q = 4$ and a shear less than that of the predominant {130} mode, including the low shear compound mode, are not observed.

The {121} twin found by Cahn, but apparently very rare, cannot be explained by the assumption $q \leqslant 4$ used in the above predictions. Crocker points out that according to the elements assigned to it by Cahn, it is a $q = 6$ mode and this does not seem too improbable in view of the $q = 6$ h.c.p. mode discussed above. In the uranium case, however, the shuffles would be much more complex since the motif unit cannot be chosen to lie in the $\mathbf{K}_1$ plane.

The twinning modes for the metallic double lattice structures other than h.c.p. are summarized in Table 4.

2.9. *Multiple Lattice Structures*

Mechanical twinning is the major deformation mechanism in some non-metallic materials with complex crystal structures of low symmetry and many atoms to the unit cell. Although the mechanism of such twinning is not well understood, it seems logical to suppose that the operative twinning modes are determined primarily by the shuffle mechanisms which depend on the structures of the unit cells rather than on lattice geometry. Metallic neptunium provides an interesting example of an intermediate case; it has an orthorhombic unit cell containing eight atoms which in a (001) projection can conveniently be represented as binary motif units of two different kinds. Rechtien *et al.*[83] considered the possible twinning modes to be limited by the condition that the lattice must be restored by the shear, i.e. $q = 1$ or 2. The two lowest shear modes are then

$$\mathbf{K}_1 = \{110\} \quad \mathbf{K}_2 = \{1\bar{1}0\} \quad \boldsymbol{\eta}_1 = \langle 1\bar{1}0\rangle \quad \boldsymbol{\eta}_2 = \langle 110\rangle \quad s = 0.068 \tag{31}$$

and

$$\mathbf{K}_1 = \{011\} \quad \mathbf{K}_2 = \{01\bar{1}\} \quad \boldsymbol{\eta}_1 = \langle 01\bar{1}\rangle \quad \boldsymbol{\eta}_2 = \langle 011\rangle \quad s = 0.630. \tag{32}$$

The very small shear of mode (31) suggests that if the shear magnitude remains an important criterion, this mode will be preferred. Experiments on polycrystalline specimens using colour metallography confirmed that deformation twins form profusely on two habit planes of each grain and an analysis of these observations combined with a study of habit plane traces in single crystals showed that all the twins were consistent with the above mode. From a detailed study of the possible shuffle mechanisms, the authors predict that the most likely orientation relationship is a 180° rotation about the $\boldsymbol{\eta}_1$ direction.

The most complex metallic structure for which a detailed analysis has been attempted is that of α-plutonium which has sixteen atoms in its monoclinic unit cell. There are many operative slip systems in this metal, but in a few specimens Spriet[84] also observed deformation twins with two different habits. The habits have not been identified because of the considerable experimental difficulties, but Sebilleau[85] suggested that they are probably (001) and $(\bar{2}01)$. In a more complete theoretical analysis Crocker[86] considered five conjugate pairs of modes with $q = 1$ or 2 and another five pairs with $q = 4$. The lowest shear mode of the second group has a slightly smaller shear (0.129) than that of the first group (0.159) but its shuffles are much more complex. Crocker examined all the shuffles with the aid of a simpler pseudo-structure with only two atoms in its monoclinic unit cell and deduced that only the conjugate pair of modes suggested by Sebilleau which have minimum shear with no lattice shuffles is likely to be acceptable. This compound mode is

$$\mathbf{K}_1 = (001) \quad \mathbf{K}_2 = (\bar{2}01) \quad \boldsymbol{\eta}_1 = [\bar{1}00] \quad \boldsymbol{\eta}_2 = [102] \quad s = 0.159. \tag{33}$$

There is no clear distinction between the two conjugate modes but considerations related to the production of twinning dislocations in the interface may favour the $(\bar{2}01)$ habit.

Intermetallic compounds of stoichiometric or near stoichiometric compositions with structures not obviously related to an ordering of a random solid solution may nevertheless deform by twinning; a recently investigated example is the compound Cu_2Sb which is the prototype of a number of A_2B compounds with the tetragonal C38 crystal structure. There are six atoms in the primitive unit cell, but deformation twinning on $\mathbf{K}_1$ planes of $\{112\}$ type was nevertheless observed in Cu_2Sb by Paxton and Entwisle[13] who were able to show by application of the Bevis–Crocker theory that this $\mathbf{K}_1$ plane corresponds to the lowest shear mode. The crystallographic elements are, in fact, identical with those of the normal b.c.c. or b.c.t. mode, but since the axial ratio is 1.526, the shear is in the opposite sense and is only about 0.15 (see Table 1). The C38 lattice is primitive tetragonal, so that only one-half of the lattice points (and hence one-sixth of the atoms) can be carried to their correct twin positions by shear alone. It is remarkable that Cu_2Sb twins so readily despite the required shuffles, and it would be interesting to investigate whether or not the other C38 structures (which fall into two groups of different axial ratios) also deform by twinning. The second group have axial ratios of about 2.0, and the $\{112\}$ mode then has a larger shear of about $2^{-\frac{1}{2}}$.

2.10. *Choice of Twin Mode*

From the above comparisons of theory and experiment, the factors which appear to determine the operative deformation twinning modes may be deduced. Bilby and Crocker[23] suggested that the operative twinning mode should:

(a) have a small shear,
(b) require only simple shuffles (i.e. have a small value of q),

(c) require, if possible, only shuffles of small magnitude, and
(d) have shuffle displacements parallel to $\boldsymbol{\eta}_1$ if large shuffles are essential.

It appears that criteria (a) and (b) generally enable the most likely twinning modes to be predicted, but (c) and (d) may have to be invoked in some cases, e.g. to distinguish between a mode and its conjugate.

Laves[87,88] defined a "shuffle parameter" as the ratio of the average shuffle displacement to the interatomic distance, but for any given structure it is not clear that this provides an adequate description of the complexities of different shuffles. In general, the shuffles might be expected to correlate either with the energy of the interface or the kinetics of its motion, or both, and thus the influence of (b), (c) and (d) on the operative modes is easy to understand in a general way. It is not so clear why a small shear should be preferred since the volume of twins required to produce a given plastic strain varies as s^{-1} and thus increases as the twinning shear decreases. However, the stress field of an enclosed lenticular twin of given aspect ratio varies as s^2, so that it should be easier to produce a given strain by a large number of small shear twins rather than a small number of large shear twins.

3. TWIN INTERFACES AND TWINNING DISLOCATIONS

3.1. *Fully Coherent Rational Twin Interfaces*

The $\mathbf{K}_1$ plane of the parent structure is the only invariant plane when the twinning shear is applied. Provided $\mathbf{K}_1$ is rational, a geometric interface between matrix and twin parallel to $\mathbf{K}_1$ may thus contain a set of lattice points common to both matrix and twin. This implies that the twin lattice points, or some integral fraction of them, are specified by eq. (1) with the origin of the coordinate system located on one of these interface lattice points. A coincident site interface of this type is similar to an intrinsic stacking fault as originally defined by Frank,[89] and the whole twin may then be regarded as a stack of such faults. This intuitive structure is almost certainly very close to the true atomic structure of a $\{111\}$ $\mathbf{K}_1$ interface in a f.c.c. twin since, with a pairwise model of the atomic interactions, differences between the various structures corresponding to ideal close-packing of spheres only appear when the computations are extended to at least third nearest neighbours. Thus the energies of an intrinsic stacking fault in the f.c.c. structure, the $\{111\}$ twin boundary and the $\{111\}_c//\{0001\}_h$ interface between the f.c.c. and h.c.p. structures are all likely to be similar and small, and this is confirmed by the calculations of Vitek[90] on stacking faults and of Sutton and Christian[91] for the cubic–hexagonal interface.

In some cases, however, the twin lattice points may be translated away from coincidence by a non-repeat vector of the lattice. The first example of a possible interface of this type came from the computer simulation by Vitek[92] of a $\{112\}$ twin boundary in b.c.c. crystals. Vitek's computation was motivated by a previous failure[90] to find any metastable configuration for a single layer intrinsic (shear-type) stacking fault on either the $\{110\}$ or the $\{112\}$ planes of a b.c.c. structure. Since a twin corresponds macroscopically to a stack of $\{112\}$ shear faults with relative displacements of $\frac{1}{6}\langle\bar{1}\bar{1}1\rangle$, Vitek next investigated the minimum number of faults which would be mechanically stable. He found this number to be four with relative displacements of approximately $\frac{1}{2}$, 1, 1 and $\frac{1}{2}$ times the expected value, and the structure of a twin interface with a large number of planes on each side of the interface was similarly found to correspond to a first plane displacement of $\frac{1}{12}\langle\bar{1}\bar{1}1\rangle$. The structure was confirmed by

Bristowe and Crocker[93] and it is shown in Fig. 8 together with the coincident site interface. The new "isosceles" interface is translated from the coincident site interface by a vector $\mathbf{t} = \frac{1}{12}\langle 11\bar{1}\rangle$, with a magnitude of one-sixth of the interatomic distance, and although the reflection symmetry across $\mathbf{K}_1$ has been destroyed at an atomic level, the new arrangement is also highly symmetrical; it is, for example, the same when viewed from either side of the interface. Note also that the interface plane is an atomic plane in Fig. 8(a), but is mid-way between two atomic planes in Fig. 8(b).

Vitek originally concluded that the configuration shown in Fig. 8(b) will have the lowest energy except possibly for very "soft" atoms which have a pairwise potential in which the repulsive part increases relatively slowly with decreasing separation. Later work, however, indicates that the computed equilibrium structure is sensitive to the boundary conditions and method of relaxation as well as to the potential, so that it is not easy to predict the equilibrium interface structure for a real material. Some calculations[93,94] indicate that the lowest energy structure may not be the same in all b.c.c. metals, and also that the difference in the energies of the two structures may be very small in some materials. The possibility of different configurations coexisting in the same interface then arises and has implications in the description of interface steps (twinning dislocations).

Simultations of the interface structures of the main h.c.p. $\mathbf{K}_1$ interfaces, namely $\{10\bar{1}2\}$, $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$, have been made by Serra and Bacon[95] using three different two body potentials. Only one equilibrium configuration was found for the $\{10\bar{1}2\}$ interface, and the parent and twin structures are mirror images in the interface. The plane of the interface is an atomic plane formed by the coalescence of two adjacent original atomic planes which make up a corrugated lattice plane of type $\{10\bar{1}2\}$, and the orientation relation is "combined", i.e. both type I and type II.

The stable interface of a $\{11\bar{2}2\}$ twin is also an atomic plane of reflection according to the calculations of Serra and Bacon, but since the motif unit lies in the $\{11\bar{2}2\}$ planes, all the lattice planes parallel to the interface are flat in this case. The interface structure is thus that of a type I twin, and was the only stable interface found for so-called equilibrium pair potentials. When non-equilibrium potentials were used, i.e. when the crystal was subjected to an external pressure which corresponded roughly to the Cauchy pressure, an additional stable interface was formed by relative translation of the two sets of atoms by

$$\mathbf{t} = \frac{1}{6(1+\gamma^2)}\langle 11\bar{2}\bar{3}\rangle \simeq \frac{1}{22}\langle 11\bar{2}\bar{3}\rangle \tag{34}$$

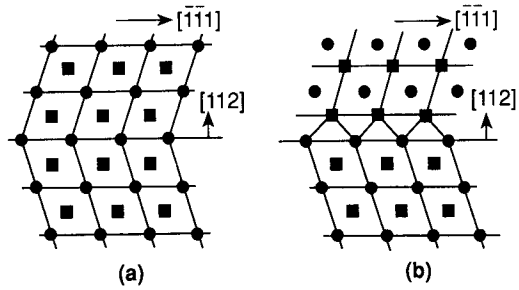

Fig. 8. Possible $\{112\}$ twin boundary structures in b.c.c. crystals. The conventional coincidence site (CSL) boundary is shown in (a) and the less symmetric 'isosceles' boundary predicted by Vitek[92] and by Bristowe and Crocker[93] from atomic simulations is shown in (b). Atoms on two successive $\{1\bar{1}0\}$ planes are represented by circles and squares.

parallel to the η_1 direction of the $q = 6$ twinning mode. This is the translation required to obtain a type II interface, but the two-fold axis is midway between two atomic $\mathbf{K}_1$ planes. This atomic symmetry might, however, be built into the pair potential model since the potentials used by Serra and Bacon do not well represent real materials. One of the non-equilibrium potentials also gave a third less symmetrical atomic model of the interface produced by an alternative displacement parallel to η_1, but this was not stable when the other potentials were used.

Two different starting configurations were considered by Minonishi *et al.*[96] for the atomic structure of a $\{11\bar{2}1\}$ interface, and these were called R and D respectively. Using a Lennard–Jones potential, they found two correspondingly stable relaxed structures for the interface, neither of which corresponds to mirror symmetry on an atomic scale. Similar results were obtained by Serra and Bacon who pointed out that the lower energy (relaxed D) interface may be obtained from the mirror interface (unrelaxed R) by moving alternate basal planes in opposite senses through $\pm\frac{1}{12}\langle 1\bar{1}00\rangle$ to change the stacking from ..ABAB.. to ..ACAC.. The configuration of the higher energy (relaxed R) interface is similar, but it has a row of vacancies in each B–C transition region. The relaxed D interface again has an atomic interface plane, but in this case it is an actual atomic plane of each crystal, not a coalesced lattice plane. Serra and Bacon point out that the atom positions are connected by a two-fold axis along η_1 although this symmetry was not present in the starting configuration.

The atomic structure of the $\{10\bar{1}1\}$ twin has been computed more recently by Serra *et al.*[97] who used the best of the pair potentials of Serra and Bacon which gives a value of $\gamma = 1.619$ for the axial ratio of a stable perfect crystal. The relaxed structure of the $\{10\bar{1}1\}$ interface is similar to that of the $\{10\bar{1}2\}$ interface and it also forms from the unrelaxed, highest symmetry form of the bicrystal by the coalescence of two separate atomic planes into a single plane. The atoms in the coherent interface plane are subjected to alternating tensile and compressive (internal) hydrostatic pressure, but the energy of the interface is quite low, and is in fact the smallest computed energy for the four h.c.p. twins considered by Serra *et al.*; the others have energies which increase in the order $\{11\bar{2}1\}$, $\{11\bar{2}2\}$ and $\{10\bar{1}2\}$.

Computer simulations of interface structures normally utilize static relaxation techniques, so that the fully relaxed structure should represent the equilibrium configuration at absolute zero. The main reservation to be made about such simulations arises from the limited validity of pairways interactions in describing the behaviour of real materials. Recent advances in basic theory and in computer technology now make it possible in principle to employ much more sophisticated "many body embedded atom potentials", but these difficult computations are not yet available. There are two further reservations about the use of simulations, namely that the static structure may change appreciably at higher temperatures or under the dynamic conditions of twin formation.

3.2. *Elementary, Zonal, Complementary and Partial Twinning Dislocations*

A step in a rational coherent twin boundary has a stress field resembling that of a dislocation in a lattice and is called a twinning dislocation. Twinning dislocations were first discussed by Vladimirskiy[98] and Frank and Van der Merwe;[99] the equivalent Burgers vector of a step of height h is

$$\mathbf{b}_T = h\, s\, \mathbf{l} \tag{35}$$

where $\mathbf{l}$ is a unit vector parallel to $\boldsymbol{\eta}_1$. Unless there are near degeneracies in the energies of different interface configurations, the flat portions of the interface separated by the step must have the same (equilibrium) structure, so that the smallest possible step height is equal to the spacing d of the *lattice* planes (not necessarily the *atomic* planes) parallel to $\mathbf{K}_1$. Such a step of minimum height is called an elementary twinning dislocation and since the elastic energy is proportional to the square of the Burgers vector, twinning dislocations with step heights which are multiples of d should tend to dissociate spontaneously into elementary twinning dislocations. However, when the lattice correspondence does not relate primitive cells of the two lattices, the two parts of the interface separated by a step between adjacent lattice planes must, in general, have different structures, and an elementary step may then be energetically unfavourable. The lattice shuffles which accompany all twinning modes with $q > 2$ imply that the interface structure repeats only at every q lattice planes parallel to K_1 if q is odd, or at every $\frac{1}{2}q$ planes if q is even, so that the Burgers vector associated with a step between two equivalent regions of coherent interface has a minimum magnitude of

$$b_T = q\,d\,s \quad (q \text{ odd})$$

$$b_T = \tfrac{1}{2}q\,d\,s \quad (q \text{ even}). \tag{36}$$

This geometrical property of a particular twinning mode was first pointed out by Thompson and Millard[100] for $\{10\bar{1}2\}$ twins in h.c.p., and they called the step of minimum height to reproduce the interface structure a "double" twinning dislocation. More generally, such steps are now called "zonal" twinning dislocations.[73,101,102]

Twinning dislocations may be of edge, screw or mixed type and have many of the properties of ordinary dislocations; in particular, they can glide in the interface plane under the action of a shear stress, enlarging or shrinking the twin as they do so. A flat, lenticular twin within a matrix (see Fig. 9) may be modelled as a series of loops of twinning dislocation, the loop diameter increasing as the central plane of the lens is approached. Such a twin can enlarge its radius simply by expansion of the twinning dislocation loops, the ratio of diameter to thickness becoming greater as it grows in this way unless new loops are formed on the central (flat) interface regions.

The dissociation of a zonal twinning dislocation into a group of q or $\frac{1}{2}q$ elementary twinning dislocations lowers the elastic energy but increases the surface energy. The elementary dislocations have parallel Burgers vectors and hence repel each other until separations are attained at which these repulsive forces are just balanced by the attractive forces due to the excess energies of the various interfaces over that of the minimum energy interface. This situation is analogous to the dissociation of a lattice dislocation into partial dislocations, and the zonal dislocation which is a repeat step of the interface may be regarded as an extended dislocation comprising partial or non-repeat steps separated by "faults", i.e. by regions of higher energy interface. If the energies of these interface faults are sufficiently small, however,

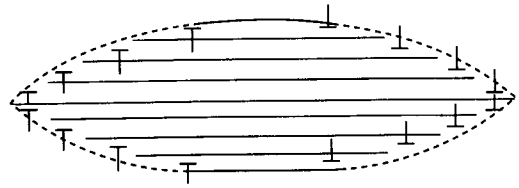

Fig. 9. A model of a lenticular twin.

the separation of the elementary twinning dislocations will become large and the concept of a zonal twinning dislocation as a separate entity is no longer required.

Zonal twinning dislocations have often been used to discuss twinning in superlattices in which the minimum step height to give an identical interface structure may be increased to some multiple of that in the disordered structure. The multiple height step is then often referred to as a zonal twinning dislocation, although this is not strictly correct, since q is now being obtained with reference to the lattice planes of the disordered structure rather than to those of the superlattice. It follows, moreover, that the formation of true twins by the motion of such steps would require interchange shuffles at the interface. The confusion arises because in the fully ordered structure there may be atomic planes parallel to $\mathbf{K}_1$ which are equi-spaced and more numerous than the lattice planes. However, in any multiple-lattice structure, it is possible to envisage interface steps between atomic planes in which the step height is smaller than that of the elementary twinning dislocation as defined above. Although it would be possible to revise the definition of the elementary twinning dislocation to make it correspond to the minimum step between atomic planes, this would cause difficulties since the twin cannot grow by motion of such a step, and the atomic planes are not necessarily equally spaced. Moreover, step defects in which the effective step height is *less* than the spacing of atomic planes may also arise in some structures by dissociation of elementary twinning dislocations. It is thus preferable to retain the definition of an elementary twinning dislocation in terms of the spacing of lattice planes, whilst noting the possibility that step defects of smaller Burgers vector may be present in some interfaces. Naturally the two interface structures connected by such a step are non-equivalent for any value of q, but in the special case of superlattice structures, this difference may be confined to changes in the chemical binding, so that the extra energy of the unfavourable interface is similar to that of an anti-phase boundary. The rather loose usage to be found in treatments which regard such a step as an elementary twinning dislocation may thus be compared with the way in which extended superlattice dislocations are often described as dissociated into "lattice" dislocations, i.e. into dislocations with Burgers vectors which are repeat vectors of the *disordered* lattice.

Various other step defects may be found in rational $\mathbf{K}_1$ interfaces. If adjacent regions of a single planar interface have different configurations of nearly equal energies, the line of separation is a step type defect with a step height equal to a fraction of the spacing of lattice $\mathbf{K}_1$ planes and hence an equivalent Burgers vector smaller than that of an elementary twinning dislocation. This applies specifically to the coherent $\{112\}$ interface of a b.c.c. twin for which the two possible structures of Fig. 8 may have very similar energies. Bristowe and Crocker[93] pointed out that this leads to the possible dissociation of an elementary twinning dislocation into two partial twinning dislocations separated by a strip of interface in the configuration which has slightly higher energy. Note that the component partials of the extended twinning dislocation have parallel Burgers vectors, as do the component elementary dislocations of an extended zonal twinning dislocation. In contrast to most extended lattice dislocations, there is thus no applied shear stress orientation which will tend to separate the partials.

When a zonal or, where appropriate, an elementary twinning dislocation is displaced along a defect-free $\mathbf{K}_1$ interface, there is no first order change in energy, other than the self energy of the dislocation, which may oscillate with the periodicity of the lattice in the direction of displacement. The dislocation may thus be described as glissile, and its motion provides a mechanism for the growth or shrinkage of the twin, as described above. In a real

crystal, there will also be both long-range and short-range additional contributions to the stress opposing motion which arise from elastic and local interactions with point, line and surface defects in the matrix. The net opposing force may be regarded as a friction stress limiting the velocity of the twinning dislocation (or, more directly, of the interface), but it is not known in most cases which interactions are most significant. The lattice resistance is a kind of Peierls–Nabarro force, and it depends strongly on the type of bonding and hence on the detailed atomic structure of the step or dislocation core. In particular, if the atomic binding is highly directional, as in materials like zirconia, the dislocation core is likely to be very narrow and the Peierls stress correspondingly high. However, for many metallic materials, the twinning dislocation core may extend over several atomic planes (i.e. the interface step is diffuse), and the lattice frictional resistance may be expected to be relatively small. Similar conclusions apply to martensite.

In early treatments of possible growth processes, it was generally assumed that the core of a twinning dislocation is similar to that of a lattice dislocation and is thus quite narrow. Some justification for this assumption arises from the magnitudes of the Burgers vectors in cubic metals and especially from the close similarity between the elementary twinning dislocation in f.c.c. metals and the Shockley partial. (The elementary twinning dislocation for f.c.c. has the same Burgers vector as a Shockley partial and a step height equal to the spacing of the $\{111\}$ planes.) Since there is probably only one stable configuration of the interface, there are unlikely to be any partial twinning dislocations in this structure, and although defects with other Burgers vectors of the DSC lattice are theoretically possible, they seem unlikely to occur in practice. For example, a step with the same height but a Burgers vector in the anti-twinning direction of twice the magnitude of a Shockley partial would be an elementary twinning dislocation of the 1.3 mode of Table 1. However, if such a step were to glide in the $\mathbf{K}_1$ plane, the atoms in successive layers would have to squeeze past each other in effectively A–A stacking, which would be energetically impossible. Thus apart from elementary twinning dislocations, the only other likely defects in f.c.c. twin boundaries are pure steps with no strain field. Pure steps can arise in annealing or growth twins, if elementary twinning dislocations with Burgers vectors in the three different but crystallographically equivalent $\langle 11\bar{2}\rangle$ directions of a particular $\{111\}$ plane are formed on successive $\{111\}$ planes and then glide together to form a triple step of zero net Burgers vector. It is probable that in a deformation twin, the vast majority of the twinning dislocations will all have the same Burgers vector, but a pure step may then be formed because three elementary twinning dislocations on successive $\{111\}$ planes have a total Burgers vector of $\frac{1}{2}\langle 11\bar{2}\rangle$ which may be cancelled if a lattice dislocation of opposite Burgers vector, or more probably two lattice dislocations with a net Burgers vector opposite to that of the three twinning dislocations, glide until they become coincident with the step. This means that, at least in principle, steps with a height of three interplanar spacings, or some integral multiple of three, may be pure steps. Pure steps may also be formed in b.c.c. twin interfaces, as discussed in Section 6.2.

Experimental evidence that small steps in twins are fairly sharp discontinuities was first provided by direct observation of elementary twinning dislocations which are visible when foils of f.c.c. copper (Mahajan *et al.*[103]) or b.c.c. molybdenum–rhenium alloys (Hull;[104] Mahajan[105–106]) containing very thin tapering twins are examined in the transmission electron microscope. However, computer calculations by Yamaguchi and Vitek[94] and Bristowe and Crocker[107] indicate that twinning dislocations, at least in b.c.c. structures, are appreciably wider than lattice dislocations, and this may have important implications for the theory of twin growth. The calculations of Bristowe and Crocker[107,108] have also revealed the possible

existence of other step defects (complementary and zonal twinning dislocations) in b.c.c. twin boundaries.

The complementary twinning dislocation was originally introduced by Sleeswyk.[109] It has the same step height as the elementary twinning dislocation but for the same sense of the step, its Burgers vector is twice as large and in the opposite direction, so that its structure is quite different. Sleeswyk considered the hypothetical dissociation of a twinning dislocation in a tapering twin into a lattice dislocation and a complementary twinning dislocation according to the Burgers vector equation

$$\tfrac{1}{6}\langle 111\rangle = \tfrac{1}{2}\langle 111\rangle + \tfrac{1}{3}\langle \bar{1}\bar{1}\bar{1}\rangle. \tag{37}$$

The reverse process of combination of a twinning dislocation with a lattice dislocation of antiparallel Burgers vector is clearly an equal formal possibility; in one case, the lattice dislocation is emitted from the interface, and in the other case the opposite lattice dislocation glides into the interface. In fact, however, with the pairwise potentials that were used by Bristowe and Crocker, an isolated complementary dislocation is unstable and will dissociate into elementary, partial and zonal twinning dislocations. Motion of a complementary dislocation along the $\mathbf{K}_1$ plane is thus an unlikely process, but if it were to occur on successive (112) planes, the twinning mode produced (see Table 1) would have a shear of magnitude $\sqrt{2}$ with $\mathbf{K}_1 = \{112\}$, $\mathbf{K}_2 = \{110\}$, $\boldsymbol{\eta}_1 = \langle 11\bar{1}\rangle$ and $\boldsymbol{\eta}_2 = \langle 001\rangle$.

Bristowe and Crocker also found a step defect of double step height but Burgers vector of type $\frac{1}{6}\langle 111\rangle$ and they called this a zonal twinning dislocation. The existence of such a dislocation in a $\{112\}$ b.c.c. twin interface was not predicted prior to the computer simulation, but it must be emphasized that this is not a zonal twinning dislocation of the usual b.c.c. twin mode. Since the Burgers vector has the same magnitude as that of the usual twinning dislocation and the step height is twice as large, it follows that propagation of such a dislocation through a series of $\{112\}$ planes will produce a shear of $\sqrt{2}/4$. The corresponding twinning mode has $\mathbf{K}_1 = \{112\}$, $\mathbf{K}_2 = \{33\bar{2}\}$, $\boldsymbol{\eta}_1 = \langle 11\bar{1}\rangle$, $\boldsymbol{\eta}_2 = \langle 113\rangle$, $q = 4$, so that one-half of the lattice points (atoms) must shuffle as the interface moves forward. (This mode is listed in Table 1.) The defect is thus correctly described as a zonal twinning dislocation of this hypothetical twinning mode with a smaller shear than the usual mode, but the usage is rather loose when the defect is present in the boundary of a deformation twin which has formed by a different shear, or in the boundary of a non-deformation twin.

The twinning dislocations found by Bristowe and Crocker for b.c.c. structures show that defects in coherent twin boundaries may be regarded in two different ways. If no restrictions are imposed on the mechanism of formation of an interface of given structure, the set of possible Burgers vectors associated with a step of fixed height in this interface is obtained by taking any representative Burgers vector of the set (given, for example, by eq. (33)) and adding to it any lattice repeat vector; these vectors form a unique set and may be derived from any representation of the lattice relations. Pure steps may be envisaged if and only if this set contains a zero Burgers vector.

It is clear that the complete set of Burgers vectors of "perfect" interface dislocations (i.e. linear defects which separate two regions of identical interface structure) is identical with the set of vectors which constitute the DSC lattice of Bollmann.[110] These vectors link the sites of the parent lattice to those of the twin when the two lattices are in a coincident orientation and position, i.e. when $\mathbf{t} = 0$. For a single lattice structure, the DSC dislocations are the only vector translations which reproduce the interface structure. The vectors are independent of $\mathbf{t}$ and each may be associated with a step of height d. However, in a general

discussion of possible defects which reproduce the structure of an interface, Pond[25-26] and Pond and Vlachavas[27] have shown that in non-symmorphic crystals (i.e. crystals containing mirror-glide planes or screw-rotation axes) additional dislocation type defects may in certain circumstances exist in an interface and reproduce the interface structure. Whereas defects in single crystals are characterized by the symmetry operations of translation, proper rotation or proper screw-rotation, interface defects are characterized by combinations of symmetry operations, one from each crystal.

In Pond's formulaton, the twinning dislocations considered above arise from the broken translational symmetry of the interface, but in some interfaces in non-symmorphic crystals, it is also possible to produce interface defects of translational character by combinations of point symmetry operations which are aligned but contain intrinsic glide components which are either not equal or not parallel. These "supplementary displacement dislocations", unlike the DSC dislocations, have Burgers vectors which are modified by any displacement **t** which breaks the translational alignment of the symmetry elements of the two crystals. Moreover, in general, such defects arise only at the junction between two differently orientated (but equivalent) interfaces and they only represent defects in a single interface when special conditions have been satisfied. The general theory of such defects is too complex to be included here, but an interesting special case arises in connection with $\{11\bar{2}1\}$ twinning in h.c.p. crystals.

In the h.c.p. structure, the only stable twinning dislocation expected for the $\{10\bar{1}2\}$ mode is the zonal dislocation of double step height first discussed by Thompson and Millard. This has a Burgers vector

$$\mathbf{b}_T = \frac{3-\gamma^2}{3+\gamma^2}\langle 10\bar{1}\bar{1}\rangle \tag{38a}$$

so that

$$|\mathbf{b}_T| = [(3-\gamma^2)/(3+\gamma^2)^{\frac{1}{2}}]a. \tag{38b}$$

The Burgers vector thus has magnitude $a/(51)^{\frac{1}{2}} \simeq a/7$ for ideal axial ratio, $\gamma = c/a = (8/3)^{\frac{1}{2}}$, but this magnitude varies rapidly with γ. Computer simulation of the structure using two body potentials shows that the width of the twinning dislocation is sensitive to the assumed potential.

As already noted, the probable twinning mode for h.c.p. $\{11\bar{2}2\}$ twinning has $q = 6$, so that the important twinning dislocation will be expected to be zonal, with a step height equal to three interplanar spacings of the $\{11\bar{2}2\}$ lattice planes. The Burgers vector of this dislocation is

$$\mathbf{b}_T = \frac{\gamma^2-2}{3(\gamma^2+1)}\langle 11\bar{2}\bar{3}\rangle \tag{39a}$$

and

$$|\mathbf{b}_T| = [(\gamma^2-2)/(\gamma^2+1)^{\frac{1}{2}}]a. \tag{39b}$$

For ideal c/a, the magnitude $|\mathbf{b}_T|$ is $(4/33)^{\frac{1}{2}}a \simeq a/8^{\frac{1}{2}}$. The core structure of this dislocation depends on the detailed shuffle displacements of 3 out of every 4 atoms, and Serra *et al.*[111] made computations for three different possibilities. The energy and width of the step were found not to be very sensitive to the shuffle model used, but to depend on the potential. Calculations were also made for two other possible step defects in this type of boundary,

having step heights of one and four interplanar spacings, respectively. These steps would be twinning dislocations of other hypothetical twinning modes for which $\mathbf{K}_1 = \{11\bar{2}2\}$; in the single step case, the mode has a high shear of ~ 1.22 and the four layer step has more complex shuffles. Thus these dislocations are probably not important in the mechanism of deformation twinning.

Since no lattice shuffles are involved in $\{11\bar{2}1\}$ twinning, an elementary twinning dislocation reproduces the interface structure. This dislocation is specified by

$$\mathbf{b}_T = \frac{1}{3(4\gamma^2 + 1)} \langle 11\bar{2}\bar{6} \rangle \tag{40a}$$

and

$$|\mathbf{b}_T| = [1/(1 + 4\gamma^2)]^{\frac{1}{2}} a. \tag{40b}$$

For ideal axial ratios, the Burgers vector is $\mathbf{b}_T \simeq (1/35)\langle 11\bar{2}\bar{6} \rangle$, and has magnitude $(3/35)^{\frac{1}{2}}a$. When this dislocation was simulated, however, Serra *et al.* found that it decomposed into two dislocations, each with one-half of the above Burgers vector, as first envisaged by Minonishi *et al.*[96] These two dislocations each have a step height equal to the separation of atomic planes parallel to the interface, i.e. to one-half of the spacing of lattice $\mathbf{K}_1$ planes. Although this ordinarily would not reproduce the interface structure, the non-alignment of the translational components of the mirror glide symmetry of the $\{1\bar{1}00\}$ plane of shear ensures that the two interfaces bounding such a step have equivalent structures and energies. This is an example of the "supplementary displacement dislocations" analysed by Pond. With two of the three potentials used, Serra *et al.* found the core width of both edge and screw twinning dislocations of this type to be very wide, implying that the steps may be very mobile.

The final h.c.p. $\mathbf{K}_1$ interface for which atomistic simulations of twinning dislocations have been made is the $\{10\bar{1}1\}$ plane. As discussed in Section 2.7, the deformation twinning mode found experimentally for this plane is, most unusually, a $q = 8$ mode, whilst the displacement of the boundaries of the observed $\{10\bar{1}1\}$ transformation twins may be regarded as a $q = 4$ mode. Thus there are two dislocations of interest with step heights corresponding respectively to $4d$ and $2d$ where d is the spacing of lattice planes parallel to $\{10\bar{1}1\}$. The Burgers vector of the zonal twinning dislocation of the deformation mode identified in magnesium and titanium is

$$\mathbf{b}_T = \frac{4\gamma^2 - 9}{4\gamma^2 + 3} \langle 10\bar{1}\bar{2} \rangle \tag{41a}$$

with magnitude

$$|\mathbf{b}_T| = [2^{\frac{1}{2}}(4\gamma^2 - 9)/3^{\frac{1}{2}}(4\gamma^2 + 3)^{\frac{1}{2}}]a \tag{41b}$$

which is $5/(123)^{\frac{1}{2}}$ for the ideal axial ratio.

The direction of Burgers vector of the $\{10\bar{1}1\}$ transformation twin is strictly irrational, so that it is not possible to write a simple analytical expression for it. However, if γ has its ideal value, the Burgers vector becomes rational but has very high indices $\langle 13,\bar{4}1,28,15 \rangle$. The magnitude of $\mathbf{b}_T$ is

$$|\mathbf{b}_T| = [3(4\gamma^4 - 17\gamma^2 + 21)/2(4\gamma^2 + 3)]^{\frac{1}{2}} a \tag{42}$$

and this is ~ 0.448 for the ideal axial ratio. Since it is necessary to have periodicity along the dislocation line in order to make possible a computer simulation of the atomic structure, this twinning dislocation, unlike the others considered above, could only be simulated in a mixed orientation, intermediate between edge and screw.

For any rational twin interface, the atomic configuration at a step will adjust itself wherever possible so as to minimize the effective Burgers vector. This implies that the structures of minimum height steps in corresponding boundaries of annealing and deformation twins are likely to be identical since the operative twinning mode of the deformation twin is likely to correspond to a minimum shear and hence to a minimum Burgers vector condition. However, in f.c.c. and some related structures, there are three crystallographically equivalent directions of the Burgers vector in the coherent interface, all of which are equally likely to be present in an annealing twin, whereas in a deformation twin, the steps will predominantly have Burgers vectors parallel to the physical $\boldsymbol{\eta}_1$ direction.

Some authors have distinguished between grain boundary dislocations and grain boundary steps for the general grain boundary, and have suggested that there is no strain field associated with an ideal step. However, it needs to be emphasized that formation of an ideal step is rarely possible even when the step height is a multiple of the interplanar spacing; a necessary condition is that the plane defined by the step length and the riser is a lattice plane of a coincident site lattice of the two crystal lattices. In the cases of coherent twin boundaries on $\{111\}$ planes of f.c.c. crystals or $\{112\}$ planes of b.c.c. crystals, pure steps are possible when the step height is some multiple of three interplanar spacings.

3.3. *Twins with Irrational $\boldsymbol{K}_1$ Interfaces*

It will be noted that except in cubic structures, the magnitude of the effective Burgers vector of a twinning dislocation depends on at least two independent lattice parameters, and is not generally an integral fraction of a lattice vector. Partial dislocations (fault vectors) of this kind are quite acceptable provided $\boldsymbol{\eta}_1$ and $\mathbf{K}_1$ are both rational. The definition of a twinning dislocation simply as a step in the coherent $\mathbf{K}_1$ interface then continues to fix $\mathbf{b}_T$ without ambiguity, as, for example, in eqs (38–40). Although it should be noted that in any dissociation model in a structure in which the shear magnitude depends upon a crystallographic parameter such as c/a, the splitting of the original dislocation also varies with the appropriate parameter, this is only what is expected from the geometry of the monolayer fault. Indeed, there is no particular conceptual difficulty in the definition of $\mathbf{b}_T$ for type I twins, in which the atomic displacements are (generally) in an irrational direction. Steps in the rational $\mathbf{K}_1$ interface can then be regarded as twinning dislocations with irrational directions of the Burgers vector, and this seems likely to be a better representation of the physical situation than a model in which two or more steps with different rational directions of displacement alternate so as to produce net displacements in the required irrational direction. However, the concept of a step in the interface finally breaks down for type II twins since if $\mathbf{K}_1$ is irrational, the spacing of lattice planes parallel to the interface is indefinitely small.

The theory of the atomic structure and of defects in irrational (or very high index) interfaces is difficult and not well developed, and the following description is simplified and partly intuitive. On an atomic scale, an irrational interface must consist of rational facets and in the general case a minimum of three differently orientated facets would be required. However, since the interface of a type II twin necessarily contains one rational direction ($\boldsymbol{\eta}_1$), it is

possible to model it as alternate facets of two rational planes. The most appropriate model will generally consist of facets of minimum size parallel to the two closest-packed planes in the zone axis of $\boldsymbol{\eta}_1$. If the smaller facets (P) all represent transitions between adjacent lattice planes of the larger facets (Q), and are spaced along Q either uniformly or in some regularly repeating sequence at multiples of the distance at which adjacent lattice planes of P intersect Q, the average interface will remain rational. However, as the period of the repeat pattern increases, the Miller indices of the interface become higher and higher. The larger facets will be those nearest in orientation to the mean interface plane, and the smaller facets may often be regarded as steps on the larger facets; by increasing the period, better and better rational approximations to an irrational plane may be obtained. For example, a first approximation to a particular interface might be produced by steps at repeated intervals of 5, 4 and 4 lattice vectors along the rational Q interface, and successive approximations might then consist of the following repeated step patterns: . . .544. . ., . . .5444. . ., . . .5444544. . ., . . .54445444544. . ., . . .544454454445444544. . ., etc. In the limit, when the period has become infinite, the interface is truly irrational, but the step pattern remains ordered. The interface is now an example of a one-dimensional quasi-crystal, since there is genuine periodicity parallel to $\boldsymbol{\eta}_1$ but the structure is quasi-crystalline[112] in the interface direction normal to $\boldsymbol{\eta}_1$. Similarly, Sutton[113] has shown that the "structural unit" model of irrational tilt boundaries with a rational tilt axis[114] may be treated as a one-dimensional quasi-crystal in which the periodic combination of A and B structural units in a rational, high indices boundary becomes quasi-periodic in the limit.

Note that if the plane of the larger facets were parallel to the true $\mathbf{K}_1$ plane, the steps would be twinning dislocations in screw orientation. For a matching irrational plane, however, they are an essential element in the structure of the boundary, and have been called "intrinsic twinning dislocations".[44] If an irrational $\mathbf{K}_1$ interface traverses a single crystal, there will be no force driving the steps in a particular direction when a stress is applied to the crystal unless a nucleating mechanism is available to supply fresh steps as required to maintain the irrationality of the interface plane. If this can be achieved, however, the steps will glide along the rational planes as the interface moves forward, and it is in this sense that they can also be regarded as twinning dislocations. This leads to the concept that steps on the rational facets could also assume edge or general orientations and local densities other than that specified by the lattice matching condition. The excess steps over the ideal model of the interface now constitute extrinsic twinning dislocations which will respond to an external stress in the same way as steps in rational $\mathbf{K}_1$ interfaces.

Extrinsic twinning dislocations are effectively steps in the macroscopic irrational interface, so that their motion displaces this interface. The magnitude of the effective Burgers vector of such a twinning dislocation is given by the twinning shear multiplied by the height of the step in the irrational plane, i.e. by the interplanar spacing of the Q lattice planes resolved in the direction of the normal to the irrational $\mathbf{K}_1$ plane. Hence the Burgers vector is

$$\mathbf{b}_T = u_i m_i s \mathbf{l} = \bar{d} s \mathbf{l} \tag{43}$$

where $\mathbf{u}$ is any vector connecting lattice points on adjacent planes of type Q, and $\bar{d}$ is the spacing of the Q planes resolved in the direction of the unit normal $\mathbf{m}$ to the irrational interface. Note that the magnitude is irrational, but the vector is parallel to the rational $\boldsymbol{\eta}_1$ direction. This step in plane Q is the type II equivalent of an elementary twinning dislocation, but the interface structure on the two sides of the step will be identical only if a primitive

lattice vector **w** parallel to $\boldsymbol{\eta}_1$ traverses not more than two lattice $\mathbf{K}_2$ planes. In other cases, the equivalent of the zonal twinning dislocation must be defined by:

$$\mathbf{b}_T = w_i m_i s\mathbf{l} = \bar{q}\bar{d}s\mathbf{l}. \tag{44}$$

It might be considered that the intrinsic steps of the irrational interface would all have a height of $\bar{q}\bar{d}$ rather than $\bar{d}$, but this cannot be assumed without modelling the actual interface structure; it is conceivable, for example, that an alternating configuration at the Q facets is more favourable than a repeated configuration.

An equivalent formal treatment of a faceted interface is to use the Frank–Bilby–Bollmann equation to calculate separately the formal dislocation content required to correct the misfit along each of the facets P and Q. This corresponds to $-\mathbf{b}_T$ for an individual step facet P, but sums to zero over a sufficient number of facets if the relative lengths of Q and P perpendicular to $\boldsymbol{\eta}_1$ give the exact $\mathbf{K}_1$ interface. Various ambiguities in the dislocation descriptions of stepped and unstepped interfaces depend on how zero dislocation content is defined, and are discussed by Olson and Cohen,[115] Olson,[116] Christian and Knowles[117] and Christian.[118]

4. NUCLEATION AND GROWTH OF DEFORMATION TWINS

4.1. *Homogeneous Nucleation*

It is usually assumed that separate consideration should be given to the formation of a small twin region and to its subsequent growth into a large twin. The reasons for this assumption are similar to those which lead to the conclusion that most first order phase transformations are divided into nucleation and growth stages, namely the spontaneous formation of a large twin is difficult to envisage, and the finite positive energy of the matrix-twin interface implies an energetic barrier to the formation of a very small volume of twinned crystal. The analogy with phase transformation may be taken further, inasmuch as twin nuclei may be supposed to form under the action of an applied stress in a region of near-perfect crystal (homogeneous nucleation) or, alternatively, may form only when a suitable defect configuration is present (heterogeneous nucleation).

The possible influence of defects on twin nucleation was studied in some classic experiments of Bell and (R.W.) Cahn.[119,120] They found that very carefully prepared and handled single crystals of h.c.p. metals may be stressed to much higher levels than those at which twins normally form in less perfect crystals, but that twins can be induced in a highly stressed crystal by pricking the surface with a pin. In later experiments on cadmium and zinc, Price[121–123] used near perfect whisker and platelet specimens strained *in situ* whilst under observation in an electron microscope and found that the stresses to induce twinning were an order of magnitude higher than those usually measured on macroscopic specimens. The interpretation of these results was that twinning is normally initiated by some defect configuration, but that in highly perfect crystals which deform at much higher stresses, homogeneous nucleation of twins may occur.

Homogeneous twinning under the action of stress alone implies a mechanical instability of the lattice, and occurs, in principle, when the applied shear stress on $\mathbf{K}_1$ resolved along $\boldsymbol{\eta}_1$ reaches a critical value, the so-called theoretical strength of the material. Recent developments in first principles calculations have made it possible to treat this problem within

the local density approximation to density functional theory, without any assumptions about interatomic force laws. Paxton *et al.*[124] considered in this way the lattice stability against twinning- and anti-twinning shear stresses for five b.c.c. transition metals and for f.c.c. Ir, Cu and Al. They found, remarkably, that the critical shear stress for twinning is $(0.12–0.17)\mu$ where μ $[=(c_{11}-c_{12}+c_{44})/3$ for cubic crystals] is the appropriate elastic modulus for shear on $\mathbf{K}_1$ in the direction $\boldsymbol{\eta}_1$. According to these calculations, the critical strain is also remarkably constant and is either equal to or slightly greater than the Frenkel value of one quarter of the twinning shear for all the metals except iridium and copper. The authors claim that these results have significant implications on, for example, the formulation of the Peierls–Nabarro model of a dislocation.

The theoretical strength is an important material parameter in theories of deformation and fracture, but it is uncertain whether it is approached in practice, even in near perfect crystals. At such high stress levels, it is also difficult to model the way in which the instability might develop; the quasi-static models of twinning dislocations are probably inapplicable, but it is difficult to envisage an instantaneous homogeneous deformation, rather than a discontinuity (a soliton wave?) which spreads outwards from some centre. This modifies the instability criterion, since either interfacial energies or gradient energy terms must be introduced.

The classical theory of homogeneous nucleation avoids such difficulties by supposing that the free energy barrier to the formation of a small twinned region is overcome by thermal fluctuations. This theory, initially applied to twinning by Orowan,[125] is considered next as a possible explanation for the experimental results on nearly perfect crystals, but it should be noted that there is no substantial experimental evidence to support a thermally-activated mechanism for twin nucleation. In particular, twins are often observed to form more readily as the temperature is decreased, even at temperatures approaching absolute zero.

In classical nucleation theory,[20] the energy of a small embryonic twin which is assumed to be separated from the parent phase by a sharp interface is calculated by assuming that the embryonic region has a defined volume and surface area and that macroscopic parameters such as surface free energy or elastic stiffness are relevant. The obvious difficulties of this model when applied to a very small twin volume have been much discussed in the analogous case of phase transformation;[20] in many circumstances, the assumptions seem to be justified provided it is recognized that the parameters introduced will not necessarily have their bulk values. The calculation is simplest if the twin embryos are assumed to be oblate spheroids with minor axis (y) normal to $\mathbf{K}_1$. A more general assumption is that the shape is an ellipsoid with three unequal axes, the two axes in the $\mathbf{K}_1$ plane being parallel to $\boldsymbol{\eta}_1$ and normal to $\mathbf{P}$ respectively. This more general assumption would be especially relevant when account is taken of elastic anisotropy, as in recent papers by Lee and Yoo[126] and Yoo and Lee,[127] but it has not been seriously tackled, presumably because the calculations then become very difficult. The simpler assumption of circular symmetry within the habit plane seems sufficiently accurate for most purposes.

The change in energy on forming an embryo of semi-axes R,R and y has a negative term representing the work τs per unit volume of embryo done by the shear stress across $\mathbf{K}_1$ resolved in the $\boldsymbol{\eta}_1^{\gamma}$ direction, a positive term of magnitude (in the isotropic approximation) Ay/R representing the elastic energy per unit volume of the constrained twin, and a further positive term for the (non-elastic) energy of the twin interfaces. In this calculation, Orowan treated the interface energy as that of the matching $\mathbf{K}_1$ planes plus that of the twinning dislocations which were assumed to have a uniform line tension, i.e. energy per unit length. Orowan assumed the constrained strain energy to be negligible on the assumption that the

matrix stresses do not exceed the yield stress. However, the energy for homogeneous nucleation, unaided by defects, is obtained by allowing the stress field of the twin to increase to whatever value is appropriate in the elastic approximation, up to the theoretical strength of the material. This is not unreasonable since there should be no dislocation sources in the small high-stressed volume around the tip of the nucleus. The strain energy may then be included by means of Eshelby's linear elastic calculation,[128] and the steps may be regarded as sections of a second interface with specific free energy σ' different from the energy σ of the $\mathbf{K}_1$ interface. The change in energy ΔG due to the formation of an embryo of volume $v = 4\pi R^2 y/3$ in an infinite matrix may then be written[129]

$$\Delta G/v = -\tau s + 3\sigma/2y + 3\sigma'/R + Ay/R. \tag{45}$$

The size and shape of a critical nucleus are given by $\partial \Delta G/\partial R = \partial \Delta G/\partial y = 0$ and this defines the saddle point in ΔG. The shape of this nucleus is defined by the equations

$$\tau s R = 2Ay + 3\sigma' \tag{46a}$$

$$\sigma R = Ay^2 + \sigma' y \tag{46b}$$

which may be solved to give the critical thickness

$$y_c = -(p+q) \pm (p^2 + q^2 - 4pq)^{\frac{1}{2}} \tag{47}$$

where $p = -\sigma/\tau s$ and $q = \sigma'/2A$. (The minimization used by Orowan corresponds to $A = 0$, whereas some other treatments effectively have $\sigma' = 0$. The equations also depend slightly on the assumed geometry of the nucleus; that used by Orowan introduces factors of 4/3 and 3/4 into the second term on the right of eq. (45a) and the first term on the right of eq. (45b), respectively.)

The factor A in isotropic approximation[128] is $\mu[\pi(2-\nu)/8(1-\nu)]s^2 \simeq \mu s^2$ and for $\{10\bar{1}2\}$ twinning in zinc, this is about $6 \cdot 10^8\ \mathrm{Jm}^{-3}$. Low estimates of σ and σ' are 20 and 100 mJm^{-2}, and with Price's measured value[121–123] of the twinning stress for zinc of $\tau = 500$ MPa, the driving force supplied by the applied stress is $\tau s = 7 \cdot 10^7\ \mathrm{Jm}^{-3}$. The critical nucleus would thus have $y_c \simeq 0.63$ nm (i.e. about ten $\{10\bar{1}2\}$ lattice planes) and the corresponding values of R_c and ΔG_c are 15 nm and 75 eV, respectively. This is clearly much too large an energy for homogeneous nucleation by thermal fluctuations to be feasible, and Price's original claim that the Orowan theory gives a nucleation barrier of only 1 eV seems to have been erroneous. Variations in the assumptions by setting either σ' or A equal to zero do not produce much improvement; the most favourable case is for $A = 0$, which corresponds to $\Delta G_c \simeq 13$ eV with the above assumptions, and an appreciably larger value with the effective value of $\sigma' = 500\ \mathrm{mJm}^{-2}$ used by Orowan.

The use of anisotropic elasticity[126,127] introduces two additional energy terms which are respectively an "inhomogeneity effect" arising from the difference in elastic constants of the twin and matrix which modifies the stress-free strain used in Eshelby's theory (the simple shear of the twinning mode) to an effective strain, and a second term which is usually described as an elastic interaction energy and is the additional work done by the applied stress because of the elastic inhomogeneity. In practice, because of the mirror plane or rotation axis of symmetry of the parent–twin relation, many elastic stiffnesses are identical in matrix and twin, and the elastic strain energy differs little from that calculated on the assumption that twin and matrix have identical elastic properties.

Lee and Yoo also discuss two separate shapes, namely the oblate spheroid with semi-axes of lengths y, R, R and the elliptic cylinder with semi-axes y, R, ∞. In both cases, the energy is treated as a function of volume and aspect ratio y/R and for the elliptical cylinder, a shape bifurcation is obtained. The equilibrium aspect ratio is predicted to be unity (i.e. the twin is a circular cylinder) below a certain linear dimension (defined as [cross-sectional area]$^{\frac{1}{2}}$), whilst above this dimension the aspect ratio decreases rapidly. This is expected since with increasing size, the surface energy term is less important, whilst the strain energy tends to zero as the aspect ratio becomes very small. The strain energy per unit volume of the twin is also found to be smaller for the flattened cylindrical plate than for the oblate spheroidal plate. However, the relevance of this result to the estimation of the energy fluctuation needed to nucleate a twin is not clear, and the calculation of the free energy barrier in an appendix to the paper on tetragonal twins[126] gives only the saddle point value of the free energy per unit length of the cylindrical twin. In order to assess the probability of homogeneous nucleation, the total free energy of formation of a twin embryo mut be calculated; this implies a minimization of the net change in free energy for a general ellipsoid shape with respect to all three semi-axes or (equivalently) to its volume and both aspect ratios. This seems to have been accepted in the results given by Lee and Yoo[127] for h.c.p. twinning where an equation is given for the energy barrier of an oblate spheroid rather than a cylindrical twin. Lee and Yoo further suggest that the active twin mode is that for which this nucleation barrier is least, and they speculate that the observed transition from predominantly $\{11\bar{2}2\}$ twinning at low temperatures to $\{10\bar{1}1\}$ twinning at higher temperatures in titanium and zirconium may be rationalized in terms of a temperature-dependent ratio of the twin boundary energies.

The general conclusion after the earlier calculation was that homogeneous nucleation of twins is improbable unless there is a combination of very high stress and very low surface and strain energies, and this remains valid in the more sophisticated recent work. Although the strain energy may have been reduced in the thin platelets used in Price's experiments, it is unlikely that the surface energies can be substantially lower than the above estimates. The alternative possibility seems to be that the true stress concentration factor at the re-entrant nucleation sites was larger than that calculated, or that the platelets contained some undetected defects which aided nucleation. Bell and Cahn similarly interpreted their results by supposing that a high stress concentration was produced by local slip on two systems. It is now considered highly probable that twinning is in fact usually initiated by defects, the role of which may be either to produce the very high stresses required for homogeneous nucleation, or to form nuclei more directly by re-arrangements in their core structures.

4.2. *Growth by Homogeneous Nucleation of Twinning Dislocations*

The model, of an enclosed lenticular twin as a series of twinning dislocation loops parallel to a (rational) $\mathbf{K}_1$ plane implies that a small nucleus of this type could extend very rapidly in all directions contained within $\mathbf{K}_1$ simply by expansion of these glissile loops. The effect of this is to produce (in principle, at least) large flat areas of coherent $\mathbf{K}_1$ interface, and further thickening of the twin then requires a mechanism for the formation of new layers. This is a problem analogous to that encountered in the theory of the growth of a close-packed face of a perfect crystal from the vapour phase, which requires (in the absence of suitable topological defects) the repeated nucleation of disc-shaped islands forming two-dimensional nuclei of new layers surrounded by closed steps. In a similar manner, a possible mechanism

for the thickening of a twin in the direction normal to $\mathbf{K}_1$ is the thermally-activated formation of a closed loop of twinning dislocation which then spreads outwards under the influence of the applied stress. This is a nucleation problem since the tendency of the stress to expand the loop is opposed by the line tension of the twinning dislocation.

With an isotropic linear elastic model, the energy needed to form a loop of radius R is

$$\Delta W = \tfrac{1}{2}\mu b^2 R \ln(R/r_i) - \pi\tau b R^2 \tag{48}$$

where r_i is the core radius of the twinning dislocation and the two terms represent respectively the line tension (or strain energy) of the dislocation loop and the work done by the applied shear stress τ. The condition for the loop of critical size, $\partial \Delta W/\partial R = 0$, then gives

$$R_c = (\mu b/4\pi\tau)\{\ln(R_c/r_i) + 1\} \tag{49}$$

and

$$\Delta W_c = (\mu b^2 R_c/4)\{\ln(R_c/r_i) - 1\}. \tag{50}$$

The activation energy at fixed stress thus depends upon the square of the Burgers vector and the stress at fixed energy varies linearly with the Burgers vector. The rate at which new loops form is proportional to $\exp(-W_c/\mathbf{k}T)$, and may represent reasonable growth rates if b is sufficiently small. Estimates show, for example, that if b is about one-tenth of the interatomic distance and τ/μ exceeds $\sim 8 \cdot 10^{-4}$, the corresponding activation energy and critical radius are ~ 0.2 eV and 10 nm, respectively, thus giving quite a high nucleation rate at most temperatures. On the other hand, if the twinning dislocation has a Burgers vector greater than (say) one-third of an interatomic distance, as in cubic metals, the probability of spontaneous (thermally-assisted) formation of new layers is almost negligible.

Twinning dislocations in face-centred tetragonal or orthorhombic structures, such as those found in indium–thallium or gold–cadmium alloys, have Burgers vectors with magnitudes in the range 0.006–0.04 nm. Birnbaum and Read[130] showed that twin boundary motion by spontaneous nucleation is quite probable in such alloys, the required activation energy being comparable to the available thermal energy at stresses and temperatures corresponding to those at which the boundaries are observed to move. In these alloys, a single crystal of the high temperature cubic phase may be transformed martensitically to give a specimen consisting of a single set of parallel twins. The twins are extremely mobile under small stresses, and deform plastically up to a limiting strain entirely by movement of the twin boundaries. The low stress required to move the boundaries is undoubtedly associated with the small shear, whether or not twinning dislocations are nucleated spontaneously. It should be noted that the calculation of the activation energy for nucleation using eq. (48) neglects the core energy of the twinning dislocation, and this may not be justified when the elastic energy becomes small. The equation also does not include any term representing the misfit energy of the area enclosed by the loop of twinning dislocation; in other words, it is appropriate to the nucleation of a new step on the surface of an existing twin, but not to the creation of a monolayer twin in a region of perfect lattice. However, if the calculation is correct, it seems that there should be no difficulty in the normal growth of a twin which is only a few lattice spacings thick.

The conclusion that thickening of deformation twins in cubic crystals by spontaneous nucleation of successive loops of twinning dislocation is not possible rests on the assumption that the interface region possesses the elastic properties of the matrix. Some authors[131–132]

have pointed out that this conclusion may be erroneous, and in particular, the effective shear modulus, μ' may be appreciably lower than the modulus, μ, for bulk material. Support for the view that the effective stress and activation energy required to nucleate a loop of twinning dislocation may be lower than the values given by the ordinary linear elastic model comes from the computer simulations of Yamaguchi and Vitek[94] and Bristowe and Crocker[93] which indicate that twinning dislocations have relatively wide cores and hence relatively small self energies. Yamaguchi and Vitek point out that the width of the core according to the Peierls–Nabarro model is proportional to the shear modulus and from the computed widths of twinning dislocations and lattice dislocations using various empirical interatomic potentials, they estimate the effective shear modulus μ' to be a factor of 3–5 times smaller than the modulus of the matrix. Sumino[131] estimated the stress needed for spontaneous twinning, i.e. virtual zero activation energy, as $\mu' b/2h$, and Yamaguchi and Vitek point out that with their potentials this is ~ 0.01–0.02μ. This is still rather a high stress for continuous growth of twins, but is lower than the corresponding estimate for formation of a twin nucleus from a screw dislocation which is $\sim 0.03\mu$ for the same potentials. Thus growth by spontaneous nucleation of new layers is considered to be a possible mechanism, even in b.c.c. metals.

4.3. *Defect-Assisted Nucleation and Growth: General Principles*

Most models of defect-assisted nucleation are based on the dissociation of some dislocation configuration into a single- or multi-layered stacking fault which then serves as the twin nucleus. Many of these models are specific to the various crystal structures, but it is useful to recognize certain common features. The fault configuration is bounded by partial dislocations of the parent crystal which can also be considered as twinning dislocations, and these can extend the fault in its own plane very rapidly. Growth normal to the $\mathbf{K}_1$ plane may be envisaged either as an orderly process in which each layer is added successively to the twin, or as the random accumulation of embryonic twin faults. Orderly growth may occur by homogeneous nucleation of steps, as described in Section 4.2, or by the heterogeneous nucleation of successive steps at some extended defect configuration such as a grain boundary, but there are other possibilities, usually described as "pole mechanisms" and "ratchet" or "cross-slip" sources.

In general, there are no crystallographic restrictions which prevent existing lattice dislocations from dissociating into any number of twinning dislocations together with a residual imperfect dislocation to conserve the total Burgers vector. However, the number of likely configurations for particular crystal structures is strictly limited and tends to be controlled by crystallographic degeneracies. Figure 10 shows some (crystallographically) possible dissociations of individual glide dislocations[133] which depend upon relations between the slip plane and direction and the twinning plane and direction. In (a), a slip dislocation lying along the intersection of its slip plane (S) and a twinning plane (T) dissociates into a single twinning dislocation which moves off into T leaving a residual imperfect dislocation along the line of intersection of the two planes. Such a dissociation can occur in any crystal structure since a glissile dislocation can always, in principle, reorient itself in its slip plane until a sufficient length also lies in the plane T. Also, in some structures, sessile dislocations may lie in a twinning plane, or long jogs may form on a slip dislocation as the cumulative result of many intersections with other dislocations of a different Burgers vector. A special case of the simple dissociation occurs if the T and S planes coincide, as shown in Fig. 10(b). The initial dislocation need not then be a straight line, and both the twinning and residual

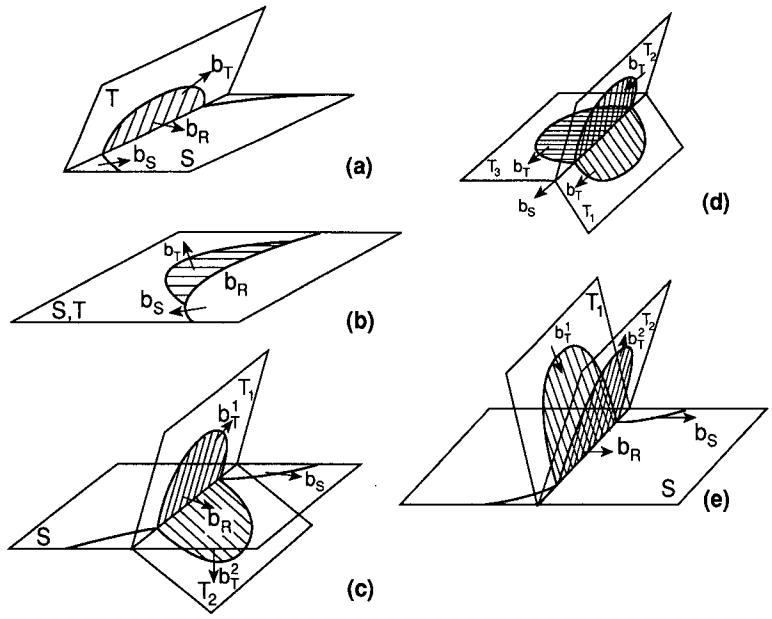

Fig. 10. Some degenerate cases of the dissociation of slip dislocations of Burgers vector $\mathbf{b}_s$ lying on slip planes **S** into twinning or transformation dislocations of Burgers vector $\mathbf{b}_T$ lying on twinning planes **T** and residual dislocations of Burgers vector $\mathbf{b}_R$. In (a) a straight segment of a slip dislocation in **S** has dissociated into a twinning dislocation in **T** and a residual dislocation along the line of intersection of **S** and **T**. In (b) the planes **S** and **T** coincide so that the dissociating slip dislocation and hence the residual dislocation may be curved. In (c) **S** and two twinning planes $\mathbf{T}_1$ and $\mathbf{T}_2$ intersect in a line so that the original slip dislocation can dissociate into twinning dislocations on both planes. In (d) a special case which is possible in b.c.c. crystals, a screw slip dislocation dissociates symmetrically into three twinning dislocations on planes $\mathbf{T}_1$, $\mathbf{T}_2$ and $\mathbf{T}_3$ with $\mathbf{b}_T = \frac{1}{3}\mathbf{b}_S$, so that no residual dislocation is required. The symmetrical situation shown in (e) with $\mathbf{b}_S$, $\mathbf{b}_T^1$, $\mathbf{b}_T^2$, $\mathbf{b}_R$ all approximately coplanar and orthogonal to the dissociating slip dislocation may occur in crystalline mercury (after Christian and Crocker[133]).

dislocations are then, in principle, glissile, since both must have Burgers vectors in the S/T plane. This case arises in f.c.c., diamond cubic and related structures, and also in b.c.c. structures when the slip plane is {112}, but not when it is {110}.

A more restrictive dissociation is shown in Fig. 10(c); the initial dislocation must lie along the intersection of two twinning planes into each of which it emits a twinning partial, leaving a stair-rod residual along the line of intersection. If the initial dislocation is a glissile slip dislocation, the line of intersection must also be contained in the slip plane. The condition is met by the basal slip plane and various pyramidal twinning planes of the h.c.p. structure,[134] and there is then an additional symmetry since the two twinning planes are crystallographically equivalent and symmetrically disposed about the slip plane, and the Burgers vectors of the slip and twinning dislocations are coplanar.

The configuration shown in Fig. 10(d) is even more symmetrical; a slip dislocation which is a pure screw lies along the common line of interaction of three twinning planes, and can thus dissociate into twinning dislocations on each of these planes. This well-known case occurs in b.c.c. structures where the Burgers vector of each twinning dislocation is equal to one third of the Burgers vector of the total slip dislocation, so that there is no residual dislocation along the original line. Early calculations by Sleeswyk,[135] however, indicated that the configuration shown in Fig. 10(d) is not stable, and the stable

structure has faults of equal length along two of the {112} planes, with the third partial along the joining line.

The symmetry relations discussed for Figs 10(c) and (d) naturally are found only in crystals of high symmetry, but Guyencourt and Crocker[44] pointed out that they also may exist in approximate form for crystals of lower symmetry with irrational twinning elements. In crystalline mercury, for example, two variants of the irrational $\mathbf{K}_1$ plane intersect in an irrational direction which lies approximately in the slip plane, and the corresponding slip and twinning directions are all coplanar and approximately normal to this direction.[44] This is shown schematically in Fig. 10(e) and suggests that dissociation of an edge slip dislocation into pairs of twinning dislocations on the two twin planes might be geometrically feasible. (The discrepancies which are ignored by such a description are all less than 2°.) A suitable rational approximation to the twinning plane suggests that each slip dislocation might dissociate into about 11 pairs of twinning dislocations, defined as discussed in Section 3.3.

It is not possible to generalize about the physical probability of the dissociations shown as geometrically possible in Fig. 10, and atomistic rather than elastic calculations will often be required to assess the energy associated with a particular configuration. It is well known, for example, that the hypothetical dissociation of Fig. 10(d) in a b.c.c. metal is strictly to be regarded as a model of the core region of the lattice screw dislocation, rather than as the formation of genuine planar faults.

The various dissociations of Fig. 10 may all (geometrically) lead to faults of indefinite extent, but in order to produce twins, some means of growth normal to $\mathbf{K}_1$ must be postulated. As mentioned above, growth might occur by random accumulation of independently nucleated faults, but orderly growth must involve either repeated nucleation of successive layers, homogeneously or at some favourable defect configuration, or a pole or cross-slip "source" mechanism which allows a single twinning dislocation to move through successive $\mathbf{K}_1$ planes.

The concept of the pole mechanism is due to Cottrell and Bilby[136] and to Thompson and Millard[100] who independently devised particular models for twinning in b.c.c. and h.c.p. structures respectively, whilst the general theory, including its extension to coherent martensitic transformation, was first given by Bilby.[137] Bilby and Christian[138] illustrated the principle of the mechanism by considering a dislocation in a parent crystal with a Burgers vector $\mathbf{b}_A$, which crosses a $\mathbf{K}_1$ interface and continues into a twin crystal as a dislocation with Burgers vector $\mathbf{b}_B$. They assumed that the two Burgers vectors are related by the simple shear of a deformation twin, i.e. $\mathbf{b}_B = \mathbf{S}\mathbf{b}_A$, and similarly that the slip plane normal $(\mathbf{m}_B)' = (\mathbf{m}_A)'\mathbf{S}^{-1}$. The components of the Burgers vectors, referred to unit cell based coordinate systems in the twin and parent respectively, are thus related by the correspondence matrix, as might also be expected if a fixed dislocation, without dissociating, is partly engulfed by a growing deformation twin. Note also that any two corresponding planes in parent and twin meet edge to edge in the interface, which is a necessary geometrical condition for the propagation of slip into the twin. However, to avoid possible confusion, it should be emphasised that, irrespective of the physical mechanism by which the configuration is attained, the Burgers vector of a parent dislocation $\mathbf{b}_A$ which crosses a $\mathbf{K}_1$ interface need not be equal to $\mathbf{S}\mathbf{b}_A$ in the twin. Other possible relations arising from the physical incorporation of slip dislocations into twins during plastic deformation are considered in Section 6.2. The assumption of corresponding vectors is made here because it is an essential condition for a successful pole mechanism.

The passage of the dislocation leaves a step in the interface of height $h = \mathbf{b}_A . \mathbf{m} = (b_A)_i m_i$ equal to the component of $\mathbf{b}_A$ (or equivalently of $\mathbf{b}_B$) in the direction of the unit normal $\mathbf{m}$ to $\mathbf{K}_1$. This step is a twinning dislocation, with a Burgers vector $\mathbf{b}_T = \mathbf{b}_B - \mathbf{b}_A = (\mathbf{S} - \mathbf{I})\mathbf{b}_A = (\mathbf{b}_A . \mathbf{m})s\,\mathbf{l}$ and it runs between two (opposite) crossing points or from a single crossing point to the periphery of the interface. Thus, each crossing point is the junction of (at least) three dislocation lines, one in each crystal and one in the interface. Bilby called this configuration, in which

$$\mathbf{b}_B = \mathbf{S}\mathbf{b}_A = \mathbf{b}_A + (\mathbf{b}_A . \mathbf{m})s\,\mathbf{l} = \mathbf{b}_A + \mathbf{b}_T, \tag{51}$$

a "generating node". Since all the planes parallel to $\mathbf{K}_1$ are now threaded by a "pole" dislocation with a normal component of Burgers vector, the set of parallel planes has been changed into a continuous spiral ramp leading from parent to twin. If the glissile twinning dislocation in the plane of the interface now glides along this plane whilst the other elements remain fixed, it must rotate about the node or nodes, and for each complete revolution, the $\mathbf{K}_1$ interface, together with the node, is displaced into the matrix or the twin (depending on the sense of the rotation) through a distance equal to $h = \mathbf{b}_A . \mathbf{m}$. Successive blocks of structure thus suffer the same vector displacement relative to each other, in order to give the macroscopic shear of the twinning relation, and any necessary shuffling presumably occurs spontaneously at the step. A dislocation which both enters and leaves a twin may do so at the same $\mathbf{K}_1$ interface or at the two $\mathbf{K}_1$ interfaces of a twin of finite thickness. Single nodes, giving a spiral step from single crossing points, and double nodes, giving closed terraces of twinning dislocation from opposite crossing points in one interface, can both be formed, as in the topologically similar models of dislocation-assisted crystal growth [139,140] and Frank–Read source[140,141] operation. (Note especially the similarity to a "cone" source.[137,140])

The dislocation configuration required for this mechanism in compound or type I twins is quite specific; the pole dislocation must have a Burgers vector component normal to the interface which is equal to qd (for q odd) or $\frac{1}{2}qd$ (for q even) where d is the spacing of the lattice $\mathbf{K}_1$ planes. Any dislocation with a Burgers vector from plane 0 to plane q or $\frac{1}{2}q$ will satisfy this condition which arises, of course, in order that $\mathbf{b}_T$, where necessary, shall be a zonal twinning dislocation and thus able to glide freely. The same condition ensures that if $\mathbf{b}_A$ is a lattice vector of the matrix, $\mathbf{b}_B$ will be a lattice vector of the twin, and together with $\mathbf{m}_B$ it defines a geometrically feasible, atomic slip system, the plane and direction of which will, however, probably have relatively high indices so that actual slip on this system may be impossible. Clearly, dislocation glide across the interface becomes a virtual rather than a physical process if the dislocation in the twin is unable to glide, but if the configuration can be formed in some other way, the resistance to slip within the twin could ensure the stability of the node. However, in many low symmetry structures with several active twinning modes, suitable pole dislocations may not exist.

It follows from this treatment that the interaction of independently formed dislocations and twins may produce a true generating node in the sense defined by Bilby and Christian[138] and Sleeswyk[142] at each crossing point. In particular, four variables listed by Venables[143] are correctly disposed so that the applied stress favouring twinning continues to drive the twinning dislocation into the matrix, whereas an opposite stress reverses the motion so as to produce de-twinning. These variables are:

(i) the screw sense of the pole dislocation,
(ii) the type of stacking fault in the parent lattice which is trailed behind the glissile partial (i.e. twinning) dislocation,

(iii) the side of the fault on which the glissile partial is situated, and
(iv) the direction in which the glissile partial moves under a fixed applied stress.

It may readily be seen that if another pole dislocation has the opposite Burgers vector (i.e. the reverse screw sense), the last two variables must also be reversed, and the left-handed rotation of the dislocation $-\mathbf{b}_T$ about the opposite pole produces the same twinning shear and displacement of the interface as the right-handed rotation of the original twinning dislocation $+\mathbf{b}_T$.

The pole mechanism is usually invoked in combined nucleation and growth models of twinning which begin with the dissociation of a lattice dislocation in, for example, one of the ways shown in Fig. 10. One simple possibility is that a glissile partial dislocation trailing a monolayer stacking fault in the $\mathbf{K}_1$ plane encounters a suitable pole dislocation threading this plane. A pole source is then produced if the partial wraps itself around the pole. The two parts of the partial then form a dipole on adjacent $\mathbf{K}_1$ planes and between these two planes, the pole dislocation is converted (formally) into the dislocation $\mathbf{b}_B$ of eq. (51). If the two opposite segments of the original partial are able to glide past each other (a very doubtful assumption with a single plane separation) they can continue to spiral upwards and downwards respectively. This mechanism is feasible only in structures where the $\mathbf{K}_1$ plane is also a slip plane, and even then it is necessary to postulate some mechanism for producing isolated partials rather than extended whole dislocations.

More elaborate discriptions suppose that an initial pole dislocation contains a superjog which dissociates in the $\mathbf{K}_1$ plane, emitting a twinning partial into $\mathbf{K}_1$ and leaving a sessile partial along the original superjog. With a correct configuration, this leads to a perfect pole in which the two ends of the twinning partial spiral upwards and downwards from the sessile partial, passing very close to it on the first turn, but never being blocked by it. Hence, a twin is formed by outwardly spreading shear on what is topologically a single helicoidal $\mathbf{K}_1$ surface wrapped around the pole dislocation. The sessile partial of the dissociation is the vector $\mathbf{b}_B$ of eq. (51) referred to the parent structure, and within the twin, this vector $\mathbf{b}_B$ defines a perfect lattice dislocation. Now suppose that the same pole dislocation $\mathbf{b}_A$ dissociates into a dislocation of Burgers vector $\mathbf{b}_B^* = [\mathbf{S}\mathbf{b}_A - 2\mathbf{b}_T]$ and a glissile partial $-\mathbf{b}_T$ which glides away from the superjog in the opposite direction to produce an identical (intrinsic or twin-type) fault. The sessile partial $\mathbf{b}_B^*$ is now given by:

$$\mathbf{b}_B^* = \mathbf{S}\mathbf{b}_A - 2(\mathbf{b}_A.\mathbf{m})s\,1 = \mathbf{b}_A - \mathbf{b}_T, \tag{52}$$

and variables (iii) and (iv) above have been reversed. The dislocation $-\mathbf{b}_T$ is still rotating about a pole $\mathbf{b}_A$ in the matrix, but the vector $\mathbf{b}_B^*$ is not a lattice vector of the twin since it differs from $\mathbf{S}\mathbf{b}_A$ (a lattice vector) by $2\mathbf{b}_T$ (not a lattice vector). Moreover, $\mathbf{b}_B^*$ for this new dislocation has the wrong screw sense since this has not changed whilst the vector of the twinning dislocation has been reversed, so that after one revolution, the twinning dislocation does not advance along the pole but returns to the sessile partial. If it recombines and then dissociates, it can continue only along its original path again, thus increasing the displacement between the same two planes and producing a high energy fault instead of a twin. This configuration, first pointed out by Cottrell and Bilby[136] in connection with a model for f.c.c. twinning, was called an "anti-generating node" by Bilby.[137] Twinning may, in principle, grow from such a node by utilising intimate cross-slip as first suggested by Venables[144] for f.c.c. metals, and later described by Hirth and Lothe[141] as a "ratchet" mechanism.

As mentioned above, there is a physical difficulty in the operation of a pure pole mechanism if the original twin is either a monolayer fault or has only a few layers. A generating node appears on both the top and bottom surfaces of the original fault, and the resulting twinning dislocation segments rotate in opposite senses and after one revolution, these two segments must glide past each other at a separation equal to the thickness of the original fault. For monolayer faults or thin twins, this would require a very large (static) stress. Bilby estimated that, for cubic twins, a nucleus of about 50 atoms thick is required before the pole mechanism can begin to operate at experimentally observed twinning stresses. Actually, the separation of the partials after the first turn is so small that linear elastic theory may considerably overestimate the stress required; there is appreciable core overlap and atomistic calculations are required. However, it does appear quite probable that the pole mechanism of growth may only be effective after a rather thick nucleus has first formed in some other way. In the analogous problem of the f.c.c. to h.c.p. martensitic transformation in cobalt and its alloys, the situation is exactly equivalent, except that the partials meet at a separation of two atomic layers. Seeger[145] suggested that the partials may acquire sufficient kinetic energy to overcome the very strong interaction and allow them to pass dynamically. This seems doublful even for cobalt where the effective stress on the dislocations from the chemical driving force may be much larger than the externally imposed mechanical stress during a laboratory test.

4.4. *The Cottrell–Bilby Theory of b.c.c. Twinning*

Cottrell and Bilby considered the continuous growth of a b.c.c. twin from an initial single layer fault formed from the dissociation of a perfect dislocation in the parent lattice. Their theory utilised the fact the the twinning dislocation of type $\frac{1}{6}\langle 111\rangle$ is common to more than one crystallographically equivalent twin plane of type $\{112\}$. Figure 11 shows a length of perfect dislocation line, initially *AOBC*, having a Burgers vector $\frac{1}{2}[111]$, and lying in the (112) plane, in which it cannot glide. The initial stacking fault is formed by dissociation of part of this line over the length *OB*, with nodes at *O* and *B*. The assumed dissociation

$$\tfrac{1}{2}[111] \rightarrow \tfrac{1}{3}[112] + \tfrac{1}{6}[11\bar{1}] \tag{53}$$

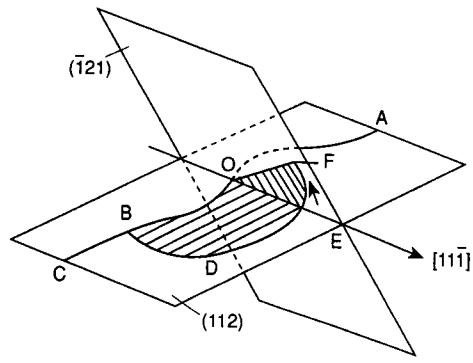

Fig. 11. The Cottrell–Bilby mechanism for twinning in a b.c.c. crystal. AO and BC represent lengths of lattice dislocations of Burgers vector $\frac{1}{2}[111]$, OB is a sessile partial dislocation with Burgers vector $\frac{1}{3}[112]$ and BDEFO is a glissile partial (or twinning) dislocation with Burgers vector $\frac{1}{6}[11\bar{1}]$. There is no dislocation line along OE (after Cottrell and Bilby[136]).

occurs by the separation of the partial dislocation $\frac{1}{6}[11\bar{1}]$ which is glissile in the (112) plane from the partial dislocation $\frac{1}{3}[112]$ which is sessile and remains along OB. The region between the two partial dislocations is a monolayer stacking fault on the (112) plane.

Since $BDEO$ is glissile, a length (EO) may lie in the $[11\bar{1}]$ direction and thus become pure screw in character. The special properties of the b.c.c. structure arise from the crystallographic condition that the $(\bar{1}21)$ and $(2\bar{1}1)$ twinning planes both intersect the (112) plane in the $[11\bar{1}]$ direction, which is a twinning (η_1) direction for all three. EO can thus move into either $(\bar{1}21)$ or $(2\bar{1}1)$, generating a new (twin type) stacking fault on these planes. Analysis shows that in order to form the correct (intrinsic) twin fault, it must move in such a direction that the new fault intersects the original fault on (112) at an acute angle.

A macroscopic twin is now assumed to grow by repeated rotation of OF on whichever set of planes it entered; the figure illustrates this for the $(\bar{1}21)$ planes. The problem of passing twinning dislocations does not arise, since the twin does not form on the plane of the original stacking fault, and it grows continuously from one side only; note particularly that there is no dislocation along the intersection EO of the two faults. However, it does encounter on each revolution the original fault on (112) which is converted into a different type of fault, almost certainly of higher energy, within the twin. If the node at O moves towards B as OF rotates, as originally stated, the sweeping (twinning) dislocation climbs along the first stacking fault, and since OB is sessile the node is firmly anchored, thus satisfying one of the physical conditions. The dislocation OB has a Burgers vector $2d\mathbf{m}$, where $\mathbf{m}$ is the unit normal to (112) and d is the spacing; since $\{112\}$ planes intersect at 60°, there is a component of magnitude d normal to either $(\bar{1}21)$ or $(2\bar{1}1)$.

As recognized in the original paper, the initial formation of a large monolayer fault on the (112) plane is improbable, and such faults are now believed to be mechanically unstable. Even if the fault is metastable, there is no first order change in elastic energy produced by the dissociation (52), so that the energy of the stacking fault represents a net increase in free energy which must be supplied by the external stress. Cottrell and Bilby estimated the shear stress needed to form the stacking fault as σ^f/b where σ^f is the stacking fault energy. This stress is reasonably small ($\sim 10^8$ Pa $\simeq 0.001\mu$ if $\sigma^f \sim 10$ mJ m^{-2}) for f.c.c. or h.c.p. metals or alloys of low fault energy, but is rather large ($\sim 0.02\mu$ for $\sigma^f \sim 200$ mJ m^{-2}, which might be an appropriate value) for b.c.c. metals. There is also an additional stress needed to bow out the twinning partial to its point of instability; this will depend on the length of OE. Stresses of magnitude $(10^{-3}$–$10^{-2})\mu$ are often applied in order to twin b.c.c. metals at low temperatures, so that with a modest stress concentration, the mechanism seemed initially feasible. There is, in fact, now good evidence that b.c.c. twins may be nucleated by dissociation of a lattice screw dislocation, but not by the Cottrell–Bilby reaction.

This combined nucleation and growth model cannot be applied to other structures, and, moreover, it now appears to be incorrect even for b.c.c. structures. The Cottrell–Bilby theory was criticized by Sleeswyk[142] who pointed out that the dislocation in the twin is imperfect and the stacking fault is not a monolayer twin fault of the dissociation (53) but corresponds instead to a $\frac{1}{6}\langle 111\rangle$ displacement in the anti-twinning direction (or equivalently to a $\frac{2}{6}\langle 111\rangle$ displacement in the twinning sense). Sleeswyk suggested this fault would be eliminated by nucleation of a dipole of $\frac{1}{6}\langle 111\rangle$ partials. One of these partials would remain in the top interface whilst the other partial glides through and removes the stacking fault and annihilates the twinning dislocation.

Hirth[146] first distinguished "pure" pole mechanisms from what were later called "ratchet" mechanisms, and Hirth and Lothe[141] pointed out that a slight modification of the Cottrell–Bilby model shows that it is actually a ratchet. The initial configuration is similar

to Fig. 11 but OE now represents a superjog in the dislocation, so that there is no stacking fault on (112) and the lines $CBOE$ and $CBDE$ are coincident and form a section of perfect dislocation CE. Dissociation of the superjog OE takes place according to eq. (52) and leads to the formation of a loop of twinning dislocation OFE which glides on $(\bar{1}21)$ or on $(2\bar{1}1)$, but after a single turn, the parts of this loop which rotate about O and E, respectively, are both blocked by the sessile partial left along OE, so that the configuration cannot act directly as a pole source. This is illustrated in Figs 12(a) and (b) which show the stacking sequence (. . .ABCDEF. . . in the perfect structure) of the $(\bar{1}21)$ planes before and after the dissociation of the superjog. If the glissile partial now winds about one or both ends of the superjog, it leaves along 1 to the right of the diagram and the two parts return along 2 and 3 to the left of the diagram. Since they are opposite in sign and very close together at this point, they cannot pass except under extremely high stresses. Thus they may form a lock of two parallel lines, or possibly mutually annihilate over some length (formally by nucleation of a jog of unit height), leaving a closed loop of fault containing a unit jog to travel outwards, and a residual part which is blocked by the sessile partial. In either event, the two ends of the twinning partial emerging from positions 2 and 3 of Fig. 12(b) run into the original sessile dislocation. In principle, they may recombine with this and immediately dissociate again, but a second revolution is not possible because the twinning partial would have to leave again along 1, thus doubling the shear displacement of the first stacking fault and creating a high energy stacking fault and not a twin. However, if the returning parts of the twinning dislocation loop can recombine with the sessile $\frac{1}{3}[111]$ dislocation left along OE to reform the original perfect dislocation, and if this now cross-slips through just one $(\bar{1}21)$ interplanar

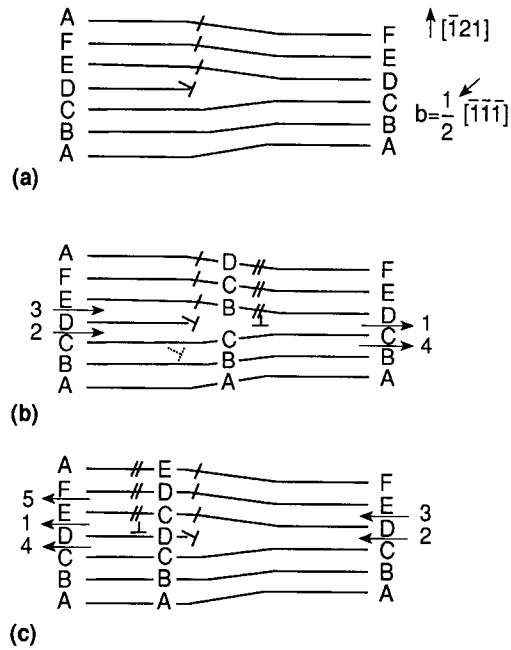

Fig. 12. The jog version of the Cottrell–Bilby pole mechanism. (a) The undissociated $\frac{1}{2}[\bar{1}\bar{1}\bar{1}]$ dislocation, (b) the configuration after its dissociation into $\frac{1}{3}[\bar{1}\bar{1}\bar{2}]$ and $\frac{1}{6}[\bar{1}\bar{1}1]$ dislocations, and (c) the situation after the first revolution of the $\frac{1}{6}[\bar{1}\bar{1}1]$ twinning partial around the pole dislocation (after Hirth and Lothe[141]).

spacing, it may then again dissociate and send out a second loop of twin stacking fault adjacent to the first loop (see Fig. 12(b)). Repetition of successive ratchet steps of dissociation, loop formation, recombination and cross-slip will then be (geometrically) possible. This mechanism requires that the dissociation (52) and its opposite recombination both take place spontaneously, and this seems rather improbable.

The fact that the Bilby–Cottrell dissociation is not a true pole was rather obscured by the initial dissociation on the (112) plane of Fig. 11. This has the result that after the first rotation of the twinning dislocation on $(\bar{1}21)$ there is no sessile partial blocking its path. Hirth and Lothe's equivalent configuration without the stacking fault on (112) is actually more probable since it avoids the disadvantages of the high energy fault discussed by Sleeswyk and it also demonstrates that the dissociation of eq. (52) does not give a true pole mechanism.

Hirth and Lothe also pointed out that a dissociation of the long jog into the opposite twinning dislocation and a larger sessile partial will give a true pole configuration. This arises because for shear on $(\bar{1}21)[11\bar{1}]$ the vector corresponding to [111] is [221] (i.e. $[00\bar{1}]_T$ referred to the twin basis), not [112]. The reaction is

$$\tfrac{1}{2}[111] = \tfrac{1}{3}[221] + \tfrac{1}{6}[\bar{1}\bar{1}1]. \tag{54}$$

The glissile partial dislocation now rotates about the two poles in the opposite sense to that of Fig. 10(b) in order to preserve the same sense of the twinning shear. Referring to Fig. 12(c), part of it leaves to the left along path 1 and returns along path 3; it is not blocked but may leave again along 5, and continues spiralling upwards to generate a twin. Similarly the other part of the glissile partial leaves along 1, returns along 2 and leaves again along 4 and continues spiralling in the opposite sense.

This example shows that geometrically a pure pole source can be obtained from the dissociation of a long jog in a single dislocation; it is clear that eq. (54) is equivalent to eq. (51) whilst eq. (53) corresponds to (52). Sleeswyk gave another example of a possible pure generating node which has a pole dislocation with a $\langle 100 \rangle$ type Burgers vector. However, it is not clear that the pure pole is a more probable growth mechanism than the ratchet. This is because the elastic energy increases in the dissociation (54) and must somehow be supplied in addition to the fault energy. An equivalent statement is that the stress field has to overcome the strong attraction between the glissile and sessile partials of eq. (54). Furthermore, although the twinning dislocation is not blocked in mechanism (54), the stress field must still overcome the strong interaction between the two ends of the twinning partial (the Bilby effect). This effect is obviously greatest after the first revolution and decreases with each succeeding revolution. These two effects together imply an exceptionally large local stress in addition to the stacking fault stress considered by Cottrell and Bilby. Thus this mechanism seems improbable physically.

The Cottrell–Bilby theory is no longer considered an acceptable model for b.c.c. twinning, partly because of the energetic difficulties but also because much experimental evidence shows that dislocations which act as nuclei for twins always give variants in which the η_1 direction is parallel to the Burgers vector of the dislocation, in contrast to eq. (53) and Fig. 11. The paper, nevertheless, constitutes a landmark in the theory of twinning and some version of the pole mechanism remains potentially significant in the growth of a twin.

4.5. *Other Dislocation Models for b.c.c. Twinning*

The peculiar crystallographic feature of b.c.c. twinning is that the possible shear directions are crystallographically equivalent to the directions of the Burgers vectors of the stable lattice

dislocations. Models of nucleation which are based on the dissociation of lattice dislocations may thus be subdivided into those like Fig. 10(d) in which the actual η_1 direction coincides with the Burgers vector of the nucleating dislocation, and those in which it does not. In the latter group are the other schematic dissociations of Fig. 10, including the Cottrell–Bilby mechanism, together with a number of proposals which are based on the assumption that twins are nucleated at intersecting slip bands.

One version of such models simply supposes that the stress concentration produced by intersecting slip is sufficient to nucleate twins homogeneously, but others depend on specific dislocation reactions. Priestner and Leslie[147] developed a model for the formation of a three-layer twin from slip on $\{110\}$ and $\{112\}$ planes. They considered attractive interactions between glide dislocations on different slip planes to form $\langle 100\rangle$ type dislocations which are believed to be sessile. The reaction

$$\tfrac{1}{2}[\bar{1}11] + \tfrac{1}{2}[1\bar{1}1] = [001] \tag{55}$$

is thus assumed to lead to pile-ups of slip dislocations on the two slip planes behind the [001] lock until the stress concentration so produced forces the [001] dislocation to dissociate again. The [001] dislocation may lie in various crystallograhic directions $\langle 100\rangle$, $\langle 111\rangle$ or $\langle 311\rangle$ depending on the two interacting slip planes. The case of interest for the nucleation of a single twin is when the slip planes of eq. (55) are $(1\bar{1}2)$ and $(\bar{1}01)$, respectively, so that the [001] dislocation lies along [131]. Priestner and Leslie show that in this case a series of hypothetical dissociations enables the $[1\bar{1}1]$ dislocation to escape and continue to glide along its original $(\bar{1}01)$ slip plane whilst the other dislocation is split into three partials each having a Burgers vector of $\frac{1}{6}[\bar{1}11]$. These partials are on successive $(1\bar{1}2)$ planes, so as they move away from the original lock, they create a three-layer fault, i.e. a thin twin. The shear of the original slip dislocation on $(1\bar{1}2)$ is thus converted into the shear of this twin nucleus. Note that there is no shear discontinuity at the site of the original lock which must formally be represented by a dislocation dipole, or rather by two twinning dislocations and one complementary dislocation (see Section 3.2). The calculations indicate that rather a small stress concentration which multiples the applied stress by ~ 40 is sufficient to dissociate the [001] dislocation in this way.

Priestner and Leslie also considered the breakdown of a [001] barrier formed at the intersection of two $\{112\}$ slip planes or two $\{110\}$ slip planes. In the former case, they predict that it is possible to form twin nuclei on each slip plane at a stress multiplication factor of ~ 15 whilst in the latter case, pairs of slip dislocations escape from the lock when this factor exceeds ~ 135. Even this relatively high barrier represents only about 12 dislocations in each pile-up.

This model for twin formation effectively uses the stress concentration of intersecting slip to force the dissociation of a lattice dislocation of mixed type into three twinning partials on successive slip planes. It does not, however, provide any obvious method for further thickening of this fault, since dissociation of a second lock formed from succeeding dislocations on the two planes would only lead to a different (high energy, or "anti-twinning") fault on the same three planes. In contrast to f.c.c. metals and alloys, there is, in fact, little experimental evidence to support the hypothesis that slip on more than one system is necessary to initiate twinning in b.c.c. metals. Small double slip bands have been observed in association with shock-formed twins in silicon–iron. However, such bands have not been found to accompany other b.c.c. shock twins and it is quite difficult to determine experimentally whether the slip bands were formed before or after the twin. Thus it seems quite possible

that the observed slip bands did not nucleate the twin but rather formed to accommodate the local high stress field of the constrained twin.

An early proposal by Sleeswyk[135] was that since an unstressed $\frac{1}{2}\langle 111\rangle$ screw dislocation has three-fold symmetry, it may be regarded as having a three-dimensional core with a $\frac{1}{6}\langle 111\rangle$ partial on each of the intersecting $\{112\}$ planes. Under stress, however, this configuration will be unstable, and the partials could rearrange to form a three layer twin on the most highly stressed of the $\{112\}$ planes. A very similar suggestion was made by Ogawa[148] who considered that edge dislocations might spread the total Burgers vector on to three successive planes, and thus give a three layer fault. Such speculations appear to be consistent with the early γ-surface calculations of Vitek[90] which indicated that very thin "twins" (strictly four layer faults since the interfaces were of the "isosceles" type, see Fig. 6b) may be mechanically stable. These theories thus by-pass the rather elaborate interactions considered by Priestner and Leslie and simply assume that rearrangements of single dislocations (albeit of special types, most probably screws) give directly the same end result.

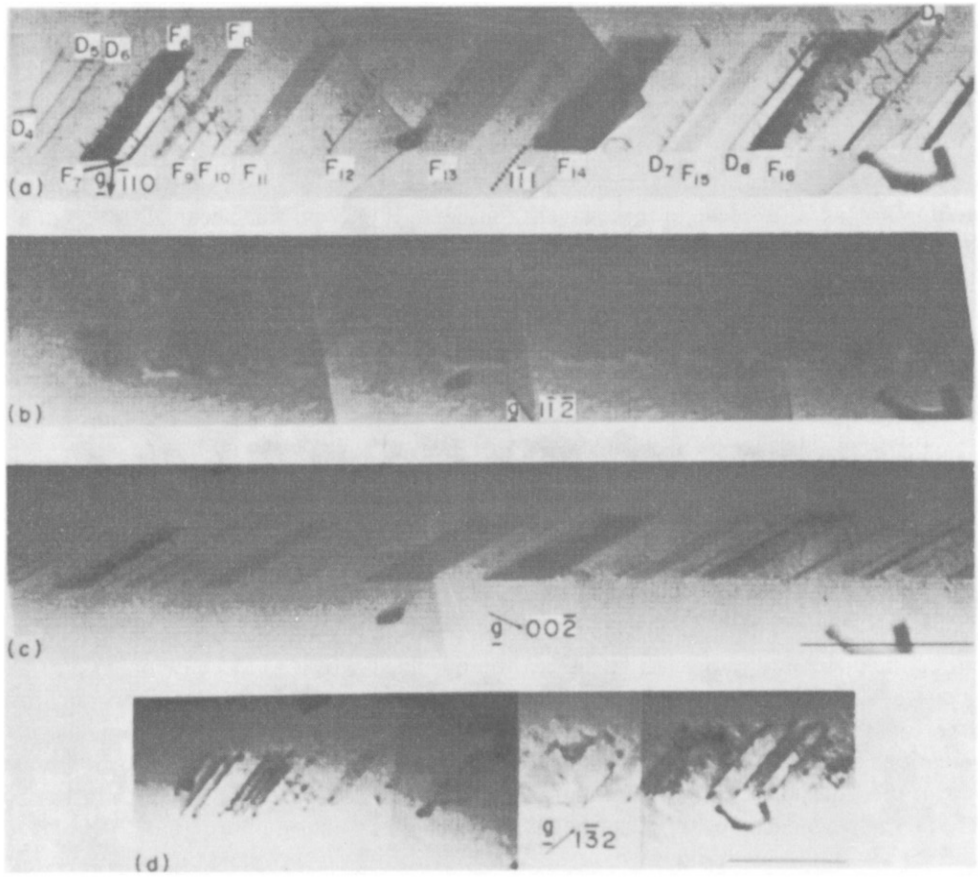

Fig. 13. Micrographs illustrating the development of faulted structures in a Mo–35at%Re alloy specimen deformed in tension at 77 K. The plane of the micrographs (a, b, c and d) are ~(111), ~(113), ~(100) and ~(111), respectively. Dotted line refers to the projection of the $[1\bar{1}1]$ vector on to the (111) plane. The markers represent 1 μm (after Mahajan[150]).

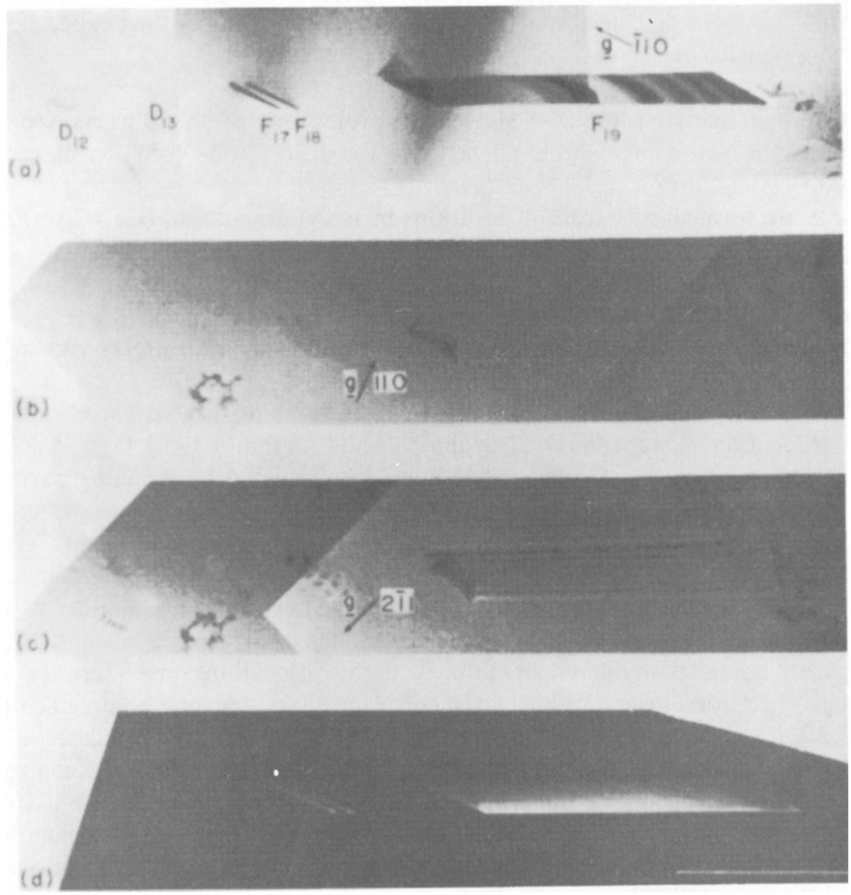

Fig. 14. Micrographs illustrating the formation of faulted structures in a Mo–35at%Re alloy specimen deformed in tension at 77 K. The planes of the micrographs (a, b, c and d) are ~(001), ~(111), ~(011) and ~(1̄15), respectively. The marker represents 1 μm (after Mahajan[150]).

Interest in the core structure of the b.c.c. screw dislocation has been stimulated by the important role assigned to such dislocations in low temperature deformation behaviour[118,149] and many computer simulations of the structure and its change when subjected to shear and/or dilatational stresses have been made. These calculations show that the core structure is quite complex and is sensitive to the assumed (two-body) interatomic potential and to both shear and non-shear components of the stress tensor. In certain circumstances, the application of stress leads to the formation of a four-layer fault, i.e. an apparent twin embryo, rather than to the movement of the dislocation as a whole. Thus, the simplest model assumes that lengths of screw dislocation, either pre-existing or left behind by previous microslip, are immobile below a certain temperature/strain rate combination, but dissociate by the Sleewyk reaction to give a four layer fault with a mobile edge.

Experimental evidence which supports this model was obtained by Mahajan[105,150] in a detailed electron microscopic examination of dislocation and twin configurations in deformed molybdenum–rhenium alloys. Figures 13 and 14 show examples of the structures observed

in foils from specimens deformed at 77 K in tension. Diffraction contrast experiments led to the following conclusions:

(1) The dotted line in Fig. 13(a) shows the projections of the Burgers vector of the dislocations in the microslip bands, so that the dislocations visible in these bands are in screw orientation.
(2) Faults are formed only from dislocations in screw orientation (see F7 in Fig. 13(a)).
(3) The fault vectors are parallel to the Burgers vector of the dislocations.
(4) Various faults are located at different levels within the slip bands.
(5) Clear faults (e.g. F8, F9 in Fig. 13) are observed.
(6) The sides of the faults are parallel to the projection of the Burgers vector.

The fault F19 of Fig. 14 terminates within the foil and is associated with faults F17 and F18 and dislocations D12 and D13. Mahajan showed that F17, F18 and F19 are all twins, and that the right hand interface of Fig. 14 is bounded by twinning partials of the same sign.

These results clearly support the view that twins originate from screw type lattice dislocations, and Mahajan extended the Sleeswyk (or Vitek) model by suggesting that the faults formed by dissociation thicken by chance encounters with one another as the faults extend in the {112} slip plane. In the original model, the three layer faults formed by dissociation are bounded on one side by three twinning dislocations on adjacent {112} planes, and on the other side effectively by two such dislocations and one complementary twinning dislocation to give zero net Burgers vector. When two such faults coalesce, a four, five or six layer fault may result, depending on the relative displacements of the centre plane of the fault. Although this seems to require a high density of dislocations to produce a macroscopic twin, Mahajan suggested that this "slip band conversion" might obviate the need for a pole type mechanism of thickening, especially if the screw dislocations are able to multiply by cross slip over short distances under the combined applied and internal stress fields. In support of this suggestion of intimate cross-slip was the observation that slip dislocations were associated with extremely small prismatic loops of the same Burgers vector, which could have formed from jogs produced by cross-slip. Also there were no indications of slip activity on any other system. Note, however, that cross-slip multiplication implies that the screws are not completely immobile, so that the dissociation into twinning dislocations has to depend either on some local pinning or on differential mobilities of the lattice and twinning dislocations. Mahajan's original description is also based on the assumption that each three layer fault will be of the type described above, but if cross-slip multiplication takes place, it is clear that closed planar faults bounded entirely by twinning dislocations may grow outwards.

It is implicit in the above model that microslip must precede the twin nucleation and must continue whilst the twin grows. Whilst the atomistic calculations provide some support for the assumption that the lattice screw dislocations may only be mobile when dissociated, it is difficult to understand how cross-slip multiplication could then occur. The rate of thickening expected from the model is also dependent on the rate of growth of the microslip band normal to the slip plane.

The sudden load drops which characterize deformation twinning at low temperatures in b.c.c. materials may be due to interactions between embryonic twins. Twins propagating in opposite directions within the nucleation region may impede each other's motion because of the attractive elastic interaction. As a result, continued deformation would require increased

stress. When the twins by-pass each other, the required stress would decrease again, leading to load drops which would continue so long as the embryonic twins were traversing the nucleation regions. However, once they propagate into undeformed regions of crystal, the probability of this "stick and slip" motion will be small, and load drops will no longer be observed. This assumes that twins nucleate during the early stages of the deformation; if the nucleation continues at moderately large strains, the load drops could persist over much of the stress vs strain curve.

Some evidence to support the coalescence theory is provided by experiments[151] on twins in niobium single crystals which had been prevented from growing to their natural lengths by a mechanical stop during the load drop. The main twin was composed of several smaller twins and apparently propagated by several discrete tips ahead of the main body. Additional microscopic evidence that small twins form from slip dislocations and then coalesce was more recently obtained from a spinodally decomposed Fe–Cr–Co alloy.[152] After room temperature deformation, interspersed slip dislocations and microtwins were visible in transmission electron micrographs, with the twinning direction parallel to the Burgers vector of the dislocations and the twins aligned along the projection of the fault vector. Recent measurements of the density of microtwins in an Fe–Ti–C alloy which was charged with hydrogen whilst being deformed at ambient temperature show both an increase in density and coalescence of microtwins as the strain increases.[153]

Coalescence theories of twin growth imply that the macroscopic twins may be highly faulted and the mixture of twinning and slip may lead to a measured shape shear smaller or greater than the theoretical twinning shear of the appropriate mode. Although it is generally assumed that twins do form with the theoretical shear, there have been few measurements reported since the work of Paxton[154] and Blewitt *et al.*[8] and careful measurements of the shear magnitude with modern techniques might now be useful.

4.6. *Twinning in f.c.c. Structures*

Cottrell and Bilby showed that their theory when applied to an analogous dissociation in a f.c.c. structure would produce only a monolayer of stacking fault, and at the time their paper was written this was in agreement with the lack of conclusive evidence for the formation of deformation twins in f.c.c. materials. Later, it was found that such twins form rather readily in metals and alloys of sufficiently low stacking fault energy, and Venables[144] suggested a modified and ingenious mechanism to allow continuous growth from a single stacking fault. Stacking fault models seem physically more realistic for f.c.c. structures since wide faults are formed in many alloys, whereas the faults postulated for b.c.c. structures are probably unstable.

Using the notation of the Thompson tetrahedron, consider the dislocation shown in Fig. 15 with a Burgers vector **AC** lying in plane *b* except for a long jog N_1N_2 lying in plane *a*. Let the part of the dislocation in *a* now dissociate into a Shockley and a Frank partial

$$\mathbf{AC} = \mathbf{A}\alpha + \alpha\mathbf{C}. \tag{56}$$

Under the action of a stress, the glissile Shockley partial $\alpha\mathbf{C}$ moves away from the sessile Frank partial $\mathbf{A}\alpha$ on the plane **a**, leaving an intrinsic fault (Fig. 15(b)) and after attaining the unstable semicircular configuration it winds rapidly around N_1 and N_2 to reach the position shown in Fig. 15(c). In this configuration, two segments of the $\alpha\mathbf{C}$ dislocation delineating the

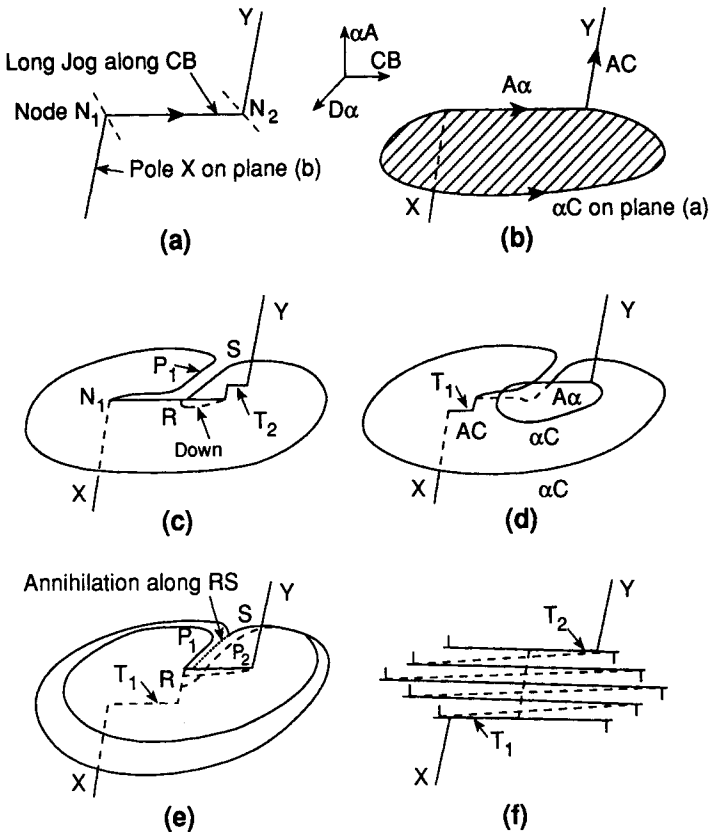

Fig. 15. Prismatic glide mechanism for f.c.c. twinning (after Venables[144]).

fault meet along RS at a separation of only one interplanar distance. These two parts of $\boldsymbol{\alpha C}$ are opposites since their line directions, originally parallel, are now antiparallel, and a very large stress would be required to force them past each other. It is important to note that the right hand element of the Shockley partial has moved downwards in wrapping itself around the pole dislocation, so that it is the lower dislocation of the dipole along RS. This element has a Burgers vector of $-\boldsymbol{\alpha C}$ when the positive line direction looks outwards from N_2, whilst the upper element of the dipole, looking outward from N_1, has a Burgers vector of $+\boldsymbol{\alpha C}$.

Venables assumed that the end element of the partial $\boldsymbol{\alpha C}$ recombines with the sessile partial $\mathbf{A\alpha}$ along the length RN_2 and the reformed dislocation with Burgers vector $\mathbf{AC}$ then glides to the next plane α and repeats the dissociation. When the second layer of fault expands, two opposite segments of its twinning partial will again meet on successive planes along RS, but each will be displaced by one plane from the initial pair. One of these segments (on the central plane) will annihilate the twinning partial left there by the expansion of the first faulted layer, thus joining the two layers into a continuous fault, and the final configuration (Fig. 15(e)) is now a double helical layer of fault terminated by twinning partials SRN_1 and SRN_2 at a separation of two atomic layers. The recombination and glide is represented in the figure as the operation of a dislocation source T_2 and an equivalent source operates at the node N_1. As shown in the figure, the cross-slip could occur formally by the formation of a unit jog

which moves along the recombined dislocation from N_2 to R, but since the length of this "cross-slip" is appreciably less than an interatomic distance, the exact mechanism will depend on the detailed atomic structure of the dislocation core. Repetition of these operations will lead to a twin limited by a helical twinning dislocation with opposing segments parallel to RS on the top and bottom surfaces. This situation again arises because of the wrong-handedness of the dislocation AC in relation to the sign and direction of motion of the twinning dislocation; a cross-section of the superjog is like Fig. 13(b) but with three-fold stacking of $\{111\}$ f.c.c. planes replacing the six-fold stacking of $\{112\}$ b.c.c. planes.

Venables pointed out that when the two partials attain a critical separation, they may pass one another under the action of the static stress field, and the twin can thicken further by the pole mechanism alone (see Fig. 15(f)). Basinski (private communication) has suggested the following simple argument to explain this transition. Suppose a single atomic jog is formed at N_2 and travels all the way to N_1. If the original superjog was on plane 0, and the new superjog is on plane 1, the two dipole partials will, in principle, become attached (i.e. form triple nodes) at the top $[+\boldsymbol{\alpha}\mathbf{C}]$ and bottom $[-\boldsymbol{\alpha}\mathbf{C}]$ of the jog. (Once again, this treatment is presented to demonstrate the correct geometry; it is, of course, physically nonsensical to imagine actual nodes within the interplanar length of the jog.) When the jog reaches N_1, the complete superjog will have reformed one plane higher, and the (infinitesimal) length of pole dislocation between the plane of the superjog and the next K_1 plane beneath it will (in principle) have a Burgers vector of $\frac{1}{3}\langle 221\rangle$. This vector is a $\langle 001\rangle_T$ vector when referred to twin coordinates and is the vector corresponding to the $\frac{1}{2}\langle 110\rangle$ type Burgers vector of the pole dislocation. In the general case, the ratchet mechanism leads to a pole dislocation between the two partials with a correct Burgers vector of type $\mathbf{b}_B$, even though the initial dissociation produced $\mathbf{b}_B^*$.

The final configuration is identical with that obtained when a partial dislocation in a stress field favouring twin formation glides on a K_1 plane one interplanar distance below the superjog until it encounters the pole dislocation, about which it wraps itself. Apart from the superjog, there is thus no clear distinction between single fault pole sources formed from the dissociation of dilocations with Burgers vectors either in or out of the K_1 planes.

Despite the initial formation of an antigenerating node, a single Venables cycle has formed from it a true generating node. Further cycles of dissociation, rotation, recombination, jog nucleation and displacement will steadily increase the length of $\frac{1}{2}\langle 221\rangle$ dislocation, i.e. the thickness of the embryonic twin, until the partials can pass, and growth by the ordinary pole mechanism can begin. In the more general case described by Venables, jogs form at both N_1 and N_2 and the twin grows both upwards and downwards. The growth transition might be prevented if the dissociation of eq. (56) is spontaneous. The ratchet mechanism avoids the difficulties of the passing of the closely spaced partials and might be regarded as a plane by plane conversion of the antigenerating node into a generating node of finite height. The same description applies to Hirth's "ratchet" version of the Cottrell–Bilby mechanism and generally to dissociations of the form of eq. (52) which are eventually converted into poles of type (51).

The above discussion verifies Venables[143] claim, contrary to an objection by Sleeswyk,[142] that the pole dislocation in the twinned region is a perfect lattice dislocation. Venables[143] also pointed out that if only one generating node (say N_2) operates, a twin in the form of a plano-convex lens, (see Fig. 16(a)) may be formed. Another rather similar configuration results if both parts of the original dislocation which are not in the plane α lie on the same side of α (Fig. 16(b)); once again, the twin is plano-convex. Some limited experimental

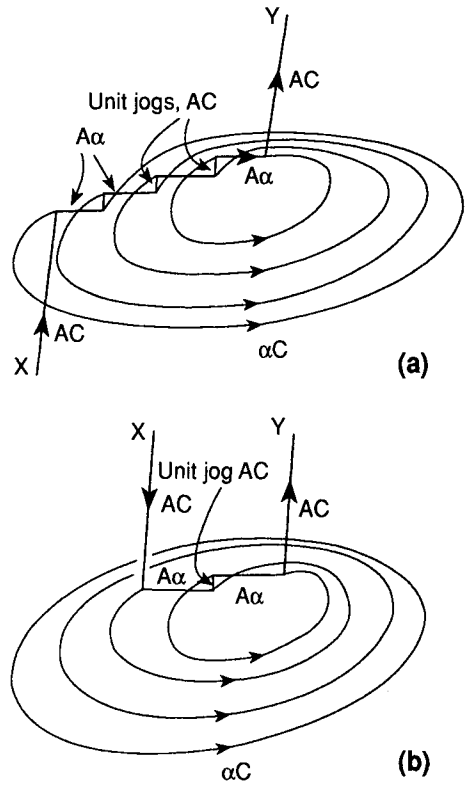

Fig. 16. Prismatic glide sources where the twinning dislocation remains at the matrix–twin interface. (a) Conventional prismatic source. (b) Source from the end of a dipole which remains on one side of the twin (after Venables[143]).

support for these later models comes from the electron microscope work of Steeds and Hazzledine.[155]

In an early discussion of Venables theory, Hirth[146] proposed an alternative dissociation to give a pure pole mechanism. However, Hirth's pole is not related to Venables' pole in the way that eqs. (51) and (52) are related, but involves dissociation of a different $\frac{1}{2}\langle 110\rangle$ dislocation AB which has a Burgers vector at $\sim 54°$ to the anti-twinning direction, whereas that of AC is at $\sim 73°$ to the twinning direction. Hirth's dissociation:

$$AB = A\alpha/BC + C\alpha, \tag{57}$$

gives the opposite twinning dislocation $C\alpha$ and a high energy sessile dislocation $A\alpha/BC$ which is of type $\frac{1}{6}\langle 411\rangle$. Hirth also pointed out that with materials of low fault energy which are likely to twin, the Frank partial of eq. (56) and the high energy partial of eq. (57) would probably themselves be dissociated, giving stair rod dislocations in extended jog configurations.

Another geometrically possible pure pole may be obtained by dissociating the lattice dislocation of eq. (56) in the manner of (51) rather than (52). Suppose that plane α is a (111) plane and the αC direction $[11\bar{2}]$. Eq. (56) is then:

$$\tfrac{1}{2}[110] = \tfrac{1}{3}[111] + \tfrac{1}{6}[11\bar{2}], \tag{56a}$$

and the corresponding pure pole from eq. (51) is:

$$\tfrac{1}{2}[110] = \tfrac{1}{3}[22\bar{1}] - \tfrac{1}{6}[11\bar{2}]. \tag{58}$$

Similarly, eq. (57) which corresponds to:

$$\tfrac{1}{2}[011] = \tfrac{1}{6}[141] - \tfrac{1}{6}[11\bar{2}], \tag{57a}$$

has a ratchet version:

$$\tfrac{1}{2}[011] = \tfrac{1}{6}[\bar{1}25] + \tfrac{1}{6}[11\bar{2}]. \tag{59}$$

The sessile products b_B with Burgers vectors $\frac{1}{3}[22\bar{1}]$ and $\frac{1}{6}[141]$ have lattice Burgers vectors $[001]_T$ and $\frac{1}{2}[101]_T$ in the twin basis whereas the products $\mathbf{b}_B^*$ with vectors $\frac{1}{3}[111]$ and $\frac{1}{6}[\bar{1}25]$ are non-repeat vectors $\frac{1}{3}[111]_T$ and $\frac{1}{6}[521]_T$ referred to the twin lattice. All these dissociations are energetically unfavourable and the elastic part of the energy varies in the order (59) > (57) > (58) > (56). The dissociations will thus take place only if there are internal stress concentrations arising from pile-ups, intersecting slip or twin bands, or other agencies. Hirth estimated that the stress to nucleate a twin via the dissociation of eq. (57) is about twice that of eq. (56), but suggested that this may be compensated by the easier growth mechanism when no ratchet is involved.

A notable feature of most pole and ratchet mechanisms is that the partial dislocation which generates the twin is formed from a dislocation with a Burgers vector which is not in the twin plane. This is described by Venables as a prismatic source. The special configuration required might be produced if AC is a slip dislocation in plane b which either has a straight length along CD or cross-slips into d and then lies along BC, or if jogs along BC are produced by dislocation intersections. Other theories which are based on prismatic sources include those of Cohen and Weertman[156] and Fujita and Mori,[157] both of which utilize the Cottrell and Bilby dissociation into Shockley and Frank partials but do not assume a pole mechanism. In contrast to this prismatic source are various theories in which the dislocation αC is produced from dislocations with Burgers vectors BC or DC which lie in α, and these may be described as glide sources. Finally, there are theories which depend upon interactions of glide dislocations of two different systems, primary and coplanar[158] or primary and cross-slip.[159]

Most of the early dislocation theories for the production of f.c.c. twins from glide sources depended on the formation of Lomer–Cottrell locks.[9,10,160] In principle this is not necessary since an extended dislocation lying in its slip plane with its ends pinned may be separated into component partials by the action of an external stress. This will happen if the first partial is able to bow out under the applied stress, as in a Frank–Read source, whilst the back partial is unable to follow it either because of its line tension or because it has a lower intrinsic mobility. The latter assumption is used in a recent theory of twinning in semiconducting materials, described in the next section. In f.c.c. metals and alloys, the intrinsic mobilities of both partials are large, and Venables pointed out that the stress-induced separation of these partials should favour twinning in tensile tests on single crystals when the stress axis is near ⟨100⟩, and this is contrary to observation. The dissociation of other glide dislocations, which would give approximately the observed dependence of twinning tendency on orientation of the stress axis, is possibly only with improbably large stresses and small source lengths.

The theories mentioned above attempt to overcome difficulties of this kind by utilizing Lomer–Cottrell barriers to anchor one of the partial dislocations. However, detailed

examination[144,161] indicates that it is impossible to devise a source of this type which will produce the correct twinning partials unless a high energy stair rod dislocation of type $\alpha A/B\beta$ is included, and this should have little strength.

Consider now the other models which assume the Cottrell–Bilby dissociation (55). Cohen and Weertman[156] suggested simply that glide dislocations in a blocked pile-up could dissociate into Frank and Shockley partials, and that glide of the Shockley partials on the appropriate $\{111\}$ planes would then give many intrinsic faults which could overlap to produce twins. In addition to the energetically unfavourable dissociation, this theory suffers from the disadvantage of all casual encounter theories that it is difficult to produce a twin which is highly perfect and has the theoretical shear. A later, rather similar model developed by Fujita and Mori[157,162–164] is described as "stair-rod cross slip" and assumes that the cross-slipping Shockleys do so in ordered sequence in order to produce a near-perfect twin. A slip dislocation in (say) the primary slip plane b is assumed to be held up by an obstacle along direction DC at 60° to its Burgers vector AC. A Shockley partial αC may cross slip to produce a wide stacking fault on the conjugate plane a, leaving a Frank partial along DC. If the stacking fault energy is sufficiently low, the Frank partial will be further dissociated into a Shockley partial on the plane b and a stair rod dislocation along the intersection of the two faults. The Shockley partial on plane a leaves a wide stacking fault but is not assumed to wrap around the remaining parts of the original dislocation (as in the Venables model) but simply to extend away from the stair rod (or Frank) dislocation. Successive slip dislocations are then assumed to pile-up behind the barrier and to cross-slip in the same way on to successive conjugate planes, thus forming a thin twin. Twins may form by the same mechanism on the primary plane if b is the conjugate plane.

There is one major difficulty with this model, namely that each glide dislocation must cross-slip only when it has been forced into the next atomic plane, at a distance of $a/\sqrt{3}$ from the Frank partial left by the preceding dislocation. The stress required to achieve this close approach is clearly extremely high, but elastic estimates are unreliable and atomistic calculations are required to give a realistic value. The situation is even worse if the Frank partial is dissociated into a Shockley partial on b and a stair-rod at the a–b intersection. This suggests that especially in materials of low fault energy, stair-rod cross slip can give only well separated single faults, as in the Cohen–Weertman model. As already emphasized, the energy required for the dissociation (52) may prevent it from occurring in practice.

Later theories of deformation twinning in f.c.c. materials, including that of Fujita and Mori, are based on the experimental result that twinning in f.c.c. does not begin until slip is activated on at least two systems. The simplest description is that of Mahajan and Chin[158] who considered a reaction between dislocations of the primary system with Burgers vectors **BC** and of the co-planar system with vectors **DC** to form three Shockley partials

$$\mathbf{BC} + \mathbf{DC} = 3\alpha\mathbf{C} \tag{60}$$

which are then rearranged on successive planes to form a three-layer fault. A small twin is obtained when embryonic three-layer twins of this kind at different heights in a slip band grow together, an approach very similar to that of Mahajan for b.c.c. crystals.

Although according to the Frank b^2 rule, the overall reaction (60) is energetically favourable, the interaction of the two $\frac{1}{2}\langle 110\rangle$ lattice dislocations may require an initial increase of energy. Moreover, when the glide dislocations are initially dissociated, an interchange of positions between the leading and the lagging Shockley partials is necessary, as shown schematically in Fig. 17. Suppose two dislocations, with Burgers vectors **DC** and

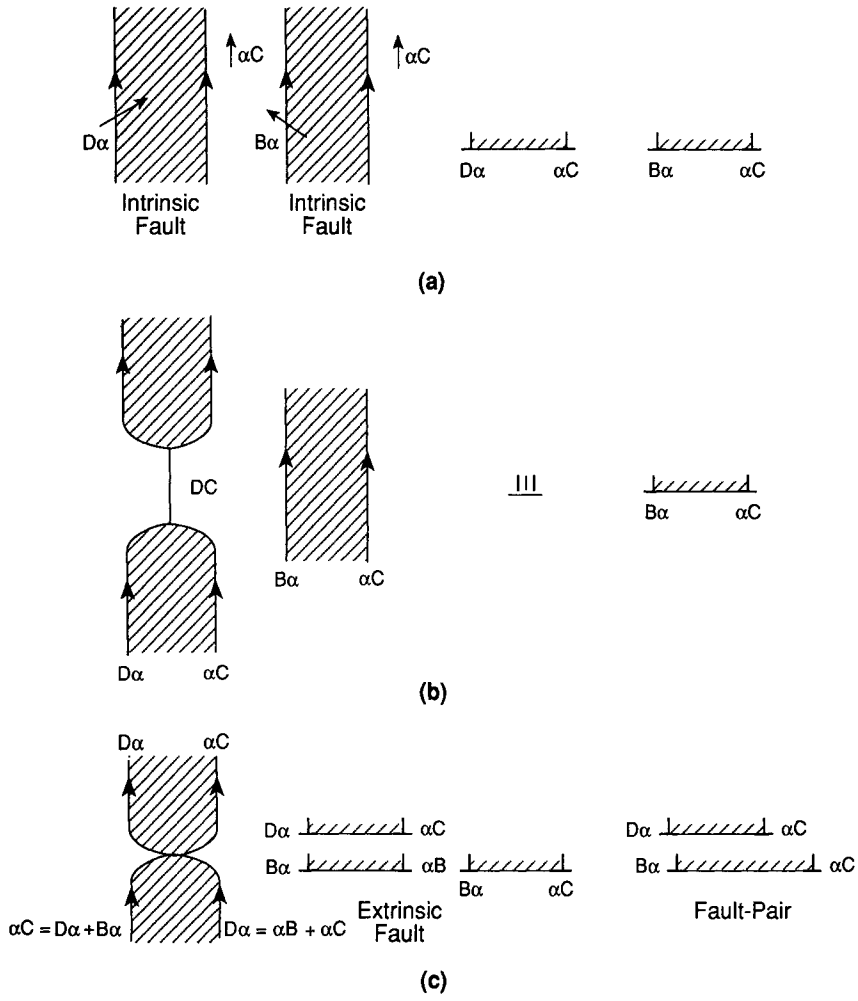

Fig. 17. Schematic illustration of the formation of a fault pair in f.c.c. crystals (after Mahajan[165]).

BC, each dissociated into Shockley partials, glide in plane *a*. The reaction (60) is opposed by the mutual repulsion of $\boldsymbol{\alpha C}$ and $\mathbf{D\alpha}$, and calculations[198] indicate that it could only occur with a very high stress concentration. Mahajan[165] later proposed that at a constriction, **DC** dissociates so that $\boldsymbol{\alpha C}$ lags behind $\mathbf{D\alpha}$; the high energy faults implied by this reversal may be avoided if the further dissociations $\boldsymbol{\alpha C} = \mathbf{B\alpha} + \mathbf{D\alpha}$ and $\mathbf{D\alpha} = \boldsymbol{\alpha C} + \boldsymbol{\alpha B}$ are assumed (see Fig. 17(b)). The partials $\mathbf{B\alpha}$ and $\boldsymbol{\alpha B}$ annihilate each other, leading to the formation of a fault-pair, as shown schematically in Fig. 17(c). Gallagher[166,167] and Mahajan[165] found experimental evidence for the formation of such fault pairs in copper and silver alloys.

It is not obvious how this fault pair converts into the three-layer twin required by eq. (60). Mahajan suggests that interaction between different fault pairs could lead to the nucleation of a Shockley loop with Burgers vector $\boldsymbol{\alpha C}$ on the adjacent plane. However, if spontaneous loop formation is possible, growth might begin from a monolayer fault and continue indefinitely without the need for the reaction (60) or the random association of faults.

More complex reactions involving slip activity on the cross-slip plane have been suggested by Narita and Takamura.[168] Their model requires the reaction of a slip dislocation **BC** with a Lomer dislocation **DA** lying along the intersection of the primary and cross slip planes to give

$$\mathbf{BC} + \mathbf{DA} = 2\alpha\mathbf{C} + \alpha\mathbf{A}. \tag{61}$$

The Lomer dislocation **DA** must be produced by reaction between dislocations of the cross slip system with Burgers vector **CA** and the coplanar system with Burgers vector **DC**, and the theory has been criticized because such Lomer dislocations are seldom observed. However, the authors maintain that there is evidence of slip activity on the cross-slip plane, and that this means that the Lomer dislocations must form, even if not observed in lightly deformed material. This model was originally developed from a hypothesis that deformation twinning in f.c.c. materials may be viewed as a stress-relief process, complementary to cross-slip, and it is claimed to agree well with the experimental results.

Attempts to find experimental evidence which will differentiate among the various models are generally based either on electron microscopic evidence for the particular reactions which have been postulated or on observed variation of twinning behaviour with external variables such as temperature, strain rate, and (with single crystal specimens) the sign and orientation of the stress axis. The microscopic technique provides more direct evidence, but suffers from the disadvantage that the foils examined may not represent bulk behaviour. On the other hand, the more macroscopic observations often permit several alternative explanations.

Figure 18 shows a tapering (111) twin F_1 with faults or dislocations F_2–F_5 ahead of it. Contrast experiments show that F_1 is bounded by two sets of partial dislocations, I with Burgers vector $\frac{1}{6}[11\bar{2}]$ and II with Burgers vector $\frac{1}{6}[1\bar{2}1]$. The more numerous and evenly spaced set I is believed to represent the twinning dislocations and to be in screw orientation, whilst set II may be formed to accommodate internal stresses (see below). The contrast behaviour of F_2, F_4 and F_5 is consistent with the assignation of an $R[11\bar{2}]$ fault vector to these faults. Dislocations L and M (Fig. 18) have Burgers vectors $\frac{1}{2}[10\bar{1}]$ and $\frac{1}{2}[01\bar{1}]$ but the contrast

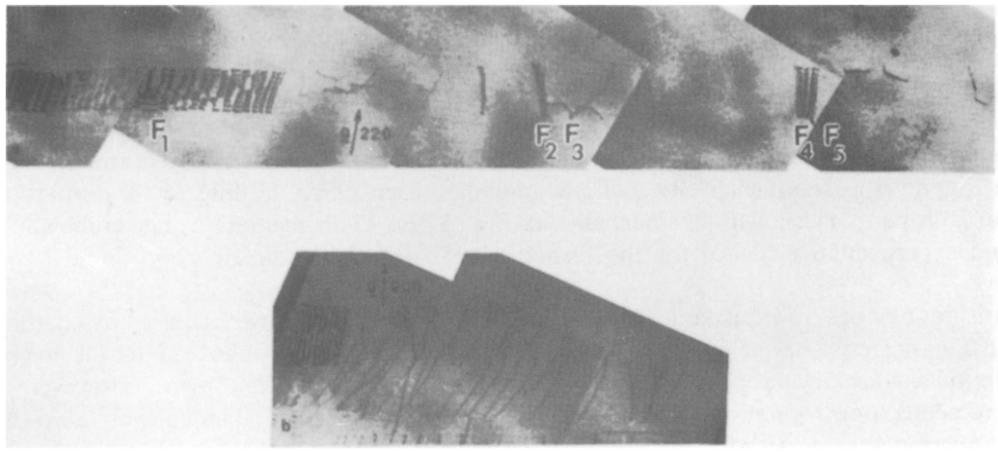

Fig. 18. Micrograph illustrating the general features of faulting and slip observed in a Co–9.5wt%Fe alloy deformed at 77 K. The plane of the micrograph is ~(001) (after Mahajan and Chin[158]).

of dislocation N is complex and Mahajan and Chin concluded that its effective Burgers vector is $\frac{1}{2}[11\bar{2}]$, and that it consists of three closely spaced $\frac{1}{6}[11\bar{2}]$ dislocations. In this figure, CD and GH represent projections of the $[10\bar{1}]$ and $[01\bar{1}]$ vectors on to the (001) plane. Comparing these projections with those of various dislocations in Figs 18 and 19, it is inferred that the portions of dislocations L and M which react to form F_3 are in screw orientation, whereas the majority of dislocations M are non-screw in character. Mahajan and Chin identified the crystallography of Figs 18 and 19 as evidence that the twin F_1 formed by a slip–twin conversion according to a reaction which is a variant of eq. (60), and they argued that it could not be explained by eq. (61). There is, however, no direct evidence that dislocation N or any of the faults has been formed by eq. (60). Similar indirect support for the Mahajan–Chin model comes from observations by Robertson[169] on a terminating twin and accompanying dislocations in nickel. The Burgers vectors of the twinning partials and of the whole dislocations were consistent with eq. (60).

In support of the stair-rod cross-slip model, Mori and Fujita[163] showed wide, overlapping stacking faults on the conjugate plane on which twinning was observed; there is, however, no direct evidence that the faults have formed by cross-slip from the primary plane. A later attempt to find such evidence was made in an *in situ* study by Mori *et al.*[164] Figure 20 shows how the twin on the conjugate plane apparently thickens by cross-slip of partials from the primary slip bands, S_1, S_2 etc. leaving stair-rod dislocations or undissociated Frank partials at A_1, A_2 etc. This micrograph clearly does not show the nucleation of the twin, but if the interpretation is correct, it does support the growth mechanism of Mori and Fujita. It is also relevant to the problem of slip–twin intersection, considered in Section 6.2.

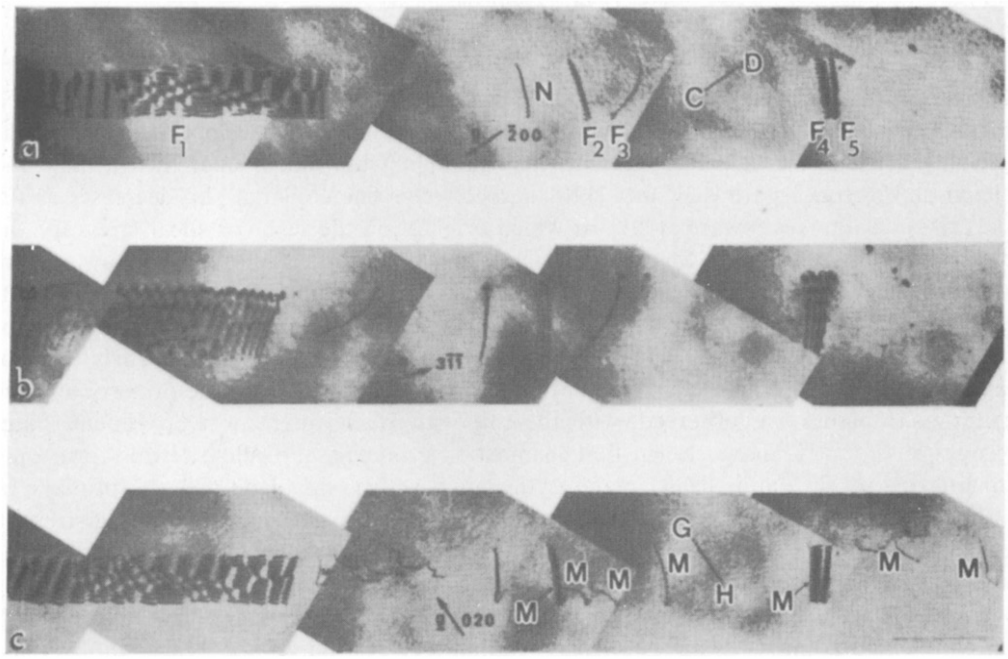

Fig. 19. Micrographs illustrating the contrast behavior of dislocations L, M and N shown in Fig. 18 for different reflections. The planes of the micrographs are (a) ~(001), (b) ~(112) and (c) ~(001). CD and GH are the projections of the $[10\bar{1}]$ and $[01\bar{1}]$ vectors on the (001) plane. The marker represents one micron (after Mahajan and Chin[158]).

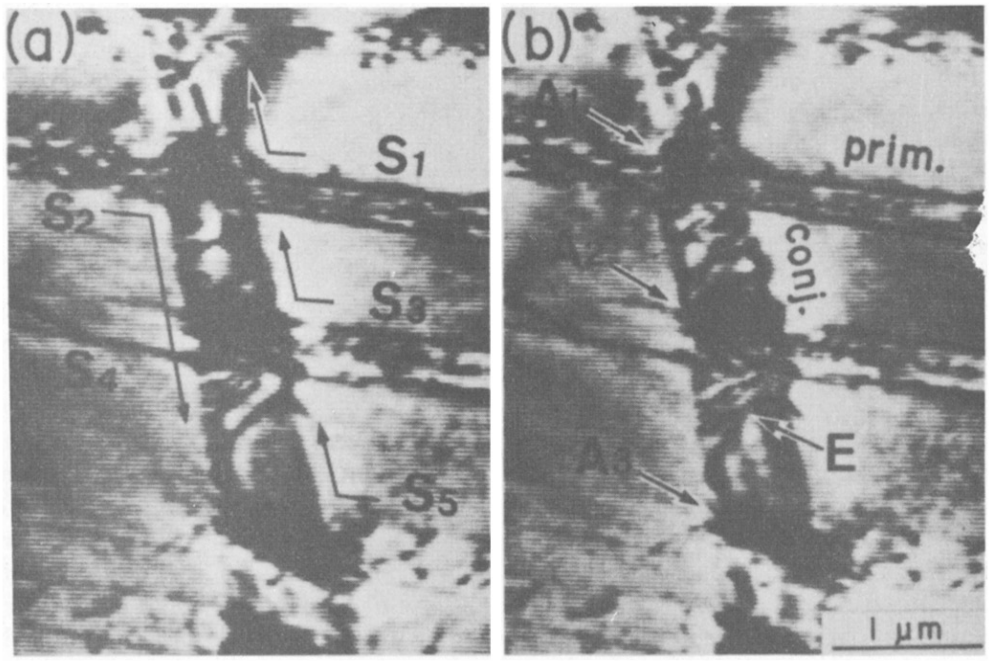

Fig. 20. The cross slip of the leading partials of the primary dislocations onto the conjugate plane. The marks S_1 to S_5 denote the primary slip bands. The marks A_1 to A_3 indicate the accumulations of the stair-rod dislocations and the following partials of the primary dislocations (or the combined Frank partials) along the intersections between the twin interfaces and the primary slip bands. Mark E shows the elastic interaction forming a dipole between the twinning partials on the opposite twin interfaces (after Mori and Fujita[163]).

The early experimental work of Suzuki and Barrett[9] on silver–gold alloy crystals showed that for a tensile axis close to $[\bar{1}11]$, twinning occurs on the primary slip plane (111) in the direction $[\bar{2}11]$, and this is consistent with the Mahajan–Chin model since the primary and coplanar slip directions are $[\bar{1}01]$ and $[\bar{1}10]$, respectively. The coplanar slip decreases as the initial stress axis moves towards [001], at which orientation the resolved shear stress for the coplanar system is zero. Thus the twinning tendency should decrease on moving away from $[\bar{1}11]$ along the $[\bar{1}11]$–[001] line and there should be no twinning for axes close to [001]. Blewitt *et al.*[8] and Suzuki and Barrett[9] reported, in fact, that twinning usually occurred only for tensile axes between $[\bar{1}11]$ and $[\bar{1}13]$. However, in both studies and also in the early work of Haasen and King[170] and Thornton and Mitchell,[171] twinning on both the primary and the conjugate slip planes was observed, with the conjugate plane often most prominent. Later investigations[7,159,168–169] have shown that in most f.c.c. metals and alloys, twins form only after appreciable slip, and the $\mathbf{K}_1$ plane is the most active slip plane (i.e. the primary or conjugate plane, depending on the amount of slip before twinning). The twinning stress in a tensile test decreases as the orientation of the stress axis approaches $\langle 111 \rangle$, and also as the temperature is lowered, provided the twinning occurs in stage III of the work-hardening curve, but is little affected by orientation and temperature in stage II. Mahajan and Chin[158] and Narita and Takamura[159] have each claimed that their respective models account for these observations.

Chin *et al.*[19] examined in some detail the behaviour of cobalt–iron single crystals under constrained deformation. A specimen was orientated for $[1\bar{1}0](110)$ plane strain compression

(i.e. the compression axis was [110]), and the specimen was allowed to elongate along $[1\bar{1}0]$ but was prevented from widening along [001]. The imposed shape change was found experimentally to be achieved by a combination of the slip systems $[\bar{1}01](111)$, $[0\bar{1}1](111)$, $[0\bar{1}\bar{1}](11\bar{1})$ and $[\bar{1}0\bar{1}](11\bar{1})$ and the twinning systems $[\bar{1}1\bar{2}](\bar{1}11)$ and $[\bar{1}12](\bar{1}1\bar{1})$. On the basis of the Mahajan–Chin model, the operative slip systems could activate the two observed twinning variants, together with $[11\bar{2}](111)$ and $[112](11\bar{1})$. However, these last two twins would elongate the crystal along [110] and so would not be expected. To obtain the observed twin systems with the "prismatic" sources of the Venables, the Cohen and Weertman or the Fujita and Mori models requires dissociation of a $\frac{1}{2}[1\bar{1}0]$ dislocation, slip dislocations with this Burgers vector cannot be activated either by the applied compressive stress along [110] or by the reaction stress along [001]. This result thus suggests strongly that the twin nucleus comes from a glide-type source rather than a prismatic type source.

4.7. *Twinning in Elemental and Compound Semiconductors*

A dislocation model of twinning in elemental semiconductors such as silicon or germanium and in semiconducting III–V or some II–VI compounds like GaAs or CdTe has been recently developed by Pirouz[14,173–174] and Pirouz and Hazzledine[175] and will be discussed next because of many similarities to f.c.c. twinning. As already noted, the diamond structure is a double lattice structure obtained by placing atoms on two interpenetrating f.c.c. lattices with the second origin at $\frac{1}{4}a\langle 111\rangle$. The zinc-blende (or sphalerite) structure of the III–V compounds is obtained by segregating each atomic species on to one of these two f.c.c. lattices. Denoting the two f.c.c. lattice sites by Roman and Greek letters respectively, both structures may also be viewed as a stacking of atomic $\{111\}$ layers in the sequence $\ldots A\alpha B\beta C\gamma\ldots$ where the close-packed planes of the f.c.c. structure are replaced by double layers α-B, β-C, γ-A. The interplanar distances α-B, etc. are one third of the separations A-α, etc. Each atom has four nearest neighbours at a distance of $a\sqrt{3}/4$; for an atom in plane α, three of these neighbours are in plane B and one of them is in plane A. The slip and twinning planes and directions are identical with those of the f.c.c. structure, but a distinction has to be made between slip on a plane midway between the closely spaced α and B layers, and slip on a plane between the widely spaced A and α layers. Lattice dislocations with Burgers vector $\frac{1}{2}a\langle 110\rangle$ may exist, in principle, in either plane, and may then be dissociated into Shockley partials. The two sets of dislocations are called the "glide" and "shuffle" sets, respectively.

The deformation behaviour of these semiconductors shows that they have relatively immobile dislocations due to high Peierls–Nabarro forces, especially for dislocations aligned along $\langle 110\rangle$ directions. Thus the important lattice dislocations are either pure screws or have their Burgers vectors at $\pm 60°$ to their line direction; when dissociated into pairs of Shockley partials, the screw dislocation consists of two 30° partials whereas a 60° dislocation consists of a 90° and a 30° partial. At low temperatures, brittle fracture usually occurs with very little evidence of plastic deformation, and at high temperatures, $\langle 1\bar{1}0\rangle\{111\}$ slip is observed. In silicon, the ductile–brittle transition is at about 700°C (varying with strain rate) but plastic deformation may be observed below this temperature, for example by subjecting the specimen to a uniform hydrostatic pressure in addition to a uniaxial compressive stress. It is found experimentally that plastic deformation at these low temperatures is predominantly by twinning even when single crystals are orientated for single slip.[15] It is an important feature of Pirouz's model that for both screw and 60° dislocations, experiments have shown appreciable differences in the mobilities of the leading and trailing Shockley partials. Moreover, since the motion is thermally activated, both mobilities are strongly

temperature dependent, and any difference in mobility will be more pronounced at lower temperatures.

Consider the dissociation of part of a screw dislocation of the glide set with Burgers vector **BA** into partials $\delta\mathbf{A} + \mathbf{B}\delta$ lying on plane a between pinning points H and H′ (see Fig. 21). If the leading partial $\delta\mathbf{A}$ has a mobility much higher than that of the trailing partial, it may be decoupled from it under the action of a suitable shear stress and by acting as a Frank–Read source, rotating about H and H′, a closed loop of stacking fault, expanding in the plane a is obtained together with a short segment of $\delta\mathbf{A}$ which approaches the trailing partial $\mathbf{B}\delta$ from the other side. Pirouz originally assumed that despite their mutual repulsion, the two partials could be forced together by the stress field to reform the perfect dislocation line with lattice Burgers vector **BA**. This line is then assumed to cross-slip on to the next {111} lattice plane, where it redissociates to produce a second layer of fault. Clearly this is a ratchet mechanism very similar to that of Venables; it was in fact considered by Venables for f.c.c. twinning, but was rejected because he considered the stress to separate the two partials of a dissociated glide dislocation to be too large. Thus although the model might, in principle, apply to f.c.c. twinning, the situation is clearly more favourable in diamond cubic and zinc-blende structures, where quite large differences in the mobilities of the two partials have actually been observed. The model does, however, have the unsatisfactory feature of all ratchet mechanisms, namely the necessity for opposite dissociation and recombination processes, which is rather suggestive of a "pulling up by bootstraps" operation. The difficulty of the recombination can partly be avoided, as was pointed out later,[175] by adopting a cross-slip mechanism due to Friedel[176] and Escaig[177] which allows the extended configuration to cross-slip without

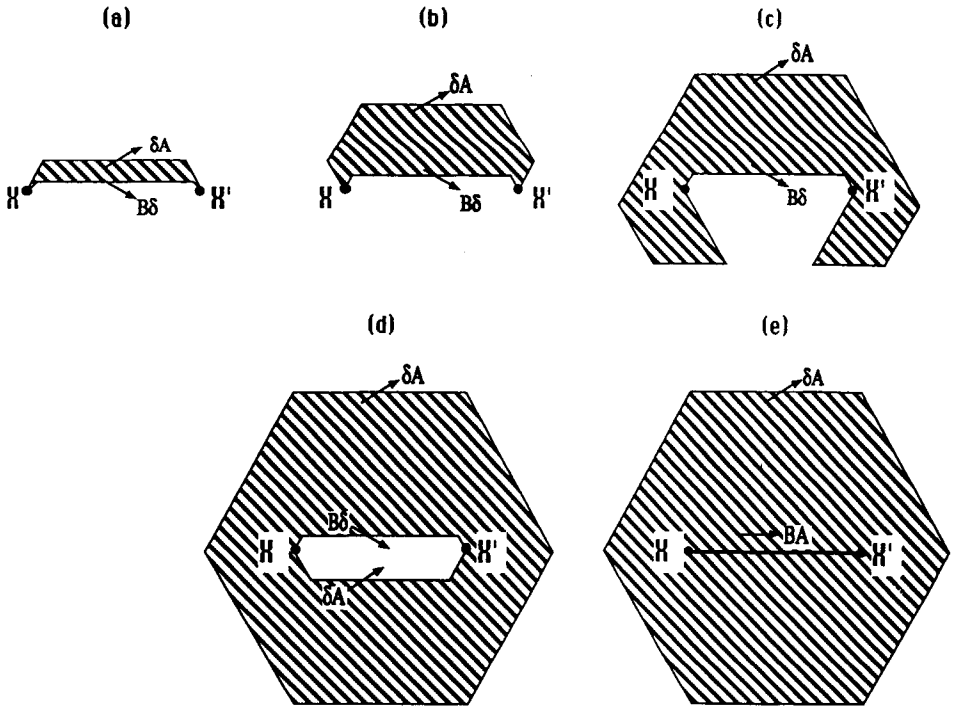

Fig. 21. Schematic illustration of the model proposed by Pirouz and Hazzledine[175] for the formation of {111} twins in diamond cubic and zinc-blende structures.

recombination over the whole length of the dislocation, and which moreover can operate without any resolved shear component of the applied stress on the cross-slip plane. Granted that this is possible, however, it is not at all clear why the cross-slipped segments should immediately move back into the next {111} plane parallel to the original glide plane. Once again, it must be emphasized that all these hypothetical displacements are taking place within the core of the dislocation and really need an atomistic description.

Note that this theory is not a pole mechanism even if the original dislocation leaves the twin plane on opposite sides at the two pinning points. This is because there is no component of Burgers vector normal to the $\mathbf{K}_1$ plane. Nevertheless, the mechanism is obviously similar to the ratchet mechanism previously described, and re-emphasizes that the latter does not actually utilize the topological properties of a pole dislocation.

Pirouz has also applied this model to compound semiconductors which are effectively long-range ordered versions of the diamond cubic structures. In the zinc-blende structure, the $A\,B\,C$ layers are occupied by one kind of atom, and the $\alpha\,\beta\,\gamma$ layers by another kind. It follows that the lattice and partial dislocations responsible for plastic deformation have the same Burgers vectors, but the core of the dislocation may consist entirely of atoms of one species. A difference in mobility of the two partials in an extended dislocation may then be enhanced. However, the experimental results of Androussi *et al.*[15] that Zn-doped GaAs crystals, oriented for single slip, twinned at ambient temperature whereas *n*-type crystals did not twin presents a difficulty for the theory. Rabier and Boivin[178] found the difference in the mobilities of the Shockley partials is much smaller in Zn-doped crystals than in *n*-type crystals, so that according to the Pirouz model the *n*-type crystals should more readily twin.

4.8. *Twinning in Hexagonal Close-Packed Materials*

The analysis of Section 2.7, summarized in Table 3, shows that the main deformation twins in h.c.p. materials have $\mathbf{K}_1$ planes of type $\{10\bar{1}2\}$ (all metals) and $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$ (Ti group metals). In addition, $\{11\bar{2}4\}$ twins which are conjugate to $\{11\bar{2}2\}$ twins have been found in Mg and Ti, and there are several other modes, notably the conjugate $q = 8$ modes $\{10\bar{1}1\}$ and $\{10\bar{1}3\}$ observed in titanium[179,180] and magnesium,[66] respectively. Transformation twinning of either type I with $\mathbf{K}_1 = \{10\bar{1}1\}$, $q = 4$ or its type II equivalent is frequently observed after the b.c.c.–h.c.p. martensitic transformation.

Twinning in h.c.p. materials was reviewed by Yoo[181] in 1981, and Fig. 22 shows his plot of twinning shear s vs c/a for the main twinning modes, with the observed modes for seven h.c.p. metals superimposed. The $\{10\bar{1}2\}$ mode is found in all cases, despite the shear reversal at $\gamma = 3^{\frac{1}{2}}$ already noted. If a uniaxial tensile stress is applied along the c axis, twins of a particular mode may form if the mode line in Fig. 22 has a negative slope, whilst a crystal or grain subjected to compression along its c axis may twin only if the line has a positive slope. This rule is reversed for the two conjugate modes, listed on the same plots as their primary modes. Thus with respect to the c axis, the $\{11\bar{2}1\}$, $\{11\bar{2}4\}$ and $\{10\bar{1}3\}$ twins are "tension" twins, and the $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ twins are "compression" twins. The $\{10\bar{1}2\}$ twin is a compression twin for cadmium and zinc and a tension twin for all the other metals.

As already noted, Thompson and Millard[100] in considering the formation of $\{10\bar{1}2\}$ twins in h.c.p. metals independently suggested a pole mechanism. Since this is a $q = 4$ mode, the expected twinning dislocation is a zonal dislocation of double step height with a Burgers vector given by eq. (38). Thompson and Millard considered that a "major" dislocation of

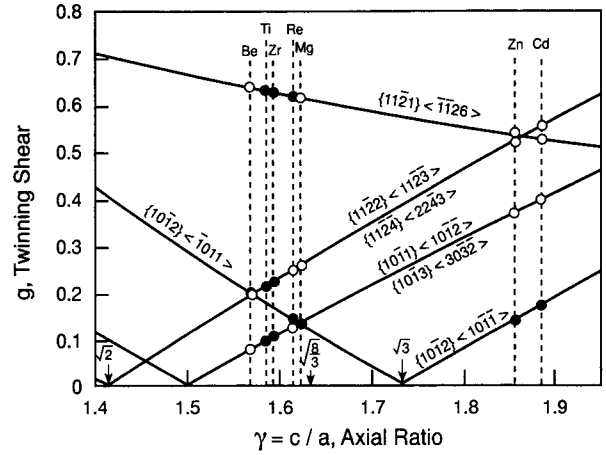

Fig. 22. Variation of twinning shear with the axial ratio for the seven hexagonal metals. A filled symbol indicates that the twin mode is an active mode (after Yoo[181]).

Burgers vector $[000\bar{1}]$ lying on the $(10\bar{1}2)$ plane of the matrix could be incorporated into a $\{10\bar{1}2\}$ twin, where it becomes a sessile dislocation with a Burgers vector of type $\langle\bar{1}010\rangle$ in the twin lattice, and it then leaves in the interface a double step, i.e. (in later terminology) a zonal twinning dislocation, of Burgers vector $f\langle 10\bar{1}\bar{1}\rangle$ where f (see eq. (38a)) is approximately $+(1/17)$ for ideal c/a and $-(1/13)$ for zinc which has $c/a \simeq (7/2)^{\frac{1}{2}}$. Thompson and Millard apparently treated the pole dislocation and the twin nucleus as distinct defects which interact, and they did not explicitly consider a combined nucleation and growth mechanisms from an initial dissociation of a single lattice dislocation. Whether or not growth begins from a single stacking fault, examination of the crystallography (very helpful equations in tensor notation are given by Saxl[182–185]) shows that the Thompson–Millard relation should be written

$$\mathbf{b}_B = [10\bar{1}0]_T = [0001]_p - f[10\bar{1}1]_p \tag{62}$$

in order to obtain a true pole mechanism. Once again, the opposite dissociation of the pole dislocation of the form of eq. (51) will give an anti-generating node. Both dissociations are energetically unfavourable, but the higher elastic energy is associated with the dissociation which gives a pure pole mechanism. If the initial nucleus is a single layer fault, or a fault of [say] 1–10 layers, there will also be the usual large stress opposing the passing of opposite elements of the twinning dislocation.

Evidence for twinning dislocations in a $\{10\bar{1}2\}$ interface in zinc has been obtained recently,[186] but the authors estimate the Burgers vector to be about $\frac{1}{4}\langle\bar{1}0\bar{1}1\rangle$ whereas eq. (38) with $c/a \simeq (7/2)^{\frac{1}{2}}$ gives a vector of about $(1/13)\langle\bar{1}011\rangle$. Thus the step height, or the "quantum" of deformation, is suggested to be 6–8 lattice planes instead of the expected two planes. There seems no obvious reason for such multiple twinning dislocations.

The Burgers vector of an elementary twinning dislocation for the $\{11\bar{2}1\}$ mode is about $(1/35)\langle 11\bar{2}\bar{6}\rangle$ in cobalt, and Vaidya and Mahajan[187] suggested the following reaction of two $\frac{1}{3}\langle\bar{2}11\bar{3}\rangle$ dislocations with a $\langle 1\bar{1}00\rangle$ dislocation would yield a multilayer stacking fault approximating to a thin twin.

$$2 \times \tfrac{1}{3}\langle\bar{2}11\bar{3}\rangle + \langle 1\bar{1}00\rangle = 12 \times \tfrac{1}{36}\langle\bar{1}\bar{1}26\rangle \tag{63}$$

The $\langle 1\bar{1}00\rangle$ dislocations might arise from interactions between dislocations with **a** type Burgers vectors, e.g.

$$\tfrac{1}{3}[2\bar{1}\bar{1}0] + \tfrac{1}{3}[1\bar{2}10] = [1\bar{1}00] \tag{64}$$

This mechanism is thus similar in concept to that suggested by Mahajan and Chin[158] for f.c.c. twinning, although the spontaneous spreading of the Burgers vector into 36 adjacent planes may not seem very probable. Moreover, in the case of $\{11\bar{2}1\}$ twinning, we have noted already that elementary twinning dislocations are probably split into steps of atomic height which are thus partial twinning dislocations (supplementary displacement dislocations) with Burgers vectors of about $(1/70)\langle 11\bar{2}\bar{6}\rangle$.

Hirth and Lothe[141] pointed out that either a true pole or a ratchet mechanism may be envisaged for $\{11\bar{2}2\}$ twinning in a similar fashion to that discussed for $\{10\bar{1}2\}$ twinning, the pole being formed from a lattice dislocation with a Burgers vector $\frac{1}{3}\langle 1\bar{2}1\bar{3}\rangle$. No specific mechanisms appear to have been suggested for the formation of the remaining h.c.p. twins, but the recent results of Serra *et al.*[97] on the structure of twinning dislocations in the various h.c.p. twin interfaces re-emphasize the possible significance of the structure and properties, especially the frictional resistance to motion (or Peierls–Nabarro force) which a twinning dislocation must overcome in order to advance the growth of the twin.

Table 5 summarizes some results for the computed energies of the relaxed $\mathbf{K}_1$ interfaces and for various structural and energetic features of steps (i.e. twinning dislocations) in these interfaces. The last column shows the applied shear strain at which the twinning dislocation was displaced along the interface. Some twinning dislocations were found to have narrow (three-dimensional) cores, $\sim a$–$2a$ in width, and did not move until the applied shear strain exceeded $\sim$1–4%. Others have wider (planar) cores (4–6a) and glide along the $\mathbf{K}_1$ interface at much smaller applied strains. The highly glissile steps are those in $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twin interfaces and the steps of low mobility are those which correspond to the observed $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ deformation twinning modes. The difference in mobility of the twinning dislocations in $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$ is striking in view of the apparent similarity of their interface structures; it is believed to be related to the magnitude and complexity of the atomic shuffles. In fact, the mobilities of the steps of height d in the $\{11\bar{2}1\}$ interface and $2d$ in the $\{10\bar{1}1\}$ interface, corresponding to the unobserved $\{11\bar{2}1\}$ high shear mode and the transformation twinning mode previously discussed, were found to be respectively very much higher and slightly higher than those of the steps in the observed modes. It follows from the table that the mobility of a twinning dislocation is not simply related to the magnitude of either its Burgers vector or of the

Table 5. Computed Energies and Properties of Some h.c.p. twin Interfaces[97]

$\mathbf{K}_1$	γ (ϵ/a^2)	$\mathbf{b}_T$ (eq.)	s	b^2/a^2	h/d	Disl. line	Energy elast.	(ϵ/a) core	Core width	Critical strain
$10\bar{1}2$	1.15	38a	0.12	1/51	2	0.1	0.1	0.0	6a	0.002
$11\bar{2}2$	0.92	39a	0.27	4/33	3	3.7	1.6	2.1	a	0.014
$11\bar{2}1$	0.73	40a	0.61	3/140	$\frac{1}{2}$	0.3	0.3	0.0	11a	0.001
$10\bar{1}1$	0.64	41a	0.15	25/123	4	4.0	2.3	1.7	a	0.02
		42	0.36	37/123	2	3.6	2.4	1.2	2a	0.006

Notes: This table is adapted, with minor corrections, from Tables 1 and 2 of Ref. (97). Only observed deformation modes plus the observed $\{10\bar{1}1\}$ transformation twinning mode are listed. The values of s and of b^2/a^2 apply to the ideal axial ratio, $\gamma = (8/3)^{\frac{1}{2}}$. The energy unit ϵ is the depth of the atomic pair potential at the nearest neighbour distance.

twinning shear, although it probably is infuenced by these quantities as well as by the complexity of the shuffles.

Why do the twins with twinning dislocations which are difficult to move form, especially when for the same $\mathbf{K}_1$ plane there is in each case an alternative mode with a more mobile twinning dislocation? Part of the answer may be that, although of course the detailed orientation variation is different for each mode, the general sense of applied stress (e.g. tension along the c axis) favours the formation of $\{10\bar{1}2\}$, $\{11\bar{2}1\}$ and the high shear $\{11\bar{2}2\}$ mode, whilst the opposite sense can lead only to the formation of $\{11\bar{2}1\}$ or to $\{10\bar{1}1\}$ twins of the observed deformation or transformation modes. Thus, as pointed out by Serra *et al.*, the high shear $\{11\bar{2}2\}$ mode is competing with two other modes, both with very glissile interface steps, so that it is not surprising that it does not form, especially as its high shear may make it difficult to nucleate. The two low mobility cases also compete with each other for the relief of compressive c-axis stresses, and in titanium[179,180] and zirconium[188] the dominant deformation mode is temperature dependent, namely $\{11\bar{2}2\}$ twinning below $\sim 400°C$ and a mixture of slip and $\{10\bar{1}1\}$ twinning above this temperature. Paton and Backofen[180] deduced that the deformation is controlled by nucleation of $\{11\bar{2}2\}$ twins at low temperatures and propagaton of $\{10\bar{1}1\}$ twins at high temperatures. The slightly more mobile twinning dislocations of the transformation twinning $\{10\bar{1}1\}$ mode have a higher shear than those of the observed deformation mode, and Serra *et al.* suggest that this may inhibit their nucleation. However, these twins form very readily during martensitic transformation, and it is not entirely clear why they should not form during deformation.

Various factors which appear to govern the choice of the observed twinning modes were considered in Section 2.10, but the physics of this choice are better represented by the statement that operative modes must be relatively easy to nucleate and must have glissile interfaces.

5. INFLUENCE OF MATERIAL VARIABLES ON DEFORMATION TWINNING

Many variables (temperature; strain rate; amount of pre-strain; specimen and/or grain size; crystal orientation or specimen texture; doping and/or alloy composition; precipitates or dispersed phases; etc.) may influence the twinning behaviour of a particular material. Some of these factors are difficult to separate, being strongly interdependent. In this section, the variables which (apparently) best illustrate the physical basis of twinning are given most attention.

5.1. *Orientation Dependence: Is There a CRSS for Twinning?*

When twinning is caused by an external stress, it is clearly necessary that the applied forces do work during the formation of the twin, i.e. that the shear stress across the twinning plane and resolved in the twinning direction should be positive. An important difference between twinning and slip deformation is that twinning is polarized, i.e. reversal of the $\boldsymbol{\eta}_1$ direction will not produce a twin. This means that for a single crystal of given orientation with respect to a uniaxially applied stress, some variants of a particular twin mode should operate only in tension, whereas others should operate only in compression. If the single crystal has completely twinned, it follows that all directions in the initially obtuse sector between $\mathbf{K}_1$ and $\mathbf{K}_2$ will have increased in length, whilst all directions in the acute sector will have decreased. However, Frank and Thompson[189] pointed out that a slightly different rule will apply to an actual tension or compression test in a single crystal which deforms initially by forming a thin

twin lamella. The average shear strain of the specimen is now fs where s is the twinning shear and f is the volume fraction of the twin. In the limit $f \to 0$, there will be an increase in length for a specimen axis in the upper right quadrant formed by $\mathbf{K}_1$ and the plane normal to $\boldsymbol{\eta}_1$ (see Fig. 1) and a decrease in length for an axis in the upper left quadrant.

An obvious hypothesis is that twin initiation or growth occurs when the externally applied shear stress across the $\mathbf{K}_1$ plane, resolved in the $\boldsymbol{\eta}_1$ direction, reaches a critical value. Such a law would be analogous to Schmid's law for slip, and several early investigations provided evidence in support of its validity. Unfortunately, the scatter in measured twinning stresses is generally too large and the range of orientations available is too small to provide an adequate test of this hypothesis, especially as the incidence of twinning rather than slip as the preferred mode of deformation is itself very sensitive to orientation. Moreover, as for slip, the observed values depend strongly on purity levels or other variables. Thus Thompson and Millard[100] reported a critical resolved shear stress (crss) of 13.5 Pa for twinning in cadmium, whereas Bell and Cahn[120] found values as divergent as 41 and 4.9 Pa for the same metal.

Experimental measurements of the "twinning stress" are subject to several reservations and their significance is limited by considerable variations in the stress vs strain curves associated with twinning. In many b.c.c. metals and alloys, deformation by twinning in tensile or compression tests of either single crystals or polycrystalline specimens is characterized by large load drops. These abrupt changes of stress are often observed from the beginning of deformation, and there is frequently little evidence of accompanying dislocation activity. The first load drop sometimes occurs during elastic loading, thus indicating that if prior slip is needed to nucleate twins, it must be microslip on a very fine scale. Figures 23 and 24 show stress vs strain curves obtained respectively in early work on polycrystalline niobium[190] and in more recent work[191] on very pure single crystals of Nb–0.33wt%Zr.

Large load drops are observed mainly during deformation at very low temperatures, where they may represent adiabatic softening accompanying a local slip avalanche rather than twinning. A detailed theory of adiabatic heating and softening was first given by Basinski[192] who showed that the effect is favoured by a high temperature sensitivity of the flow stress and a low work-hardening rate. Thus, it is always desirable to obtain metallographic evidence to support a conclusion that observed load drops are due to twinning. Siedersleben and Taylor[193] found, for example, that load drops in single crystals of Li–48at%Mg deformed in tension at 10 K were associated with twinning, but that no twins were visible after

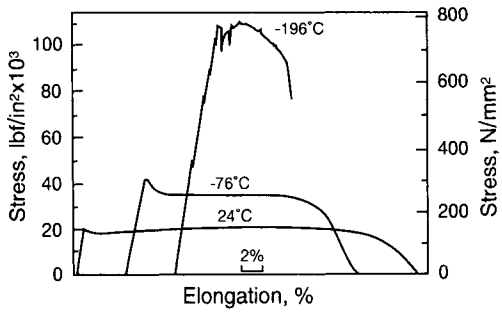

Fig. 23. Typical stress/strain curves for annealed polycrystalline niobium at various temperatures (after Farrell and Evans[190]).

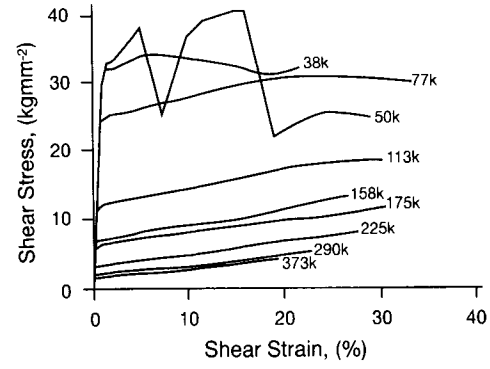

Fig. 24. Shear-stress vs shear-strain curves of Nb–0.33wt%Zr alloy crystals deformed at different temperatures (after Botta *et al.*[191]).

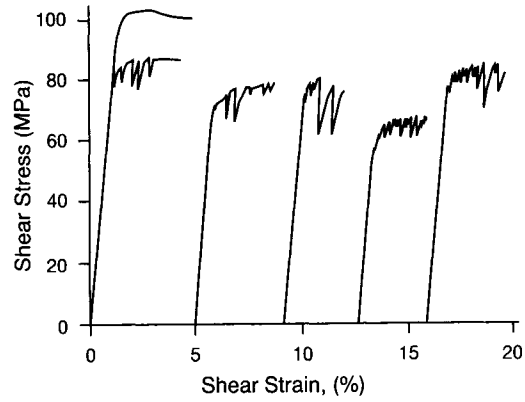

Fig. 25. Shear-stress vs shear-strain curves of Li–57at%Mg alloy crystals deformed in tension at 10 K (after Siedersleben and Taylor[193]).

somewhat larger load drops in crystals of Li–57at%Mg (see Fig. 25). The small magnitude of the serrations in Li–48at%Mg may indicate a difference, much smaller than in the niobium case, between the stresses needed for twin nucleation and twin growth. The tendency towards a smooth stress vs strain curve is even more pronounced in Fe–~25at%Be alloys which were intensively investigated by Bolling and Richman and their coworkers,[38,194–196] and by Green and Cohen.[39] Alloys quenched from a high temperature are random b.c.c. solutions, but long-range order develops on heat treating in the range 325–425°C. As noted in Section 2.6, the ordered structure was originally believed[194,196] to be homogeneous DO_3, but the later work of Green and Cohen and others showed that it is a two-phase mixture of the α-solid solution and an ordered B2 phase.

Bolling and Richman concluded that disordered alloys deform almost entirely by twinning, a condition which they called continual mechanical twinning and defined as deformation under conditions such that the flow stress for twinning is less than that for

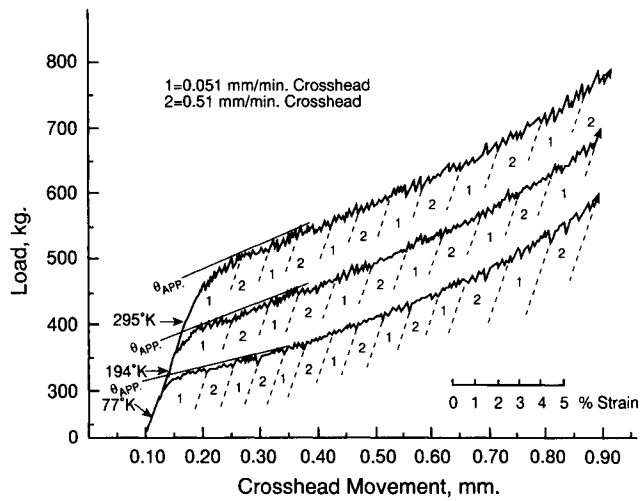

Fig. 26. Load-contraction curves for three Fe–25Be crystals of the same size and orientation deformed at different temperatures (after Bolling and Richman[194]).

macroscopic slip. The deformation is thus produced mainly (an estimated 99% in the case of Fe_3Be) by twin formation, giving a serrated stress vs strain curve but no large load drops. Figure 26 shows load vs contraction curves for disordered crystals of the same size and orientation deformed at three different temperatures with cyclic alternation of two different strain rates (crosshead velocities). Although the curves are not smooth, the amplitude of the jerky flow is only a small fraction of the stress level. In contrast to most cases of slip deformation, there is a positive temperature dependence and negative strain rate sensitivity of the flow stress. Similar effects have been reported in polycrystalline specimens of some other iron alloys.[38,195]

Bolling and Richman considered the ordered alloys to deform by b.c.c. pseudo-twinning of the DO_3 structure and pointed out that the strain after loading was almost completely recovered on unloading (Fig. 27). This remarkable 'pseudo-' (or 'super-') elasticity is part of a more general set of related phenomena which have been much studied in martensitic shape memory alloys.[21,197] As described in Section 2.6, Green and Cohen were able to show that the ordered alloys deform by pseudo-twinning of the B2 regions to give effectively an orthorhombic martensitic product. The B2 regions were much smaller than the twins, so that each twin sheared a region of matrix which contained an appreciable number of coherent B2 regions. The twinning strain is accommodated elastically by the untwinned portion of the α matrix, so that there is both an elastic and a chemical contribution to the driving force for the reverse ('un-pseudo-twinning') transformation on unloading.

Whether or not a superlattice will deform so as to produce a pseudo twin depends essentially on the additional free energy of the new structure, or at very low temperatures on its extra internal energy or enthalpy. If a B2 structure is progressively sheared on a $\{112\}$ plane in a $\langle\bar{1}\bar{1}1\rangle$ direction, there is no symmetry condition which requires the energy to have an extremum at $s = 2^{-\frac{1}{2}}$, even though in the b.c.c. case there is *no* excess energy at this (twin) configuration. Paxton[198] has recently used density functional theory to calculate energy vs shear magnitude curves at 0 K for various B2 alloys. These curves show local minima near to $s = 2^{-\frac{1}{2}}$ for CuZn (β-brass) and FeBe, but for NiAl and NiTi the energy continued to rise smoothly through this value. These results indicate that the pseudo-twin phase is mechanically unstable at 0 K in these latter two systems, but a monoclinic (slightly distorted orthorhombic) phase is metastable in CuZn and FeBe. However, Paxton concludes that the calculated energy difference between the B2 and the sheared structure is too large for pseudo-twinning to be feasible. The pseudo-twinning in Fe_3Be is thus attributed to the non-stoichometric composition and the very small (< 10 nm) particles of the B2 phase.

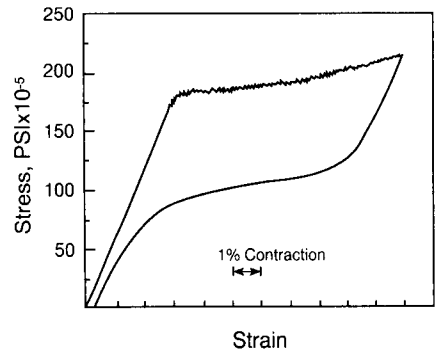

Fig. 27. Typical engineering stress-strain relation for an Fe_3Be single crystal (after Richman[38]).

As previously discussed, twins in f.c.c. metals and alloys usually form on either the primary or the conjugate slip planes (probably depending on which of them is currently most active) but only after the tensile axis has been rotated near to, or beyond, the $\langle 001\rangle$–$\langle \bar{1}11\rangle$ symmetry line where the primary and conjugate systems are equally stressed. The detailed crystallography has already been presented in Section 4.6 and typical stress vs strain curves are shown in Fig. 28. The onset of twinning is usually signalled by a rather small load drop at quite a high strain and stress level, attained as a result of work-hardening (see Fig. 28). At very low temperatures, faulting and twin nucleation may become copious and there are then no load drops and only a small inflection in the curve marks the onset of twinning.

In h.c.p. metals and alloys, twinning may occur without apparent load drops. Figure 29 shows stress vs strain curves for polycrystalline specimens of magnesium tested in tension and compression at three different strain rates.[199] There is a strong fibre texture in the extruded specimen rods with the basal plane parallel to the axis; this is a favourable orientation for $\{10\bar{1}2\}$ twinning in compression but not in tension; see text relating to Fig. 22 which is described in terms of a stress axis normal to the basal plane. The very large difference in the stress vs strain curves in tension and compression is thus attributable to the utilization of the $\{10\bar{1}2\}$ twinning mode to assist in the compressive deformation. Another example of the effects of the polarity of twinning is provided by the h.c.p. metals titanium and zirconium. These are remarkably similar in most of their structures and properties, including stress vs strain curves at relatively high temperatures where slip dominates as the deformation mechanism. However, for some reason, $\{11\bar{2}2\}$ twinning occurs much more readily in titanium than in zirconium, and at 77 K, the incidence of twinning leads to very different stress vs strain curves.[199]

The above examples illustrate the difficulty of defining a 'twinning stress' from the measured deformation behaviour, and with the prospect of abrupt load drops, very hard machines may be required in order not to lose part of the change. The classical experiments of Bell and Cahn[120] showed that it may be necessary to consider separately the stress needed for nucleation of a twin and the (usually lower) growth stress. The initiation of twinning probably depends on nucleation if large, discontinuous load drops are observed during normal tensile or compression tests, as in most b.c.c. metals at very low temperatures. In

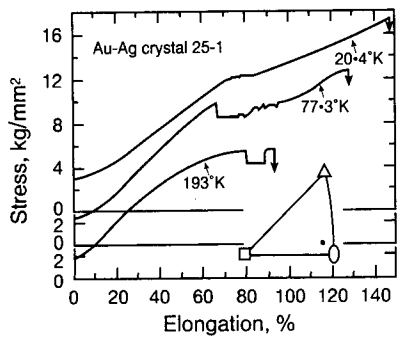

Fig. 28. Stress–strain curves of the silver–25at%gold alloy crystals (after Suzuki and Barrett[9]).

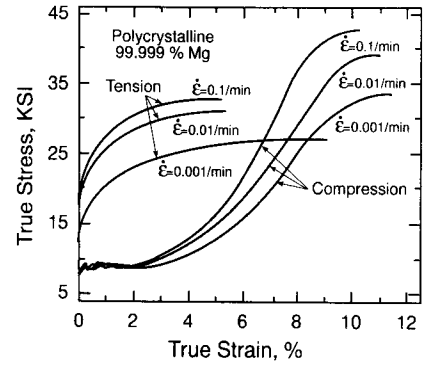

Fig. 29. Stress–strain curves of strongly textured polycrystalline magnesium showing differences under compression and tension. The difference in the compressive and tensile curves is due to the $\{10\bar{1}2\}$ twinning that occurs in compression (after Reed-Hill[199]).

many of the nucleation models already discussed, twins form at intersections of slip lines, or in other configurations where the external stress is enhanced, so that the true local stress cannot be measured. Thus tests of a possible crss law for nucleation have to be made with great care to avoid such stress concentrations. Although the upper and lower stresses of a load drop may be related respectively to the nucleation and propagation stresses of the twins, the discontinuity in stress may nevertheless have been increased by adiabatic softening which is as likely to be triggered by rapid twin formation as by a slip avalanche.

Tests on b.c.c. metals give contradictory results on whether or not a crss law applies, but the majority of the evidence is that the orientation dependence is more complex. Body-centred cubic metals twin readily (without appreciable prior slip) only at low temperatures and/or high strain rates, and under these conditions analysis is complicated by peculiarities in the slip behaviour which include breakdown of the Schmid law of crss for slip and large orientation dependences and asymmetries. Some early results on polycrystalline niobium[199] indicated no differences between tensile and compressive tests at relatively high temperatures where deformation involved usual slip modes, but the first twin formed in compression at 77 K at a stress below the yield stress for slip in tension, and the first tensile twin formed at 20.4 K at a higher stress, but considerably below the extrapolated yield stress for slip. In very pure metals, later work has shown that the situation may be much more complex; and major components of the total strain may result from slip on unpredicted (so-called 'anomalous') variants of the usual slip system. These effects are believed to be a consequence of the core structure of the screw dislocation in b.c.c. metals.[118,149]

Conflicting evidence for and against a crss law for f.c.c. twinning may also be found in the literature. An early comprehensive analysis was carried out by Venables[161] who pointed out that because of the large strains undergone by most f.c.c. crystals prior to twinning, it is difficult to calculate accurately the axis rotation, and hence the Schmid factors for either slip or twinning. In copper alloys of low stacking fault energy, this problem is further complicated by 'overshoot', i.e. continued deformation by slip on the primary slip plane after the symmetry axis is reached. The data available to Venables consisted of results on pure copper and silver and on copper alloys and Ag–Au alloys. He made plots of the variation of twin stress against the ratio of the critical resolved shear stress for slip to that for twinning at the onset of twinning and found for both copper and silver that the twinning stress apparently decreases slightly with increasing values of this parameter in the range 0.9–1.1. However, as he emphasized, there is a very large scatter in individual results and little reliance can be given to these conclusions, which are further complicated by the orientation dependence of the occurrence of twinning. In the Ag–Au alloys,[9] twinning becomes easier as the original tensile axis approaches ⟨111⟩ or the ⟨111⟩–⟨110⟩ zone; most of the twinning occurs between ⟨311⟩ and ⟨111⟩. Similar results have been reported for copper and for copper alloys;[170–172] in the case of copper, Blewitt *et al.*[8] found the twinning stress at 77 K to be so high that fracture occurred before twinning except for orientations very close to ⟨111⟩.

An observation which has been reported very frequently and for many different materials is that when the orientation of the stress axis is varied in single crystals subjected to tension or compression,[200–203] or in polycrystalline materials with a texture,[204] the first twins to form are almost always those of the variant for which the resolved shear stress is largest. In b.c.c. crystals, for example, with a stress axis within the unit triangle defined by [001] [011] and [$\bar{1}$11], the two variants in tension should be (1$\bar{1}$2) [$\bar{1}$11] near [001] and ($\bar{1}\bar{1}$2) [111} near the [011]–[$\bar{1}$11] boundary, whilst in compression the single variant ($\bar{2}$11) [111] should operate over the whole triangle. The different variants imply an asymmetry in the applied stress for twinning in tension and compression and this carries over to polycrystalline textured materials, as shown

for iron by Richards and Reid.[204] For materials without a texture, no difference in the twinning stresses for tension and compression was found, but the twinned volume fractions and the fraction of grains containing twins were both appreciably larger in compression than in tension. The authors point out that on average the grains, even in a random aggregate, are more favourably orientated for twinning under an applied compressive stress than under a tensile stress. Similar results apply to f.c.c. metals and alloys where twins form on either the primary or the conjugate $\{111\}$ slip planes, or in the case of constrained deformation, on the most highly stressed system.[19] This confirms that the applied shear stress in the $\mathbf{K}_1$ plane and the $\boldsymbol{\eta}_1$ direction is the most important stress component, but nevertheless leaves open the possibility of a variation with stress axis orientation of the critical value of this stress at which twins first form. Twinning is essentially antisymmetric, inasmuch as an oppositely directed (i.e. 'anti-twinning') shear stress of comparable magnitude to that needed to produce twinning will generally have no effect. This contrasts with slip deformation in which the crss for forward and reverse deformation is comparable (but not necessarily identical unless the slip elements possess certain point group symmetries) in most materials. Both twinning vs anti-twinning slip asymmetries and those due to the influence of other components of the stress tensor on dislocation core structures were first discussed for b.c.c. metals,[118,149] but are now known to be significant at low temperatures in very many structures in which the dislocation core can loosely be described as three-dimensional rather than two-dimensional, i.e. not spread along the slip plane, as in dissociated f.c.c. dislocations. These recent investigations on slip have the effect of making it seem rather improbable that a crss law ever holds for twinning.

5.2. *Temperature*

Twinning in most b.c.c., f.c.c. or h.c.p. metals and in intermetallic compounds, semiconductors, etc., increases in importance as the temperature is lowered. This is often formally represented by a twinning stress vs temperature curve which increases less steeply at low temperatures than the yield stress or the flow stress for plastic deformation by slip; in some cases, the measured twinning stress actually decreases slightly with decreasing temperature. Mahajan and Williams in their 1973 review suggested that b.c.c. metals have a negative dependence of twinning stress on temperature, whilst f.c.c. metals actually have a positive, albeit smaller, temperature sensitivity. However, Reed-Hill[199] emphasized the positive temperature dependence found by Bolling and Richman[194] for a b.c.c. Fe–25at%Be alloy (see Fig. 26) and after reviewing the available literature, he concluded that whenever the deformation occurs mainly by twinning, the flow stress tends to have a positive temperature dependence and a negative strain rate dependence.

In any event, if the twinning stress rises less rapidly with decreasing temperature than the flow stress, a transition to twinning can be expected. The temperature effect is likely to be most pronounced in materials (e.g. b.c.c. metals) for which the increase in (dislocation) yield or flow stress with decreasing temperature is large, and less obvious in materials such as f.c.c. metals which have yield stresses less sensitive to temperature. In the latter case, the flow stress may ultimately reach the twinning stress by work-hardening, and the transition from slip to twinning as the temperature is reduced is governed, at least in part, by the strong temperature dependence of the work-hardening rate in such materials.

In both polycrystalline specimens and pure single crystals of b.c.c. metals, the effect of temperature on the stress vs strain curve is often dramatic; Figs 23 and 24 illustrate a general tendency for the transition from slip to twinning as the main deformation mode to occur at

lower temperatures in single crystals than in polycrystals and also at lower temperatures in metals or substitutional alloys free of interstitial impurities. Similar results have been obtained for the other transition metals with a b.c.c. structure and also, in a quite different temperature range, for b.c.c. alkali metals, e.g. lithium–magnesium[193] and potassium.

Although, as already described, twinning in f.c.c. metals and alloys frequently occurs without large load drops and only after appreciable glide deformation, the contribution of twinning to the overall deformation nevertheless increases as the temperature is reduced. The first unambiguous experimental evidence for deformation twinning in a f.c.c. material[8] was made on copper deformed at 4 K, but in alloys of lower stacking fault energy, twinning at or above room temperature is quite common. In f.c.c. metals and alloys, temperature affects not only the competition between slip and twinning, but also the type of twin that is formed. Alloys with very low fault energies (e.g. 70:30 brass or Cu–8%Al) may at low temperatures undergo localized twinning on a very fine scale, and the resultant, almost homogeneous deformation becomes, in the limit, indistinguishable from the copious formation of individual faults. At higher temperatures, or with higher fault energies, conventional large twins may form with load drops in a tensile test, and localized flow of the specimen. This is indicative of a transition to a nucleation-controlled twin stress, as in b.c.c. metals. There is sometimes an intermediate range in which bands of local flow contain twins on the primary and conjugate slip systems.

Early, very careful work by Suzuki and Barrett[9] on single crystals of silver–gold alloys of varying compositions but fixed orientation established three regimes similar to those described above. Their results are shown in Fig. 30; in region I (relatively high temperatures) a localized band of twins is formed on the primary or conjugate slip planes and spreads across the specimen into two opposite quadrants. This is followed by a second band of twins on the other (conjugate or primary) planes and this band grows into the other two quadrants. Twinning is accompanied by load drops. In region II twin bands form on either the

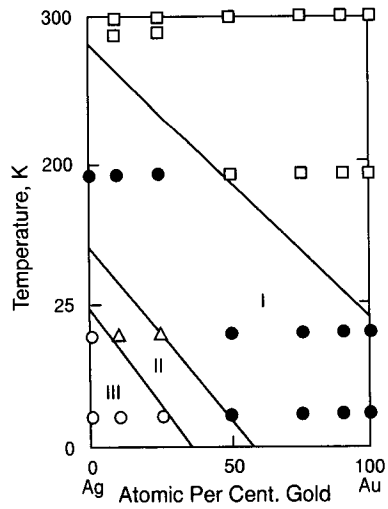

Fig. 30. Temperature–concentration diagram showing the occurrence of twinning in Ag–Au alloys. In domain I, twinning occurs on the primary slip plane. In domain II, twins are observed on the primary as well on the conjugate planes but in different regions. In domain III, the two types of twins coexist in the same region. Failure to twin in the main part of the specimen is denoted by the squares (after Suzuki and Barrett[9]).

primary or the conjugate plane in different parts of the specimen, and grow until they impinge on each other. In region III, which was found only in silver-rich alloys at low temperatures, twins form copiously on both primary and conjugate planes, as already indicated, and there are no sharp load drops. Figure 30 is a temperature–composition diagram illustrating these changes.

In general, the size of the load drop due to f.c.c. twinning increases with increasing temperature and stacking fault energy, and this may indicate an increasing ratio of nucleation stress to propagation stress. The load drops, though not usually so pronounced as those in b.c.c. materials, nevertheless make measurements of the true stress to initiate twinning very difficult. A lower yield stress for twinning can, however, be defined in circumstances where there is apparently a Luders band type deformation following the yield drop.

Twinning in polycrystalline h.c.p. metals and alloys often arises because of the lack of an adequate number of slip systems to effect an imposed strain. The measured twinning stress decreases slightly with decreasing temperature for most h.c.p. modes, except for $\{10\bar{1}1\}$ where an increase has been reported. In an investigation of polycrystaline zirconium, Reed-Hill[199] found that room temperature deformation at moderate strain rates is accomplished mainly by $\{10\bar{1}0\}$ prismatic slip and $\{10\bar{1}2\}$ twinning, together with infrequent $\{11\bar{2}1\}$ twins. At 77 K, the amount of $\{10\bar{1}2\}$ twinning was considerably increased and there were many more $\{11\bar{2}1\}$ twins and also some $\{11\bar{2}2\}$ twins. Similar conclusions by Paton and Backofen[180] were mentioned at the end of Section 4.8.

As already noted in Section 4.7, both elemental and compound semi-conductors apparently deform at low temperatures by twinning rather than slip, although the behaviour is complicated in most cases by the ductile–brittle transition. In Pirouz' model which has already been discussed, the transition to twinning is attributed to the high Peierls force and hence very low mobility of lattice dislocations at low temperatures, combined with a greater difference in the mobilities of different partials.

The slow variation of twinning stress with temperature and the prevalence of twinning at low temperatures together support the conclusion that twin nucleation is not thermally activated but rather occurs at places of high stress concentration. Once nucleated, there is evidence that over an appreciable temperature range, twins can grow more readily than slip can propagate. In very general terms, this is because partial or twinning dislocations do not become immobilized so readily as lattice dislocations, either through the intrinsically sessile nature of some core structures or because of work-hardening. Overall, twinning is a much more regulated process than is slip.

5.3. *Strain Rate*

Strain rate and temperature effects in materials science are usually coupled by an Arrhennius type equation, which is characteristic of a thermally activated process. A rapid rate of change of some property with temperature then indicates that the same property has a high sensitivity to an imposed rate, and vice versa. The expected general equivalence of high strain rates and low temperatures is certainly valid for twinning, but as already noted, the tendency to substitute twinning for slip, and the actual magnitude of the twinning stress, change rather slowly with temperature but are very sensitive to the strain rate. Indeed under shock loading or severe impact conditions, all b.c.c. and many f.c.c. and h.c.p. materials deform solely by twinning. Face-centred cubic materials with high stacking fault energies, especially aluminium alloys, do not twin under normal deformation conditions, but twinning

has been observed in shock-loaded Al–Mg alloys[11] and even, emanating from a crack, in a foil of pure aluminium.[205]

The general equivalence of low temperatures and high strain rates is also shown, in particular in b.c.c. structures, by the dislocation structures of untwinned matrix regions examined by thin foil electron microscopy after deformation. A characteristic structure after shock loading consists of a uniform distribution of long screw dislocations.[206,207] This is quite different from the tangled dislocation structures found after room temperature deformation at normal strain rates, but is very similar to the well known screw dislocation structures observed after deformation at low temperatures. As discussed in Section 4.5, the immobile screw dislocations are often assumed to dissociate into twin embryos.

As shown in Fig. 26, a twin stress which increases with increasing temperature will decrease with increasing strain rate, both changes being opposite to those observed when slip is thermally activated. Such correlated effects of temperature and strain rate have been fund experimentally in other alloys, e.g. Cu–5at%Ge.[208] Following Reed-Hill's suggestion[199] that this behaviour is always observed when twinning is the main mode of deformation, it is possible that the twinning stress always has this intrinsic dependence, but that it is masked when twinning and slip occur together and slip produces the major part of the strain.

A possible interpretation of the positive temperature and negative strain rate sensitivity was suggested by Bolling and Richman.[194] They considered that an enclosed lenticular twin must always have some accommodating slip near its edge because of the high stress concentration, and that the applied stress needed to propagate the twin will increase with an increase in this slip activity. If dislocation glide is thermally activated, as is often assumed, then the normal sensitivity to temperature and strain rate will govern the slip, but will be inverted as far as twinning is concerned.

Experiments show that individual twins frequently form with effective interface velocities which are appreciable fractions of the velocity of sound, and this makes nonsense of some of the theories of growth described above. A full understanding of why a twin can apparently form much more rapidly than a slip band is not yet available, but if dislocations are still utilized in the growth, it follows that they must have unusually high mobilities, possibly because the core structure of a twinning dislocation is very diffuse.

5.4. *Grain Size*

The lower yield stresses for both slip and twinning in polycrystalline b.c.c. metals and alloys often obey a Hall–Petch relation[209,210] of the form

$$\sigma_y^s = \sigma_0^s + k^s d^{-\frac{1}{2}} \tag{65}$$

and

$$\sigma_y^t = \sigma_0^t + k^t d^{-\frac{1}{2}} \tag{66}$$

where d is the mean grain diameter, σ_y is the yield or flow stress, σ_0 represents a friction stress opposing the motion of the dislocations or twins, and the superscripts s,t denote deformation by slip and twinning, respectively.

A conventional explanation of the usual Hall–Petch equation is based on the assumption that the slip deformation will be halted at a grain boundary until the stress acting on a near-by source in the next grain at a distance r_c^s from the head of the pileup is large enough to unpin

or otherwise activate this source. Since the effective stress acting on the dislocations is $\sigma_y^s - \sigma_0^s$, the stress at the source is $(\sigma_y^s - \sigma_0^s)(d/r_c^s)^{\frac{1}{2}}$ and at yielding or flow this must equal some critical value, σ_c^s. This gives the Hall–Petch eq. with $k_y = \sigma_c^s(r_c^s)^{\frac{1}{2}}$. The material parameter σ_c^s may be identified with the yield or flow stress needed to unpin a pre-existing dislocation source, or, to create spontaneosly a dislocation source. Clearly a similar interpretation may be advanced for a twinning stress which satisfies eq. (66).

Not all experimental results support the Hall–Petch equation and there are differences even in quite similar alloys. Vöhringer[211] found a good Hall–Petch relation for Cu–5at%Sn alloys at 295 K but for Cu–15at%Zn alloys at 77 K (over a similar range of grain sizes) the twinning stress increased linearly with d^{-1} rather than $d^{-\frac{1}{2}}$.

5.5. *Chemical Composition*

Many investigations have been made of the effects of substitutional or interstitial solutes on the twinning behaviour of single phase alloys; the results are complex and difficult to summarize, but certain important parameters have been identified. The effect of interstitial solutes in b.c.c. metals and alloys is almost invariably to decrease and ultimately to remove twinning as a deformation mechanism. As pointed out by Magee *et al.*,[212] this may be a simple consequence of the crystallography of twinning. In a disordered b.c.c. interstitial solid solution, the interstitial atoms occupy octahedral sites $\langle \frac{1}{2}00 \rangle$ and $\langle \frac{1}{2}\frac{1}{2}0 \rangle$ in a random fashion, but only 1/3 of these sites are translated directly by the shear into equivalent octahedral sites of the twinned structure. Figure 31 shows that in the absence of shuffling, the other two-thirds of the sites are carried into twin positions of type $\langle \frac{1}{4}\frac{1}{4}\frac{1}{4} \rangle$, i.e. midway between two nearest neighbour solvent atoms. If this actually happened, it would be analogous to 'pseudo-twinning' in ordered alloys, but clearly the additional energy of an

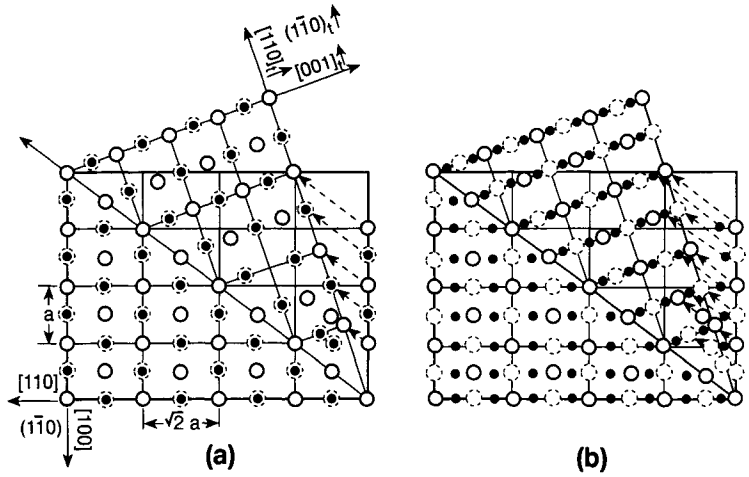

Fig. 31. The effect of the (112) twinning shear on the octahedral interstitial sites in a body-centred cubic lattice. (a) [$\bar{1}$10] projection showing only those octahedral sites which are sheared to octahedral sites in the twin. O: substitutional atoms in plane of projection; ●: possible interstitial atom positions in plane of projection; O: substitutional atoms $a/\sqrt{2}$ above (and below) plane of projection. (b) [$\bar{1}$10] projection showing the octahedral sites which are sheared to sites along the close-packed directions in the twin. O: substitutional sites in plane of projection; ●: possible interstitial atom positions $a/2\sqrt{2}$ above (and below) plane of projection; O: substitutional sites $a/\sqrt{2}$ above (and below) plane of projection (after Magee *et al.*[212]).

interstitial in such a site would be prohibitive, and when twins form in interstitial b.c.c. alloys, the presumption must be that those atoms which would be sheared to the wrong sites have to undergo shuffles in addition to the transformation shear. Whilst such shuffles appear perfectly feasible, they nevertheless represent a constraint not required of twinning in the pure solvent, so that this crystallographic circumstance may account for the inhibition of twinning and/or the increase in the twinning stress which is found experimentally in many interstitial alloys. Sites for interstitial solutes in f.c.c. and h.c.p. materials are also carried to non-equivalent sites by the twinning shear so that similar effects might be expected from the interstitial atom shuffling during twinning. However, the differences in twinning behaviour will make it more difficult to isolate the effect of a small concentration of interstitial solutes in the close-packed structures.

Substitutional solutes often increase the tendency of b.c.c. metals to deform by twinning, although the effects of different solutes are variable. The outstanding example already mentioned is that of iron–beryllium alloys with about 25at%Be, but Bolling and Richman[195] subsequently found many other alloys of iron which show a similar transition from slip to twinning as the main mode of deformation when the concentration of solute, c, exceeds a critical value which decreases with increasing values of the solid–liquid distribution coefficient, k_m, at the melting point of iron. (k_m is merely a convenient parameter for differentiating solutes on the basis of their misfit.) At room temperature, the yield stress initially increased monotonically with $c|\ln k_m|$. The initial deformation mode at 77 K was generally twinning, and as already noted, the twinning stress at this tempeerature was slightly lower than that at room temperature, but in non-ordered alloys was independent of solute concentration and type. Similar promotion of twinning is found when vanadium is dissolved in niobium[213,214] and in the group VIA metals molybdenum and tungsten, twinning is greatly enhanced by additions of rhenium,[215] the so-called 'rhenium effect'. All of these observations can be explained by the hypothesis that the substitutional solute affects the core structures and hence the mobilities of the screw dislocations.

Substitutional solutes often have a pronounced effect on the deformation twinning behaviour of f.c.c. metals, and in an early discussion, Venables found an apparent correlation between the twinning stress and the measured stacking fault energy (see Fig. 32). Such a

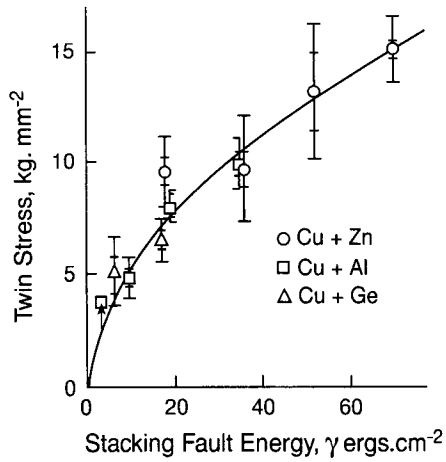

Fig. 32. The dependence of the twinning stress on stacking fault energy for copper-base alloys (after Venables[161]).

relation would be expected if the twin stress were indeed a nucleation stress, and nucleation involved either spontaneous faulting or faults produced by the dissociation of a lattice dislocation. One difficulty with this simple model is that cobalt–iron alloys with 8–9.5wt%Fe twin more readily, at equivalent strains, than many copper alloys,[216] even though the latter have lower stacking fault energies. A possible reason is that twinning in f.c.c. is favoured not specifically by low fault energy but by a tendency to planar slip. The works of Gerold and Karnthaler[217] and of Hong and Laird[218] show that planar slip is prominent in alloys which exhibit short range order and/or clustering, as well as in those of low fault energy. A correlation of twinning with planar slip might well be expected from models which postulate single or coplanar slip on the currently active slip plane.

Both elemental and compound semi-conducting materials are brittle at low temperatures, but they may often be induced to deform plastically under a confining pressure, a method which was first used successfully for minerals.[219] This method has been used recently to study the effect of doping on the mechanical properties of GaAs single crystals.[15,220,221] Figure 33(a) shows stress vs strain curves at various temperatures for intrinsic GaAs crystals oriented for single slip, whilst Fig. 33(b) shows comparable curves for n- and p-type crystals doped with $2.2 \times 10^{24}\ m^{-3}$ atoms of Se and 2×10^{24} atoms of Zn, respectively. The stress required to deform the intrinsic compound is very dependent on the temperature, as is expected since the covalent and ionic bonding will result in a high Peierls–Nabarro force, but there are also marked differences between the p- and n-doped crystals, deformed under comparable conditions of temperature, grain size, etc. (see Fig. 33(b)). Auxiliary experiments[220] have shown that the higher stress levels of the p-type crystals are not due to the constrained testing. Similar tests have also been made on isoelectronic substitutions, such as In and these show that such crystals are softer than the intrinsic crystals which themselves are softer than the p-type crystals.[15]

Transmission electron microscopy shows that in the zinc-doped crystals and to a lesser extent in the intrinsic material, twinning on the primary {111} slip plane co-exists with slip, and the twinning shear in the $(1/6)\langle\bar{2}11\rangle$ direction was confirmed by measurement of surface tilts.[15] On the other hand, no twins ere found in the indium-doped and n-type crystals. As

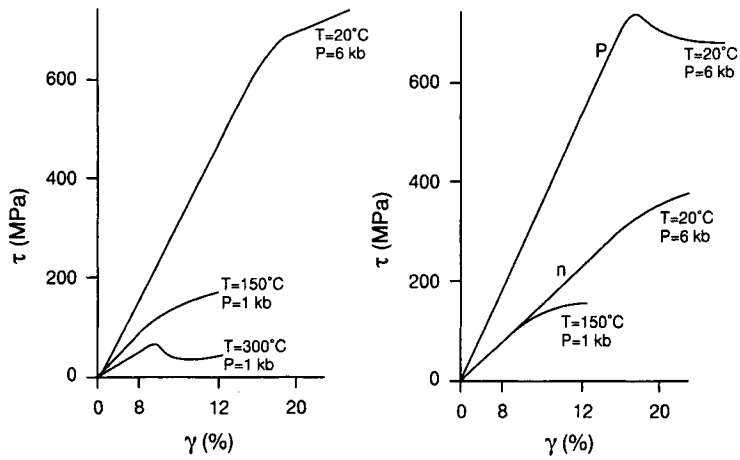

Fig. 33. (a) Stress–strain curves under confining pressure for intrinsic GaAs oriented for single slip ($\epsilon^* = 2 \times 10^{-5}\ s^{-1}$). (b) Stress–strain curves under confining pressure for n- and p-type GaAs oriented for single slip (after Boivin *et al.*[220]).

discussed in Section 4.7, these differences may be due to changes in the relative mobilities of different partial dislocations induced by doping, but the measurements[178] indicate that the mobility difference is smaller in the p-doped crystals than it is in the n-doped crystals. It may be that cross-slip is inhibited in the p-doped material and the fine planar slip then leads to twin formation by a coplanar mechanism.[158]

5.6. *Prestrain*

Numerous observations show that twinning in iron,[201,202,222,223] niobium[151,190,224,225] and chromium[210] can be suppressed by a strain previously applied at a higher temperature. The formation of shock twins in iron[226,227] and molybdenum[228] can also be suppressed by prestraining, and a comparison of these results with those of Rosenfield *et al.*[229] shows that the amount of prestrain needed to suppress twinning depends on the strain rate subsequently imposed. The twinning behaviour of prestrained iron can be restored by aging.[226,229]

Boucher and Christian[151] examined the effect of dislocation substructure on the twinning behaviour of niobium crystals and found (i) after very small prestrains of the order of 0.5%, more twins were observed than in the crystals which were not prestrained, (ii) the prestrain required completely to suppress twinning at 77 K is smaller when the substructure produced is a homogeneous distribution of screw dislocations, and larger when the distribution is heterogeneous, and (iii) the prestrain to suppress twinning also depends on the final testing temperature, and increases as the testing temperature decreases. A discussion of these results led to the conclusion that the principal effect of the existing substructure is to inhibit twin growth. However, the experiments of Mahajan[227] on the shock loading of heavily prestrained iron showed that the substructure causes fragmentation of twins but does not appear to affect their growth rate significantly. On this basis, prestrain inhibits nucleation rather than growth. It is also possible that the homogeneous dislocation substructure led to very fine twins which escaped detection, rather than to elimination of twinning.

5.7. *Precipitates and Second Phase Particles*

The influence on the twinning behaviour of the size, distribution and volume fraction of second phase particles, as well as that of factors such as the coherency of the interphase interface has not been systematically investigated. Interstitial elements in excess of their solubility limits, tend to suppress twinning in niobium.[230] Aging or precipitation in many other alloys, e.g. Ti–5.1wt%Zr,[230] also leads either to delay in formation or to suppression of twinning. In some cases, part of this effect is undoubtedly due to the difficulty or impossibility of propagating a twin across a partly coherent or incoherent boundary, and part may be due to the complex dislocation structures produced when the composite begins to deform. Mahajan *et al.*[152] investigated the deformation of a spinodally-decomposed iron–chromium–cobalt alloy, and found that after aging inside the spinodal, microtwins formed during subsequent deformation at ambient temperature.

The suppression of twinning by incoherent b.c.c. particles has been compared to that by pre-strain, since rather similar dislocation substructures are formed around the particles. Mahajan *et al.*[152] have suggested a more elaborate explanation of the microtwinning in the spinodally decomposed alloy; this twinning is attributed to differential friction stresses (or Peierls–Nabarro forces) in the Cr- and Fe-rich regions. According to Gray,[1] thoria particles dispersed in nickel also prevent twinning, even under shock-loading conditions. However,

rather opposite results are quoted by Gray for twinning in Fe–4.6at%Be alloys. In the initial stages of precipitation, when finely dispersed clusters have formed, twinning is completely suppressed, but twins pass apparently unimpeded through isolated $FeBe_2$ particles when these have formed at a later stage of precipitation.

6. TWIN ACCOMMODATION, TWIN-SLIP AND TWIN–TWIN INTERACTION

6.1. *Twins Terminating Within a Crystal*

Very high stresses are generated in the immediate vicinity of a deformation twin which is confined within an externally stressed crystal or a polycrystalline aggregate. These stresses and the associated strain energy arise from the resistance of the matrix to the macroscopic change of shape in the twinned volume. If the surrounding matrix is either defect-free or sufficiently strong, the twinning shear may be accommodated without any plastic deformation, and this leads in the ideal case to the phenomena of elastic twinning and pseudo-elasticity,[3,20,21,231,232] which have been described in outline in Section 5.1 (see Fig. 27). Strains much larger than normal elastic strains are produced by twin formation as a specimen is loaded, and are then removed again spontaneously, albeit with some hysteresis, on unloading, during which the twins shrink and eventually disappear. The elastic twinning of calcite and of some non-metallic compounds was extensively studied in the early Russian work of Garber and his coworkers,[16] and was comprehensively reviewed by (R.W.) Cahn.[3,4] Twinning in minerals was later reviewed by Turner[17] and further work on calcite was described by Williams and Cahn.[231] Most metals are too soft for elastic twinning, but it has been detected in antimony, bismuth, and zinc by Startsev and Kosevich[232] and also in tin.[233] A related phenomenon, the formation of thermoelastic martensite, has been widely studied, especially in 'shape memory' alloys. Thermoelastic martensite, was discovered and discussed by Kurdjumov and Khandros;[234] in addition to the stored elastic energy, there is a chemical contribution to the driving force for removal of strain on unloading. As already emphasized, 'pseudo-twinning' in ordered alloys is properly regarded as a special type of martensitic transformation and the resultant chemical term (i.e. the extra energy of the incorrectly ordered 'twin') may thus facilitate super-elastic behaviour as shown in Fig. 27. Elastic twinning in some minerals may also actually be due to formation of pseudo-twins as has been suggested for certain feldspars.[235]

If a twin is formed without substantial plastic flow, the magnitude of the stress field may be calculated approximately from the well known linear elastic model of an inclusion developed by Eshelby.[128] An isolated, plate-shaped twin is most conveniently modelled as an oblate spheroid, and the elastic energy of the constrained system per unit volume of twin (Section 4.1) is then approximately equal to $\mu(y/R)s^2$. The most important component of the elastic stress field is the shear stress resolved on the plane and in the direction of the twinning shear. Both in the plane of the plate and in the central plane normal to $\boldsymbol{\eta}_1$, this is the only non-zero stress component, and for any aspect ratio its value in the matrix tends to infinity as the tip of the plate in the $\boldsymbol{\eta}_1$ direction is approached. The resolved shear stress in the plane through the centre of the plate normal to $\boldsymbol{\eta}_1$ is negative up to a distance of the order of R, after which it becomes positive if y/R is adequately large. Thus, as is physically obvious, the field of an enclosed twin tends to reduce the sharp discontinuity in shear strain either by further extending the twin in its own plane or by inducing slip ahead of the twin in a direction or directions close to $\boldsymbol{\eta}_1$. On the other hand, in the matrix close to the centre of the twin plate, the stress field opposes the twinning shear, i.e. it favours an additional shear

on, as nearly as possible, the same system but oppositely directed. In general, this reverse shear may be accomplished only by slip, since twinning is uni-directional and reverse twinning is not possible. If some accommodation of this kind is feasible, the average shape change across the twin edge is near zero.

Eshelby treated the twin and matrix as linear-elastic objects, and this is difficult to justify in view of the rather large strains involved, especially in cubic twinning. An alternative method of calculation is based on the Orowan model of a twin (Fig. 9). Provided the angle of taper is small, the stress field may be attributed to a single or double pile up of circular or elliptic loops of twinning dislocation. Unfortunately, the mathematical equations arising from this configuration do not have convenient analytical solutions and it is necessary to resort to numerical methods in order to make quantitative predictions.[236,237] In principle, the most reliable estimates should be obtained from a computer model of a tapered, enclosed thin twin, but with realistic interatomic potentials this would probably be formidably difficult and expensive in computer time.

The pile-up model of a blocked twin has very recently been criticized by Müllner and Solenthaler,[238,239] who suggest that such a twin will not have a lenticular shape. Their alternative proposal is that straight twinning dislocations in edge orientation will be aligned in a planar array, forming an incomplete wall, normal to $\mathbf{K}_1$ and to $\boldsymbol{\eta}_1$. They consider first whether the maximum repulsive force acting in the glide plane between the first two dislocations of a tapering twin can be overcome by the stress field acting on the second dislocation. This field is the resultant of the applied stress and the effective pile-up of all the subsequent twinning dislocations. A numerical example suggests that for an austenitic steel, the shear component of the applied stress acting on the $\mathbf{K}_1$ plane and in the $\boldsymbol{\eta}_1$ direction must exceed about 125 MPa if there are ~ 50 dislocations in the pile-up and 12.5 MPa if there are 500 piled-up dislocations. (The number of lattice planes is of the order of 500 for twin lamellae of observed thickness ~ 100 nm.) It follows that the second dislocation should be able to overcome the maximum repulsive force with a pile-up of ~ 60–70 dislocations at an applied (tensile or compressive stress) about one-half of the experimental yield stress of ~ 200 MPa. The authors then assume that if the second dislocation overcomes the repulsion of the leading dislocation, most of the other dislocations will follow it, so that the pile-up will be converted into an (incomplete) wall. An appropriate description of such a blunt-ended configuration is a wedge disclination dipole rather than a dislocation pile-up.

In a second paper,[239] an attempt is made to estimate what fraction of the total number of twinning dislocations enter the wall. For N dislocations, of which M are within the wall, the force between the wall and the $(M + 1)$th dislocation may be equated to the pile-up force of the $(N - M - 1)$ remaining dislocations, and the authors conclude that over 80% of the dislocations will be in the wall. They also believe that this change of predicted shape may have a large effect on, for example, twin–twin intersection processes.

There are some difficulties with this model. The authors themselves point out that the maximum force is calculated to occur at a very small distance from the edge of the wall, so that linear elastic theory should not apply, and also that the use of the pile-up model overestimates the forward stress on the dislocation just outside the wall. They claim, without any detailed justification, that these effects balance to give a small residual error. Another difficulty is that the force between the wall and the next twinning dislocation is entirely repulsive in the final equation and the maximum force occurs at a distance which is independent of M. These defects possibly appear because the calculations were made with the assumption that the last dislocation of the wall and the first one outside it are on the same slip plane rather than on immediately adjacent planes. A rather similar recent

calculation by Kamat and Hirth[240] dealing with the formation of multiple height ledges in phase transformations gives similar results for the maximum elastic force but shows correctly that the force becomes attractive at very small distances, so that the wall configuration is metastable in the absence of stress, and the stress needed to add a further dislocation to the wall increases with the height of the wall, i.e. with M.

However, the greatest difficulty in adopting this model is that it is valid only for straight edge dislocations; a single set of screw dislocations does not form a low energy configuration of this kind, and so the model seems to imply a rectangular twin plate with planar edges normal to η_1 and tapering edges parallel to η_1. This morphology has not been reported, but it presumably would only develop when the growth parallel to η_1 was halted by an intersecting twin or some other obstacle. Twin–twin intersection is discussed in terms of this model in Section 6.3.

Whether or not plastic accommodation actually occurs depends on a number of material parameters, notably the magnitude of the twinning shear, the yield stress and the elastic stiffness appropriate for shear on $\mathbf{K}_1$. Ling and Owen,[241] considered the similar problem of the martensitic transformation in Fe_3Pt alloys, and used a von Mises' yield criteria to plot contours showing the regions of the matrix which would yield for given degrees of long-range order, since the above parameters change appreciably with the order. Figure 34 shows calculated yield contours for an ellipsoidal plate with varying degrees of long range order (S) and aspect ratios. For $S = 0$, yield occurs all round the plate, even for aspect ratios as low as 0.02, and this is the expected condition for a high shear twin in a soft matrix. For high values of S, i.e. a relatively strong matrix, plastic deformation is confined to a very small region around the sharp edge of the plate, and may not occur in practice, thus giving thermoelastic transformation or elastic twinning.

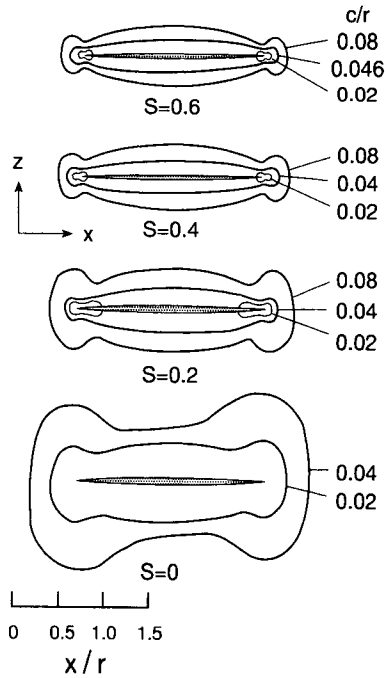

Fig. 34. Matrix yield stress contours of an oblate spheroidal plate of Pt_3Fe lying in the x, y plane with the transformation shear in the x direction (after Ling and Owen[241]).

The pioneering work on plastic accommodation ahead of the twin came from Sleeswyk[109] who first developed the well-known theory of emissary slip (Fig. 35). He pointed out that in a b.c.c. structure, every third twinning dislocation with a Burgers vector $\frac{1}{6}\langle 111\rangle$ could, in principle, dissociate into a lattice dislocation with a Burgers vector $\frac{1}{2}\langle 111\rangle$ and a complementary dislocation with a Burgers vector $\frac{1}{3}\langle \bar{1}\bar{1}\bar{1}\rangle$ vector (see eq. (37)). If the lattice dislocation now glides into the matrix on the $\mathbf{K}_1 = \{\bar{2}11\}$ plane, which is a quite common slip plane in b.c.c. structures, it leaves three adjacent elementary steps in the twin interface, two of which are twinning dislocations and the third is the complementary dislocation. These three steps thus have zero net Burgers vector, and they may combine to form a "pure step" with no observable shape discontinuity across the three planes. Repetition of this process every three

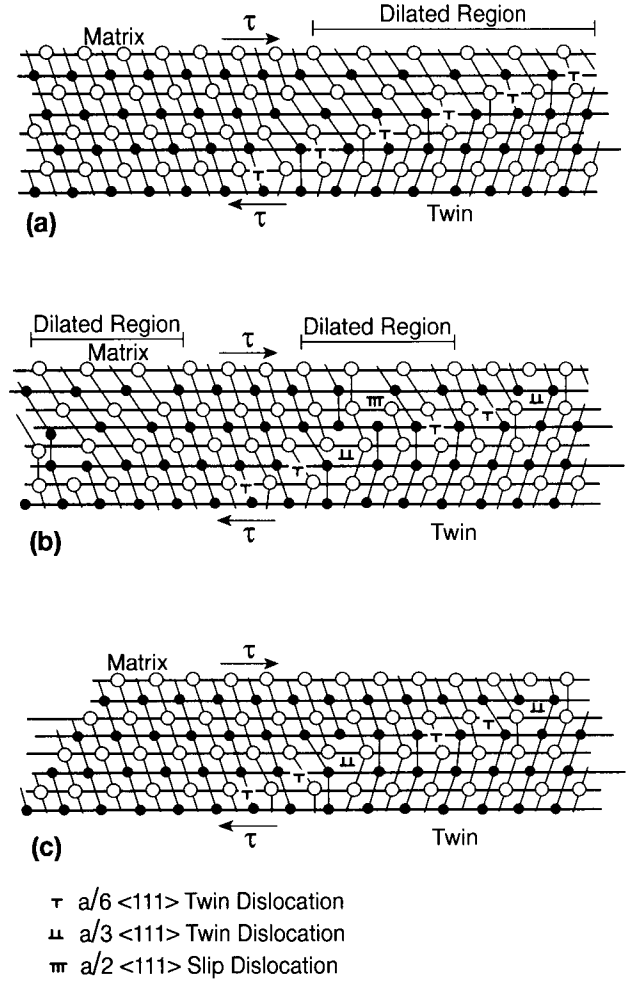

Fig. 35. Dissociation of a non-coherent twin boundary in the b.c.c. lattice (after Sleeswyk[109]). Two layers of atoms are projected on a $\{1\bar{1}1\}$ plane. In (a), the boundary between twin and matrix is represented as an array of $\frac{1}{6}\langle 111\rangle$ twinning dislocations on successive $\{112\}$ planes. In (b), the dissociation has produced slip (emissary) dislocations which move away from the boundary under the influence of the stress, and 'complementary' $\frac{1}{3}\langle \bar{1}\bar{1}\bar{1}\rangle$ type twinning dislocations. The residual boundary shown in (c) has one complementary dislocation to every two twinning dislocations, and produces no far-reaching strains in the lattice.

planes will lead to a terminating twin with no shear discontinuity across that part of its edge from which slip dislocations have been emitted. The discontinuity has, in fact, been transferred to the matrix surface which forms the limit of the slipped region.

According to Frank's rule, reaction (37) is energetically unfavourable, but the Frank stability criterion is unlikely to be applicable to a dissociation entirely within the core structure of the interface. Although it was noted in Section 3.2 that an isolated complementary dislocation is probably unstable, this need not apply to a complementary dislocation flanked on each side by an elementary twinning dislocation. An apparent slight modification of Sleeswyk's dissociation was a suggestion by Hull[209] that three adjacent twinning dislocations could associate to form a triple step, and their Burgers vectors could combine to form the $\frac{1}{2}\langle 111\rangle$ type emissary dislocation, leaving a triple step with no Burgers vector. However, this is not really distinguishable from Sleeswyk's proposal that the three single steps are aligned normal to $\mathbf{K}_1$ following the formation of the emissary dislocation; the two final configurations of the pure step will be identical. Moreover, repetition of this reaction every three steps over a relatively large distance, will allow all the steps to be aligned and thus to form a stress-free facet normal to $\mathbf{K}_1$. There is an alternative reaction in which a lattice dislocation of opposite Burgers vector is emitted from a matrix source, or is created spontaneously as a dipole or a closed loop. If the $\frac{1}{2}\langle\bar{1}\bar{1}\bar{1}\rangle$ dislocation travels towards the twin and eventually combines with one of the twinning dislocations to give a complementary dislocation, the final configuration is indistinguishable from the emissary model. However, the probability of the matrix dislocations being nucleated at exactly three plane intervals must be very low, so that if this is the physical mechanism, the slip shear will only approximately equal the twinning shear. The final shape change occurs around the periphery of the combination of twin + slipped region, as indicated in Fig. 35.

The transfer of the shear discontinuity from the limit of the twin to another internal surface may not greatly reduce the strain energy, and for an isolated, stopped twin, a substantial reduction can only be accomplished if the emissary dislocation, or the other half of a dipole or loop, continues to move until it encounters a free surface (or, possibly, an incoherent, high-angle grain boundary). This produces the familiar tilting of the surface and allows much of the strain energy to be released.

When it is mechanistically possible, plastic accommodation by reverse shearing of a region adjacent to the twin is also efficient in reducing the strain field. In some martensitic transformations, there is a near degeneracy in the crystallography such that adjacent, nearly parallel plates may have nearly opposite shape changes so that their fields largely cancel. Ling and Owen found that in a case where the entire matrix adjacent to the surface of an isolated partly ordered plate of Fe_3Pt of given aspect ratio (would yield plastically), yielding would be confined to a small region close to the extreme tip when two such plates were side by side and in contact along their central planes normal to $\boldsymbol{\eta}_1$. The yield region is further reduced when more plates are added, thus making eventually a parallel array of plates with common $\mathbf{K}_1$ interfaces. As explained above, it is not possible to form twins with oppositely directed shears, but a closely-related effect is found in many martensitic transformations in which the product regions consist of arrays of parallel mutually twinned regions with (on average) a fixed ratio of twin volume to matrix volume. The function of these twins is to combine the deformation obtained from the lattice change with the volume averaged twinning shear in order to obtain an average macroscopic deformation which is an invariant plane strain, as required by the crystallographic theory of martensite. Twinning and detwinning in such arrays is often important in thermoelastic deformation and pseudo-elasticity.

Returning to the case of the isolated twin, it was recognized long before Sleeswyk's work that side by side accommodation can result from slip or in certain cases kink band formation. Figure 36 illustrates some of the possible effects.

In b.c.c. crystals, the slip and twinning directions coincide and the $\mathbf{K}_1$ plane is a frequently observed slip plane; this simplifies the problem of plastic accommodation and makes it possible to envisage exact continuation of the twinning shear. Figure 37 due to Sleeswyk provides evidence for the propagation of the shear forward from a stopped twin; a sub-boundary ahead of the twin acts as a 'marker' and is seen to have been sheared. However, extensive studies have shown that although slip at the tips of twins in b.c.c. materials is frequently observed, the actual accommodation processes may be more complex. Hull[104] found that in silicon–iron the slip direction was always the same as the twinning direction, but the slip frequently takes place on the {110} type planes containing this direction. In a detailed study of slip patterns in a Mo–35at%Re alloy, Mahajan[106] found evidence for both simple emissary slip on the twinning plane, as in the Sleeswyk model, and for slip on two planes which was then not confined to the region directly ahead of the twin. However, the slip near some twins was much more complex and dislocations with Burgers vectors not parallel to the twinning direction were involved.

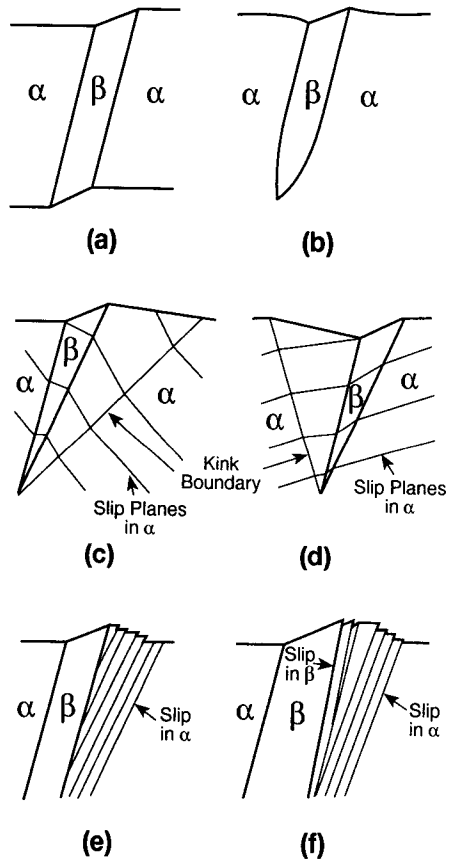

Fig. 36. The accommodation of the shape change due to twin formation (schematic): (a) unconstrained twin forming in a single crystal; (b) lenticular twin accommodated elastically in the matrix; (c) and (d) accommodation by kink boundaries in matrix; (e) accommodation by slip in the matrix; (f) accommodation by slip in matrix and twin. The twin is labeled β (after Christian[20]).

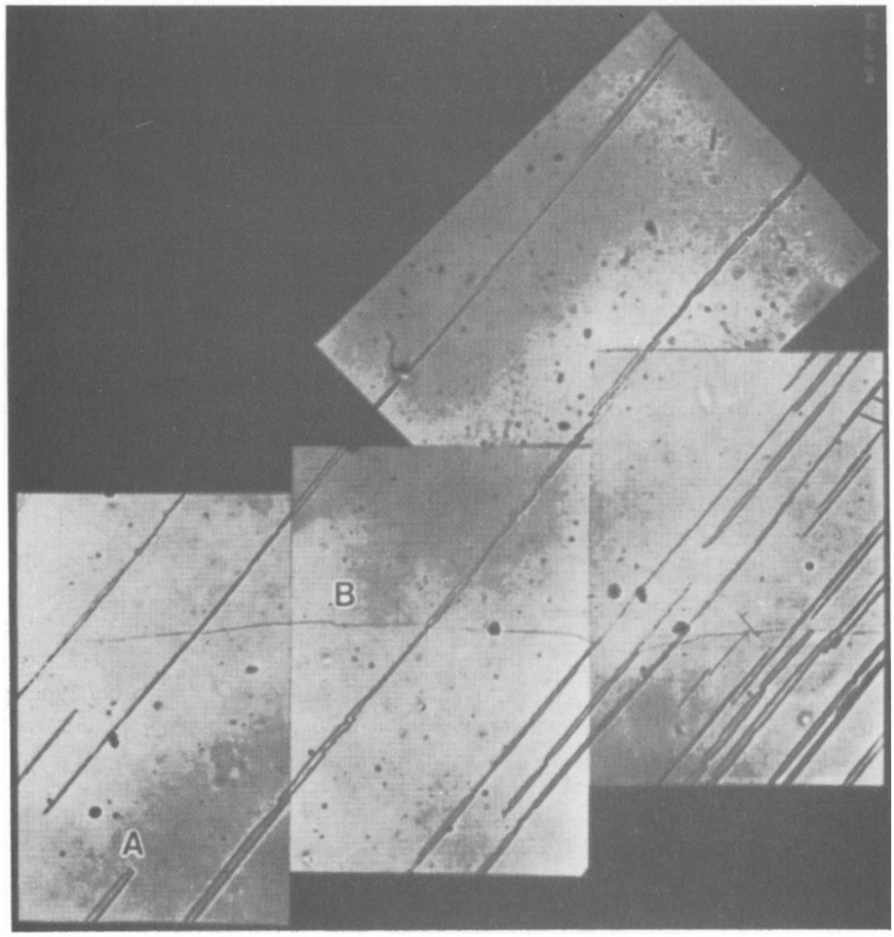

Fig. 37. Deformation twins formed in pure Fe during compression at 77 K showing the displacement of a subboundary of B ahead of a twin which has stopped at A (after Sleeswyk[109]).

The theory of emissary slip implies a physical separation of the shape change associated with twin formation and the change of lattice orientation. Sleeswyk considered separation during growth, so that two distinct interfaces, one representing a shear strain discontinuity and the other an orientational discontinuity, move independently through the parent crystal as it is consumed by the twin. However, if the emissary slip has been efficient, there will be virtually no driving force to displace the true twin (change in orientation) boundary. This growth model thus seems less probable than the alternative assumption that emissary slip is initiated only after the twin interface has been halted.

The general shape of the twin boundary may be expected to be either a doubly convex or a plano-convex lens, as shown in Fig. 38, and evidence for these types of twin has been obtained by Sleeswyk for iron and and by Votava and Sleeswyk[242] for molybdenum–rhenium alloys. However, some twin shapes are observed to be much less regular, possibly as a result of obstacles which hold up the twin–matrix interface in a local region. Figure 39 shows how, by removing the stress field of the interface, emissary slip allows irregular morphologies to develop with only small energetic penalties. Slightly different results were

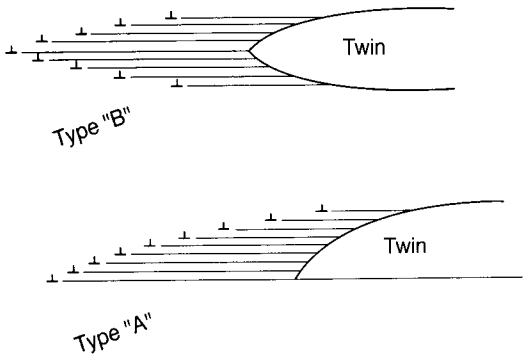

Fig. 38. To illustrate the two types of emissary dislocation array and associated twin front observed in α-iron and molybdenum-rhenium alloys (after Votava and Sleeswyk[242]).

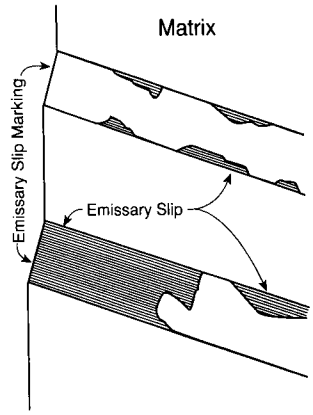

Fig. 39. Schematic drawing to show that twins may occupy only parts of the regions of emissary slip (after Sleeswyk[109]).

obtained by Hull,[104] probably because he studied silicon–iron alloys which slip mainly on {110} planes rather than {112} planes. He found that even in the ideal case where a twin traversed the entire cross-section of a single crystal, only one of its two interfaces was completely planar. The other interface intersected the free surface in a series of zig-zag markings (see Fig. 40) which Hull showed were the traces of {110} + another type (possibly {112}) slip planes. This morphology results when the appropriate interface is halted just below the free surface and its stress field is relieved by matrix slip, on the protruding side of the tilted surface.

Although the crystallography may be more complex, the phenomenon of emissary slip has been observed in other crystal structures, and as detailed by Mahajan and Chin[243] should be of general application except when the twinning shear is very small. For f.c.c. materials, the twinning $\mathbf{K}_1$ plane is the normal slip plane, but slip has never been observed in the $\boldsymbol{\eta}_1$ direction. However, the equivalent of $\langle 11\bar{2}\rangle$ emissary slip is obtained if two slip dislocations with Burgers vectors $\frac{1}{2}\langle 10\bar{1}\rangle$ and $\frac{1}{2}\langle 01\bar{1}\rangle$ glide away from each three-plane group at the twin tip. Mahajan and Chin[243] have analyzed the slip structures ahead of twins in thin foils of a Co–Fe alloy and found them to be equivalent to resultant slip on the twinning plane. The same result was obtained by Vaidya and Mahajan[187] for $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins in single crystals of hexagonal cobalt. Accommodation by primary kink bands, formed from arrays of basal plane dislocations, as shown in Fig. 36, is very common in h.c.p. metals[244–247] and

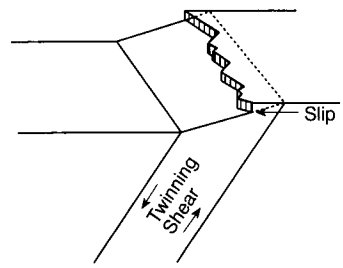

Fig. 40. Schematic representation of the shape of the serrations that may develop at the surface due to emissary slip when a twin terminates below the surface (after Hull[104]).

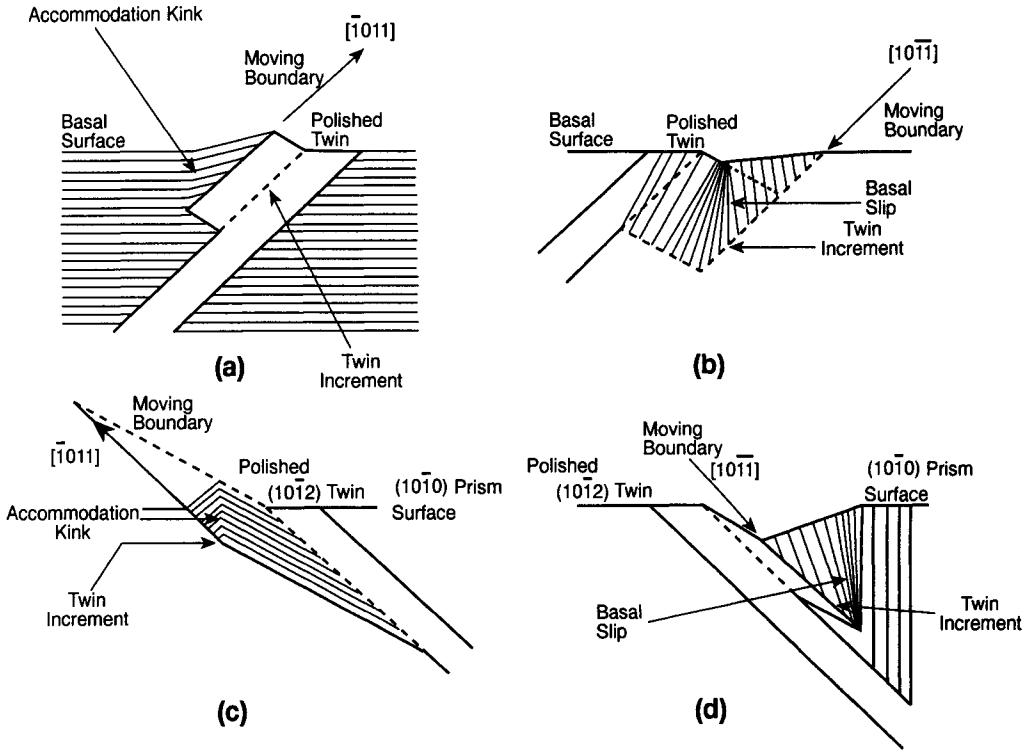

Fig. 41. Schematic diagram in the plane of shear illustrating the form of accommodation of a $(10\bar{1}2)$ twin; the angles and surface tilts are exaggerated. (a and b) Movement of opposite twin boundaries as observed on an (0001) surface. (c and d) Movement of opposite boundaries as observed on a $(10\bar{1}0)$ surface (after Roberts and Partridge[249]).

in some cases there are several kinks each corresponding to an abrupt change in twin thickness below the surface. Secondary kinks formed from non-basal plane dislocations[248] are also commonly observed.

Roberts and Partridge[249] made a very detailed study of the accommodation around individual $\{10\bar{1}2\}$ twins and interacting pairs of $\{10\bar{1}2\}$ and $\{\bar{1}012\}$ twins in magnesium, and found that the accommodation depends on the position of the moving twin boundaries and on the orientation of the free surface. As in the silicon–iron crystals studied by Hull, opposite boundaries of a single twin behave differently as a free surface is approached. On one side of the twin, the surface tilt is accommodated mainly by $\{10\bar{1}0\}$ kink bands in the matrix, but on the other side, the principal accommodation is by basal slip within the twin (see Fig. 41). Two interacting twins were found to grow independently if each was able to utilize its own accommodating deformation, but when one twin effectively blocked the other, additional kink bands were formed inside the obstacle twin which ultimately led to the twins being in contact over a common surface.

6.2. *Interaction Between Slip and Twinning*

A growing twin which encounters a pre-existing slip line or band with few remaining dislocations will presumably propagate unhindered through the slipped region. If the slip extends to a free surface, the slip traces (like any other fiducial marks) will be deviated into

a new orientation in the twinned region. This is the basis for one standard method of measuring the twinning shear. If, however, the slip band is work-hardened, i.e. if it contains dislocations, the twin may have difficulty in penetrating it, and when penetration does occur, the individual interactions of dislocations with the twin interface have to be considered.

An external slip-band or a growing twin may first encounter an obstacle twin, B, either along the notionally flat matrix–B interface or along the edge or rim of B. Edge to edge encounters will be rare if the in-plane growth velocity is high, as is often the case. When edge-to-edge intersection does occur, the incident lattice or twinning dislocations may wrap around the barrier twin (if it is not too thick) and hence form pile-ups pressing against both faces of B. Equally, a slip-band or a twin meeting a planar interface of B not too far from the edge of B may wrap around this edge and so form a pile-up on the opposite face. Thus with either initial configuration, interactions with both the fully coherent $\mathbf{K}_1$ interfaces and the edge of B may have to be considered. In some cases edge to edge intersection may lead to branching of the twins. However, the major part of the published theoretical and experimental work deals only with propagation of slip or twinning across the planar $\mathbf{K}_1$ interface.

The systematic treatment of this problem, and of its frequently considered inverse, the penetration of slip dislocations into a twin which forms an obstacle in the path of the slip, began with the work of Sleeswyk and Verbraak.[250] A pinned dislocation line which is engulfed by a growing twin will be reorientated within the twin because of the twinning shear; an obvious assumption is that the new direction of the dislocation line and its new Burgers vector are the corresponding direction and vector produced by the lattice deformation **S**, and this means that the slip plane in the twin will be the plane corresponding to the parent slip plane. As mentioned previously, it is also possible that the twin interface will cause the dislocation to dissociate into other dislocations, and various possible reactions are discussed below for the inverse process in which a gliding dislocation crosses a stationary twin interface. Many such reactions are energetically unfavourable and in the absence of a sufficient stress concentration, the matrix dislocation might then act as an obstacle to the continued growth of the twin. Under these circumstances, a highly dislocated region may lead to fragmentation of the twin, i.e. islands of untwinned region, as is frequently observed in b.c.c. materials. Sleeswyk proposed that this might be a result of emissary dislocations bypassing the obstacle, leaving shear loops around it, and the model is obviously similar to that of Fig. 39 for the production of twins with irregular shapes. A difficulty arises when the Burgers vector of the dislocations is not parallel to the composition plane of the twin so that they cannot cross-slip on to this plane, and the propagation of the twin would then result in a high jog density. Mahajan[207,227] suggested that this difficulty could be avoided if the propagating twinning partials loop around the deformed regions, and that this was the reason why fragmented twins are frequently observed in some materials.

Consider now the penetration of an existing twin by slip dislocations of the matrix. It is immediately obvious that slip is unlikely to continue undeviated into the twin since even in cubic structures the original slip plane and direction do not constitute a physically convincing, atomic slip system in the twinned lattice. For example, if a dislocation with a Burgers vector of $\frac{1}{2}\langle 110\rangle$ gliding on a $\{1\bar{1}\bar{1}\}$ plane of a f.c.c. matrix were, without dissociating, to cross the $\{111\}$ composition plane of a twin, its slip plane would then be $\{\bar{5}11\}$ and its Burgers vector $\frac{1}{6}\langle 114\rangle$ referred to the twin basis. (There are, however, some exceptional cases where there is experimental evidence that slip inside twins has been forced to take place on physically improbable systems.) Sleeswyk and Verbraak considered dislocation–twin interactions in

b.c.c. materials, with the assumption that the matrix slip plane, like the $\mathbf{K}_1$ plane of the twin, is of type {211}, and they showed that a lattice vector of the parent may dissociate into a lattice vector of the twin (with reasonably low indices) plus a number of elementary twinning dislocations. Note that if the twin is considered just as an obstacle, it is irrelevant whether it is a deformation, an annealing or a growth twin, provided they all have interfaces with identical atomic structures. Variation in the orientation of the applied stress will thus allow any slip band to interact with a twin of particular orientation. However, a deformation twin which has formed under the same applied stress as that which is now responsible for the slip will probably be subject to matrix slip on only a limited number of systems, namely those for which the resolved shear stress has the same sign as that producing the twin.

Sleeswyk and Verbraak considered only Burgers vectors, and thus failed to recognize an important geometrical constraint on the slip plane in the twin; if a dislocation is to glide into the twin on some plane, thus continuing to propagate at least part of the original matrix slip shear, the slip planes in matrix and twin must intersect the twin–matrix interface along a common direction which is the orientation of the dislocation as it crosses the interface. A systematic general theory, applicable to all crystal structures was given by Saxl.[182–185] Much of the theory is implicit in the early work on pole-mechanisms, so that the following description may be considered along with the previous accounts in Sections 4.3, 4.4 and 4.6.

It is useful first to distinguish one special case of slip across a twin boundary, namely when the Burgers vector of the slip dislocations, $\mathbf{b}_A$, is parallel to the twin interface and hence to the line of intersection of the slip and twinning planes. The dislocations then encounter the interface in screw orientation, and they may (geometrically) cross-slip into the twin on any plane in the zone of $\mathbf{b}_A$ without leaving a step in the interface. The Burgers vector in the twin has the same matrix representation as in the matrix, or is trivially reversed, depending on how the orientation relation is defined, i.e. how the twin axes are labelled. (Rotations IV or II of eq. (6) are generally preferred to reflections, I or III, in order to keep both sets of axes 'right-handed'.)

In all other cases of slip propagation, the component of $\mathbf{b}_A$ normal to $\mathbf{K}_1$ means that a step must be produced along the length of an originally flat interface which has been crossed by a dislocation. If the dislocation glides into the twin, the only geometrical restrictions are that it must do so on some plane in the zone of the line of intersection and that it must have a Burgers vector which is a lattice vector in that plane. The original Burgers vector must thus dissociate to give a new slip vector within the twin, and in this case the step at the interface will be a twinning dislocation with a Burgers vector equivalent to an integral number of elementary twinning dislocations;[182–185] this follows simply since the components of the slip vectors in parent and twin normal to $\mathbf{K}_1$ are equal. For a type I (or compound) twin, one of the geometrically possible slip planes in the twin is the mirror image in $\mathbf{K}_1$ of the matrix slip plane, and these two planes are thus crystallographically equivalent. Similarly, for a type II twin, a plane with the same crystallographic indices as the primary slip plane is obtained by a 180° rotation about $\boldsymbol{\eta}_1$. (Note that types I and II are here distinguished solely on the basis of the orientation relations in order that the result be not confined to deformation twins.) For both orientations, this symmetry-related twin plane is likely to be the preferred slip plane provided the angles between slip and twinning planes and directions are not too large to permit an external stress to give a reasonably large resolved shear stress on each system. Another possibility is that slip in a deformation twin will be on the plane and in the direction specified by the lattice corespondence. However, the correspondence has special

significance only if the twin is actually growing; a {111} f.c.c. twin interface, for example, might represent an annealing twin or any one of three possible deformation twin variants. In general, the matrix slip plane and the plane in the twin which is related to it by the lattice correspondence will only be crystallographically equivalent planes when the slip plane is actually the $\mathbf{K}_2$ plane or the slip direction is the $\boldsymbol{\eta}_2$ direction of an appropriate deformation twinning mode. Corresponding slip was represented in eq. (51) where the dislocation has Burgers vector $\mathbf{b}_A$ in the matrix, and $\mathbf{b}_B$ (the corresponding vector to $\mathbf{b}_A$) in the twin. The remaining dislocation $\mathbf{b}_T$ is then a step in the coherent twin interface representing an elementary or zonal twinning dislocation of the deformation mode with the assumed correspondence. This situation was discussed by Saxl who emphasized that for $q > 2$, a lattice vector of the parent may have a corresponding vector which is only a partial lattice vector of the twin, so that in order to continue the slip, an integral number of parent dislocations must combine to produce a single glissile dislocation in the twin. When this condition is satisfied, the step left in the interface necessarily represents a zonal rather than an elementary twinning dislocation. The twinning dislocation must remain in the interface but must move away from the original line of intersection if successive dislocations of a pile-up are to penetrate into the twin. As it moves away, the twin, over the area swept, increases or decreases in thickness by the step height. If a limited length of dislocation crosses into the twin, the twinning dislocation may rotate about either or both crossing points, and the configuration is that of a generating node, as already discussed. If the dislocation $\mathbf{b}_B$ glides right through the twin to the opposite $\mathbf{K}_1$ interface, it may there reform the matrix dislocation $\mathbf{b}_A$ by the inverse of the reaction (51) and glide away into the matrix, leaving a step or ledge in the second interface of Burgers vector $-\mathbf{b}_t$. There may then be a generating node on each interface.

In most cases, slip on a corresponding system is unfavourable since the slip plane and direction are not close-packed; for example, a $\frac{1}{2}[110]$ dislocation on a $(1\bar{1}\bar{1})$ slip plane in a f.c.c. structure corresponds to a dislocation with a [001] Burgers vector on a (010) slip plane of a $(111)[11\bar{2}]$ deformation twin. Penetration into the twin on such a slip system seems unlikely (although unusual slip systems have been observed in some metals) so that it is generally believed that further decomposition into glissile systems will occur. Decompositions of single dislocations are often unfavourable (as judged by the Frank rule), but if an external stress causes a dislocation pile-up on a slip plane intersecting a twin, the stress concentration may be sufficient to initiate the decomposition of the leading dislocation at the interface. The work done by the applied stress when this dissociation just enables the lead dislocation to escape, and to be replaced by a new dislocation at the tail of the pile-up, is readily seen to be proportional to the number of dislocations in the pile-up. Thus if this number is sufficiently large, i.e. if the applied stress is high enough, the work done will outweigh the Frank imbalance of energy.

For b.c.c. crystals, detailed analysis is complicated by the observation that glide planes of different crystallographic types are frequently found to be operative in the same material under different conditions, and macroscopic glide may also occur on high index or irrational planes, which are not necessarily those of maximum resolved shear stress. At an atomic level, slip is usually regarded as confined to {110} and/or {112} planes, although, in some cases, reasonably good experimental evidence for {123} slip has been obtained,[118,251] and experiments on slip–twin interaction (see below) have confirmed that slip on {123} planes does occur when there is a suitable stress concentration. Note that a {112} plane contains only one $\langle 11\bar{1} \rangle$ direction, so that there is a unique screw dislocation which is able to cross the twin without leaving a step; if the obstacle twin is a deformation twin, there is only one possible

mode for each interface and the Burgers vector of the cross-slipping dislocation is parallel to the η_1 direction of this mode. However, in the b.c.c. case, the mirror image of the primary slip plane is not the only crystallographically equivalent plane of the twin on which this dislocation might glide. Three matrix planes of type $\{011\}$ intersect the $\{112\}$ twinning plane in the $\eta_1 = \langle 11\bar{1}\rangle$ direction, as do two $\{\bar{1}21\}$ planes, and the same numbers of possible slip planes in the twin meet along this direction. The possibility that the matrix slip plane is identical with the $\mathbf{K}_1$ interface of the barrier twin is excluded here as slip on this plane could only either enter or leave the twin along its edge or periphery; this has already been considered in connection with emissary slip. However, it is possible, in principle, for the screw dislocations to cross-glide along this interface rather than enter the twin. Finally, there are two $\{123\}$ planes in the $\langle 11\bar{1}\rangle$ zone of both matrix and twin, and these could, in principle, also act as atomic slip planes.

This means that for any twin obstacle, there are up to five different $\{110\}$ or $\{112\}$ slip systems in which the glide dislocations are in screw orientation when they meet the interface in the η_1 direction, and even more possible twin systems which can continue the slip. A simple criterion might be that the slip plane pair will normally be two planes of favoured type (e.g. both $\{110\}$ or both $\{112\}$) for which the lower of the two resolved shear stresses is greatest. Experiments by Tomsett and Bevis,[252] Partridge and Peel[253] and Vallance and Bevis[254] first established the importance of the resolved shear stress acting on the slip systems of both matrix and twin, but the actual choice of the system most able to penetrate the twin is likely to be quite complex, because the preferred slip plane in the twin may not be crystallographically equivalent to that in the parent matrix. Mathewson and Edmunds[255] pointed out as long ago as 1928 that matrix slip in the η_1 direction on any plane should be able to cross the twin, but although it has frequently been suggested in the literature that such cross slip should encounter only a small resistance, there is little experimental evidence available to support the theory in b.c.c. materials.

When considering the other possible interactions, it is convenient first to list the various directions in which the matrix slip plane meets the interface, since these are the zone axes of possible slip planes in the twin. Two of the three $\{110\}$ type planes which are not in the η_1 zone of a $\{2\bar{1}1\}$ twin have $\langle 131\rangle$ type intersections with the $\mathbf{K}_1$ plane, and the remaining $\{01\bar{1}\}$ plane has an $\langle 011\rangle$ intersection normal to the plane of shear. Consider the [131] intersection of a $(10\bar{1})$ slip plane with a $(2\bar{1}1)$ twin; the only usual slip planes in the [131] zone are $(10\bar{1})$ and $(1\bar{1}2)$. Thus, dissociations of the Burgers vector into other vectors representing dislocations which are glissile on these two planes in the twin should be considered first. However, the incident slip plane is at $\sim 73^\circ$ to the $\{2\bar{1}1\}$ $\mathbf{K}_1$ plane, as is the $\{10\bar{1}\}$ slip plane in the twin. This large angle implies either that the applied shear stress on the $\{10\bar{1}\}$ plane in the twin is opposite in sign to that on the matrix slip plane, or that both these slip planes have resolved shear stresses much smaller than that on the $\mathbf{K}_1$ plane. For this reason, slip on the $\{1\bar{1}2\}$ plane of the twin (at only $\sim 33^\circ$ to $\{2\bar{1}1\}$) may be the only possibility.

Similarly, in addition to the $\langle 11\bar{1}\rangle$ intersections of $\{112\}$ slip planes with a $\{2\bar{1}1\}$ twin plane, there are nine further intersections, namely one parallel to $\langle 011\rangle$, four (not all equivalent) to $\langle 35\bar{1}\rangle$, two to $\langle 10\bar{2}\rangle$ and two to $\langle \bar{1}13\rangle$. In every case, of course, the $\{112\}$ plane in the twin which is the mirror reflection of the matrix slip plane is one possibility, but experiment shows that this plane is not necessarily that which is operative.

Although the b.c.c. structure has many slip planes, it has only four $\langle 111\rangle$ slip directions; two of these directions are η_1 $(=[11\bar{1}]$ for a $(2\bar{1}1)$ twin) and η_2 $(=[1\bar{1}1]$ for the same twin) and their corresponding vectors are also $\langle 111\rangle$ type vectors of the twin. Since η_1 is an

invariant vector it has identical (or reversed) indices in the twin coordinates, as discussed above; all the other three vectors are of type $\frac{1}{6}\langle 5\bar{1}1\rangle$ in the twin lattice and so must decompose if slip is to continue into the twin. Consider the possibility of slip on the corresponding plane and direction of the twin. For any of the three matrix $\{110\}$ planes with slip direction parallel to $\boldsymbol{\eta}_2$ (including the plane of shear) or any of the three $\{112\}$ planes (including $\mathbf{K}_2$), the corresponding planes in the twin have identical (or reversed) indices, so that the physical conditions for slip are also fulfilled, subject to the proviso that the shear stress on both matrix and twin systems is adequate and of the correct sign. However, since the various slip planes with an $\boldsymbol{\eta}_2$ Burgers vector intersect the $\mathbf{K}_1$ plane in different directions, the only geometrically possible slip on a $\{110\}$ or $\{112\}$ plane of the twin is in each case on the twin plane corresponding to the matrix slip plane; this is, of course, the mirror image of the matrix slip plane. Thus, provided the Schmid factors are favourable, matrix slip parallel to $\boldsymbol{\eta}_2$ should be able to cross the twin on a corresponding slip system in which both slip plane and direction are crystallographically equivalent to the plane and direction of the incident slip.

The other two matrix $\langle 111\rangle$ directions correspond to $\langle 110\rangle$ vectors of the twin, with corresponding twin glide planes of type $\{001\}$. Since slip on a $\langle 010\rangle\{001\}$ system is extremely unusual in b.c.c. materials, it seems likely that the incident dislocation will dissociate in some way other than that of eq. (51) in order to cross the $\mathbf{K}_1$ interface. Other possibilities may be examined by allowing further dissociations, all of which must satisfy the geometric criteria that the slip planes in matrix and twin meet edge to edge in the plane of the interface, that the Burgers vector of the slip dislocation in the twin is a repeat vector of the twin lattice and has the correct sign to continue rather than oppose the shear produced by the matrix slip, and that the slip plane is defined by the line of intersection and the Burgers vector of the new dislocation.

Consider now a particular slip–twin interaction when the slip plane is $\{112\}$ and the slip direction is not parallel to $\boldsymbol{\eta}_1$ or $\boldsymbol{\eta}_2$. Mahajan[256] made one of the first detailed TEM investigations of dislocations at twin boundaries in a b.c.c. Mo–35at%Re alloy. Figure 42 shows a slip–twin interaction for which the arbitrary assumption (consistent with the Bilby–Crocker sign convention) that $\mathbf{K}_1 = (2\bar{1}1)$ and $\boldsymbol{\eta}_1 = [11\bar{1}]$ has been made. With a 180° rotation about $[2\bar{1}1]$ to define the coordinate axes in the twin, the slip planes in the matrix and twin respectively were found from the projected directions of AA′, BB′, CC′ and DD′ to be (211) and $(2\bar{3}1)_T$. (Indices relative to the twin lattice are given the subscript T.) This indicated the following reaction which was first suggested by Sleeswyk and Verbraak; in addition to the Burgers vectors, slip plane indices are specified as:

$$\tfrac{1}{2}[\bar{1}11]_{(211)} = \tfrac{1}{6}[\bar{1}51]_{(10.1.5)} + \tfrac{1}{3}[\bar{1}\bar{1}1]_{(2\bar{1}1)} \tag{67}$$

where

$$\tfrac{1}{6}[\bar{1}51]_{(10.1.5)} = \tfrac{1}{2}[111]_{T(2\bar{3}1)_T}. \tag{67a}$$

Thus the matrix slip plane intersects the twin in the $[\bar{1}02] = [10\bar{2}]_T$ direction and is propagated into the twin as a lattice dislocation on the slightly unusual $(2\bar{3}1)_T$ plane. The complementary dislocation $\frac{1}{3}[\bar{1}\bar{1}1]$, if stable, forms a double step in the $\mathbf{K}_1$ interface which may prevent further slip if it remains along the original line of intersection. If it glides along the interface, the $\frac{1}{3}[\bar{1}\bar{1}1]$ step will decrease the volume of the twin. The decomposition is energetically unfavourable, but could occur when the stress concentration at the head of a pile-up of dislocations on the matrix (211) slip plane reaches a sufficient value.

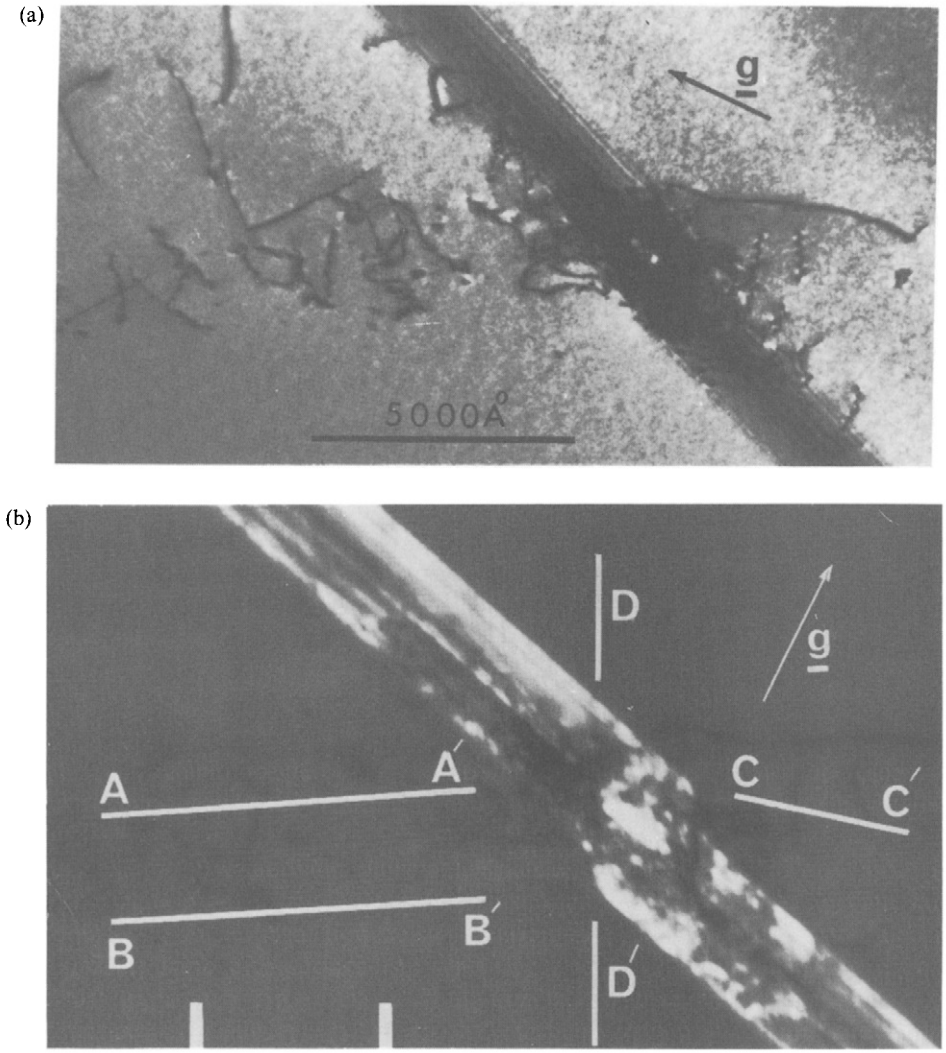

Fig. 42. (a) A propagating slip band interacting with a deformation twin in a Mo–35at%Re alloy sample. (b) Dark-field image of the twin in (a) AA′ and BB′ are traces of the slip plane within the matrix with the (115) plane, whereas CC′ is the trace of the slip plane within the twin with $(\bar{1}11)_T$ plane. DD′ is the projection of the line of intersection of the (211) and $(2\bar{1}1)$ planes on the (115) plane. Distance between markers is 250 nm (after Mahajan[256]).

Other possible slip planes in the twin must contain $[10\bar{2}]_T$ in which the primary slip plane meets the twin. There are no {110} planes in the $[10\bar{2}]$ zone, so that if the slip continues into the twin on an atomic slip plane of a type normally observed in b.c.c. materials, it must do so on the $(2\bar{3}1)$ plane which was observed in the experimental work, or on either of the only remaining {112} and {123} planes in the $[10\bar{2}]$ zone, namely $(211)_T//(2\bar{7}\bar{1})$ (which is the symmetry-related plane) and $(231)_T//(\bar{2},\bar{1}\bar{1},\bar{1})$. Mahajan pointed out that the required decompositions could be represented by

$$\tfrac{1}{2}[\bar{1}11]_{(211)} = \tfrac{1}{6}[115]_{(2\bar{7}\bar{1})} + \tfrac{1}{6}[\bar{1}\bar{1}1]_{(2\bar{1}\bar{1})} + \tfrac{1}{2}[\bar{1}1\bar{1}]_{(231)} \qquad (68)$$

where

$$\tfrac{1}{6}[115]_{(2\bar{7}1)} = \tfrac{1}{2}[1\bar{1}\bar{1}]_{T(211)_T} \tag{68a}$$

and

$$\tfrac{1}{2}[\bar{1}11]_{(211)} = \tfrac{1}{6}[\bar{5}1\bar{1}]_{(\bar{2},\bar{1}\bar{1},\bar{1})} + \tfrac{1}{6}[\bar{1}\bar{1}1]_{(2\bar{1}1)} + \tfrac{1}{2}[111]_{(2\bar{3}1)} \tag{69}$$

with

$$\tfrac{1}{6}[\bar{5}1\bar{1}]_{(\bar{2},\bar{1}\bar{1},\bar{1})} = \tfrac{1}{2}[\bar{1}1\bar{1}]_{T(231)_T}. \tag{69a}$$

The slip represented by eqs (68) or (69) is energetically less favourable than that of eq. (67) and in addition new perfect dislocations of the parent lattice are produced at the interface, thus reducing the effective shear produced by the incident twin. If these dislocations move back along the slip plane, they must do so against the applied stress; alternatively, they will block the shear transmission and lead to high stress concentrations if they remain in the interface between the matrix and the barrier twin. Movement against the applied stress is possible in the stress field of the pile-up, but should cease after a limited amount of reverse slip because of the formation of a pile-up of these matrix dislocations.[257] In view of the energetic and mechanistic differences, it is not surprising that only dissociation (67) has been clearly observed.

In f.c.c. materials, there are only three matrix $\{111\}$ slip planes, each of which intersects the remaining $\{111\}$ plane (the $\mathbf{K}_1$ plane of the twin) in a $\langle 01\bar{1}\rangle$ direction. Each slip plane contains three of the six $\langle 1\bar{1}0\rangle$ vectors which are normally observed to be the only slip vectors, and one of these three directions thus meets the $\mathbf{K}_1$ plane in screw orientation so that, as already discussed, it may cross-slip into the twin without leaving an interface step. There are thus three slip systems which can potentially cross the twin in this way. Each of the three $\{111\}$ matrix planes may be regarded as the $\mathbf{K}_2$ plane of a hypothetical deformation mode, so that its corresponding plane (rotated but undistorted by the twinning shear) is a $\{111\}$ plane of the twin; all three $\langle 110\rangle$ directions in this plane similarly have corresponding $\langle 110\rangle$ twin vectors. Thus any of the slip dislocations in a matrix slip plane can (geometrically) cross the twin on an equivalent slip system which may be regarded as the corresponding slip system of one of the three deformation modes sharing the same $\mathbf{K}_1$ plane. However, the angle between the $\mathbf{K}_1$ plane and the incident slip plane is always $\sim 70^\circ$ in f.c.c. crystals, so that it is difficult to obtain large shear stresses on both the slip plane and its mirror image plane in the twin.

Twinning in f.c.c. crystals is conveniently shown in a double Thompson tetrahedron[258] (see Fig. 43) in which the matrix planes and directions are represented by **ABCD** and a twin on plane d is represented by **A′B′C′D′** where $\mathbf{A} = \mathbf{A}'$, $\mathbf{B} = \mathbf{B}'$, $\mathbf{C} = \mathbf{C}'$ and **D′** is the reflection of **D** in d. Dislocations on planes a, b or c with Burgers vectors **BC**, **CA** or **AB** cross slip as screws on to the twin planes a', b' or c', whereas dislocations with other Burgers vectors must decompose in order to cross the interface. Dislocation reactions or dissociations may be represented by Burgers vector equations expressed in terms of the double tetrahedron, but for those who prefer algebra to geometry, the same equations will be given in vector form.

Mahajan and Chin[259] suggested the following dissociations for a dislocation with a $\frac{1}{2}\langle\bar{1}01\rangle$ Burgers vector on a $\{111\}$ slip plane encountering a $\{\bar{1}11\}$ twin boundary:

$$\mathbf{DB}_{(a)} = \mathbf{C'D''}_{T(b')_T} + \mathbf{A}\boldsymbol{\delta}_{(d)} \tag{70}$$

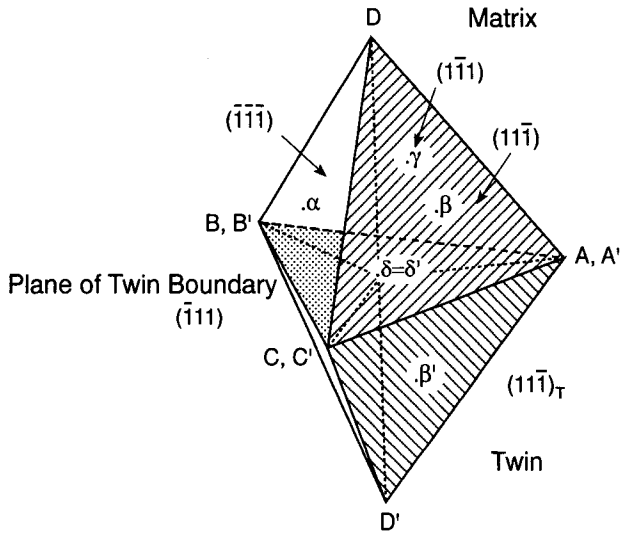

Fig. 43. The double Thompson's tetrahedron for the twin-matrix orientation relationship. With an origin at δ, the co-ordinates of A, B, C, D and D′ are, respectively, $\frac{1}{6}[211]$, $\frac{1}{6}[\bar{1}\bar{2}1]$, $\frac{1}{6}[\bar{1}1\bar{2}]$, $\frac{1}{6}[2\bar{2}\bar{2}]$ and $\frac{1}{6}[\bar{2}22]$ (after Remy[260]).

and

$$\mathbf{DB}_{(a)} = \mathbf{BD}'_{\tau(a')_T} + 2 \times \boldsymbol{\delta}\mathbf{B}_{(d)} \tag{71}$$

or in vector form

$$\tfrac{1}{2}\langle\bar{1}01\rangle_{\{111\}} = \tfrac{1}{6}\langle\bar{1}14\rangle_{\{5\bar{1}\bar{1}\}} + \tfrac{1}{6}\langle\bar{2}\bar{1}\bar{1}\rangle_{\{\bar{1}11\}} \tag{70a}$$

with

$$\tfrac{1}{6}\langle\bar{1}14\rangle_{\{511\}} = \tfrac{1}{2}\langle 1\bar{1}0\rangle_{\tau\{111\}_T} \tag{70b}$$

and

$$\tfrac{1}{2}\langle\bar{1}01\rangle_{\{111\}} = \tfrac{1}{6}\langle\bar{1}41\rangle_{\{511\}} + \tfrac{1}{3}\langle\bar{1}\bar{2}1\rangle_{\{\bar{1}11\}} \tag{71a}$$

with

$$\tfrac{1}{6}\langle\bar{1}41\rangle_{\{511\}} = \tfrac{1}{2}\langle 10\bar{1}\rangle_{\tau\{111\}_T}. \tag{71b}$$

In both cases, the predicted slip in the twin is on the symmetry-related plane, and in view of the strong preference for $\{111\}$ slip in all f.c.c. materials, it is improbable that any other slip plane in the twin could be activated. Both reactions are energetically unfavourable according to the Frank rule, the increase in elastic (i.e. line) energy being one third of the initial energy for eq. (69) and four thirds for eq. (70). On the other hand, an approximate calculation by Mahajan and Chin[259] indicates that the compatibility of the strain produced by the various defects in the interface region is almost complete for dissociation (71) but not for (70). However, the dislocation with Burgers vector $\mathbf{A}\boldsymbol{\delta}$ of eq. (70) is an ordinary twinning dislocation, whereas $2\boldsymbol{\delta}\mathbf{B}$ in eq. (71) is the f.c.c. equivalent of Sleeswyk's complementary dislocation and may be unstable.

Experimental verification of slip inside a twin on the mirror image of the parent slip plane has been obtained from slip band traces on the surfaces of a single crystal of a Co–8wt%Fe

which had been deformed in compression under constraints designed to enforce plane strain conditions. Examination by optical microscopical techniques[259] showed, as anticipated, that two deformation twin variants and two or four slip variants had formed in the deformed region, and that the slip traces within twins were always on the {111} plane symmetrically related to the incident slip plane. In a later electron microscopic study of the interaction of dislocations with a thin annealing twin, Remy[260] was able to identify the Burgers vectors of the various dislocations. In the electron micrograph shown in Fig. 44, dislocations marked I are piling up against the lower twin interface, whilst two dislocations (II) within the twin are clearly gliding on the symmetry related plane, and the twinning dislocations (III) left at the interface are also visible. Analysis showed that this situation was equivalent to eq. (70), thus supporting the lower energy condition.

In grain boundary theory, it is often assumed that a lattice dislocation entering a boundary should dissociate into components with Burgers vectors given by vectors of Bollmann's DSC lattice. In the case of a f.c.c. twin, for which the reciprocal fraction of coincidence sites, $\Sigma = 3$, this implies that a dissociation of type (59a) into a Frank plus a Shockley partial, involving no change in elastic energy, should be preferred to one like eq. (70). However, the grain boundary theory is not concerned with the compatibility of the slip deformation produced by the glide of the dislocations up to the interface; the dissociation of eq. (59) obviously does not allow the slip to be propagated past the interface since the Frank partial is sessile. Gleiter[261] has even suggested that in circumstances where there is a large unrelieved strain on one side of an interface, existing interface dislocations with DSC vectors might amalgamate to form lattice dislocations which can then partly relax the strain. The relation between grain boundary theory, especially Bollmann's O-lattice and DSC lattice descriptions,

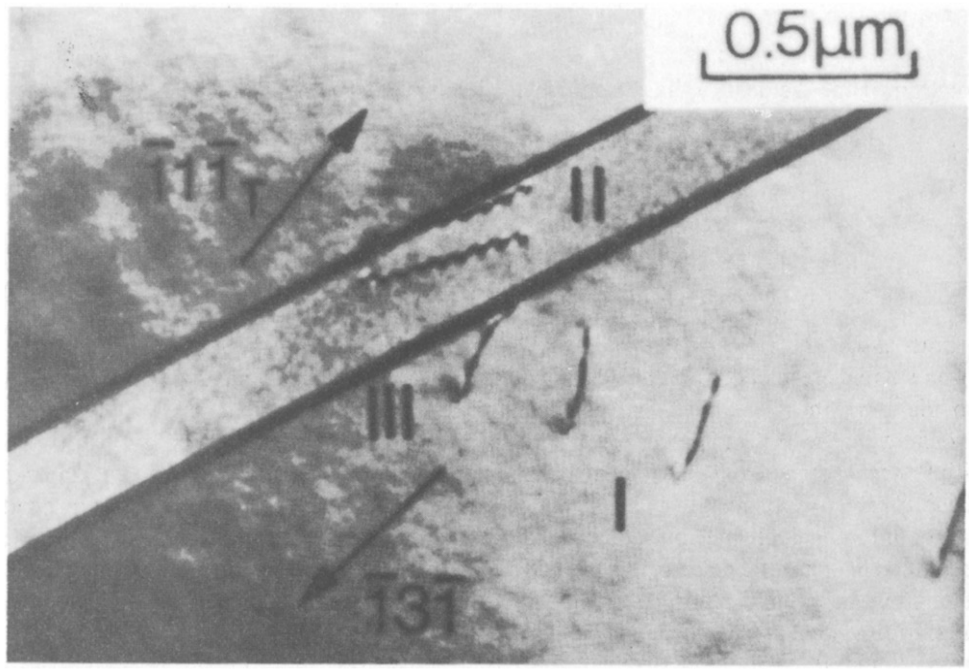

Fig. 44. Electron micrograph showing the interaction of slip dislocations with a thin coherent twin boundary in an f.c.c. crystal (after Remy[258]).

and the theories derived from the Sleeswyk and Saxl papers is reviewed in more detail by Rémy.[258]

The edge to edge interaction between the twinning dislocations in the tip of a tapering deformation twin which is growing into a dislocation array has been considered by Fontaine[262] and Bushnev.[257] The reaction between a lattice dislocation and an individual twinning dislocation may take the form of eq. (70), which now represents a 25% reduction in energy since it is effectively

$$\tfrac{1}{2}\langle\bar{1}01\rangle + \tfrac{1}{6}\langle 2\bar{1}\bar{1}\rangle = \tfrac{1}{2}\langle 1\bar{1}0\rangle_{\mathrm{T}}. \tag{70c}$$

Other possible reactions lead to larger reductions in energy, but again give sessile configurations which, if stable against stress, would halt the deformation. Thus eq. (59) can be written as the reaction between a lattice dislocation and an opposite Shockley partial to give a Frank sessile dislocation (giving an energy reduction of 50%) and a further reduction in elastic energy is possible if the Frank partial dissociates into a stair rod of type $\frac{1}{6}\langle 110\rangle$ and a Shockley partial in the matrix. It has been suggested that such sessile configurations help to prevent untwinning or unloading, but in general they are believed to be unstable against pile-up stresses in the edge to edge configuration in the same way as in the planar interface interactions.

Yoo and Wei[263] gave the first analysis of slip–twin interactions in h.c.p. materials. They considered the most common $\{10\bar{1}2\}$ twin mode and basal slip in the matrix in a $\langle 11\bar{2}0\rangle$ direction (often called *a* slip). A basal dislocation with a $\frac{1}{3}\langle 11\bar{2}0\rangle$ Burgers vector can encounter the $\{1\bar{1}02\}$ twin in screw orientation, and may then simply cross-slip on to either a prism plane $\{1\bar{1}00\}$ or the basal plane of the twin. This is simply represented as

$$\tfrac{1}{3}\langle 11\bar{2}0\rangle_{(0001)} = \tfrac{1}{3}\langle\bar{1}\bar{1}20\rangle_{\mathrm{T}(0001)_{\mathrm{T}}\text{ or }\{1\bar{1}00\}_{\mathrm{T}}}. \tag{72}$$

However, if the dislocation has one of the other two Burgers vectors of *a* type, a dissociation reaction such as

$$\tfrac{1}{3}\langle\bar{2}110\rangle_{(0001)} = \tfrac{1}{6}\langle 11\bar{2}\bar{3}\rangle_{\mathrm{T}\{1\bar{1}00\}_{\mathrm{T}}} - \mathbf{b}_{\mathrm{t}} \tag{73}$$

must take place. However, the dissociation (73) has a product dislocation in the twin which is not a lattice dislocation, so that it would trail a stacking fault if it were to glide along the $\{1\bar{1}00\}_{\mathrm{T}}$ plane. This can be avoided if matrix slip dislocation combine in pairs to give the dissociation

$$2 \times \tfrac{1}{3}\langle\bar{2}110\rangle = \tfrac{1}{3}\langle 11\bar{2}\bar{3}\rangle_{\mathrm{T}} - 2\mathbf{b}_{\mathrm{t}} \tag{73a}$$

where $2\mathbf{b}_{\mathrm{t}}$ is an appropriate zonal twinning dislocation.

Experimental confirmation of both eq. (72) and eq. (73) was obtained by Tomsett and Bevis[252] who made an electron microscopic study of twin–slip interactions in zinc crystals which had been deformed in such a way that twinning preceded slip. It is particularly noteworthy that the decomposition (73) was confirmed experimentally since this represents a previously unreported slip system which arises directly as a result of the interaction. Figure 45 is a striking electron micrograph in which dislocations in the matrix

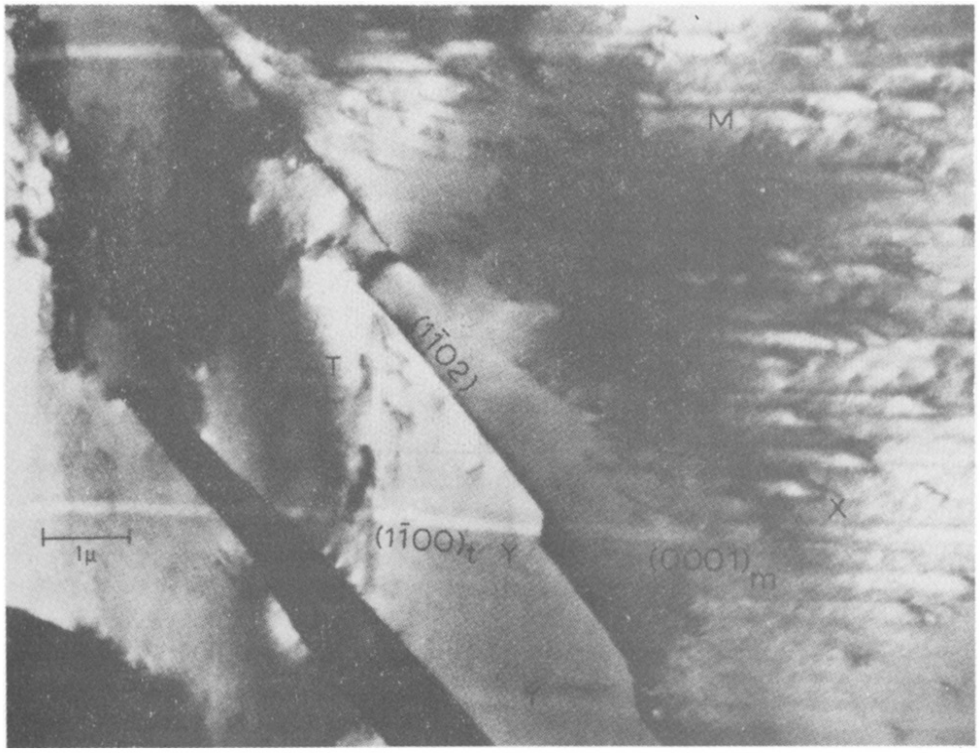

Fig. 45. Electron micrograph showing slip transferred from the matrix basal plane $(0001)_m$ to the $(1\bar{1}00)$ plane of a $(1\bar{1}02)$ barrier twin in zinc (after Tomsett and Bevis[252]).

and the twin are visible at X and Y, and traces of the slip plane in matrix and twin and of the twin plane are all clearly visible. Burgers vector analysis confirmed that eq. (73) was indeed valid. Later work by the same authors showed, however, that the decomposition is influenced by the applied stress. The single crystals used in observations such as those of Fig. 45 were orientated so that the slip planes in both matrix and twin were at approximately 45° to the tensile axis, thus maximizing the resolved shear stress on both systems. Experiments on polycrystalline specimens showed that a different dissociation leading to the formation of basal plane stacking faults within the twin can sometimes occur. Dissociations alternative to (74) are represented by

$$2 \times \tfrac{1}{3}\langle\bar{2}110\rangle = \tfrac{1}{3}\langle 11\bar{2}0\rangle_T + [000\bar{1}]_T - 2\mathbf{b}_t \tag{74}$$

and

$$2 \times \tfrac{1}{3}\langle\bar{2}110\rangle = \tfrac{1}{3}\langle 10\bar{1}0\rangle_T + \langle 01\bar{1}0\rangle_T - 2\mathbf{b}_t. \tag{75}$$

The slip planes are not given in these equations, but in eq. (75) both product dislocations may, in principle, glide on the basal plane and their Burgers vectors are the h.c.p. equivalent of Shockley partials. Equation (75) describes many experimental results when the resolved shear stress is much greater on the matrix slip system than on $\{1\bar{1}00\}_T$. The importance of the Schmid factor on both primary and twin slip systems was confirmed by the experimental investigations of Partridge and Peel[253] and Vallance and Bevis.[254]

The above reactions all concern the commonest h.c.p. twin, $\{10\bar{1}2\}$, but Yoo[181] has also examined theoretically interactions with $\{10\bar{1}1\}$, $\{11\bar{2}2\}$ and $\{11\bar{2}1\}$ twins. He showed, using anisotropic elastic theory, that in zinc and cadmium, non-screw basal plane slip dislocations are attracted by the $\{10\bar{1}2\}$ twin interface, but similar dislocations in the other metals are repelled because of the reversal of the twinning shear.

6.3. *Twin–Twin Interactions*

An existing deformation or annealing twin in the path of a growing deformation twin is an obstacle which may be difficult to overcome. Very often, however, the growing twin manages to force some or all of its shear strain into, across and beyond the obstacle twin. In (R.W.) Cahn's classical paper[80] on twinning in uranium, he stated two restrictive conditions which, if satisfied, will allow a deformation twin (A) to cross another twin (B) by creation of a secondary twin (C) in the crossed region. These well-known conditions are (1) the $\mathbf{K}_1$ planes of A and C must intersect that of B in the same direction and (2) the direction $\boldsymbol{\eta}_1$ and the magnitude and sense of shear in A and C must be the same. The first condition corresponds to the geometrical condition for the propagation of slip; the second ensures complete shear compatibility, and later work has shown that it may be partly relaxed if some accommodation by slip is also involved. However, twin propagation by secondary twinning is frequently impossible because of the directionality of the twinning shear, a complication which does not occur with slip. Sleeswyk's theory of emissary slip first provided an explanation of the crossing of obstacle twins by internal slip rather than twinning in b.c.c. materials, and the theory of inter-conversion of twinning and slip dislocations has since been generalized to account for some twin–twin intersections in other structures.

The simplest way in which the crystallography can conform to Cahn's condition occurs if the shear direction of A and C is parallel to their mutual line of intersection with B so that there is no displacement of B normal to its $\mathbf{K}_1$ plane. The twinning dislocations of A meet the interface of B in screw orientation so that they can simply cross-slip into B on the $\mathbf{K}_1$ interface between B and C. This is thus the equivalent of the simple cross-slip case in the propagation of slip. Liu[264] pointed out another possible geometry in which the $\mathbf{K}_1$ planes of A and C are parallel, so that the crossing twin A is undeviated but the A–B interface plane is inclined to the matrix–B interface. This tilting is the net effect of the steps left in the matrix–B interface by successive twinning dislocations of the matrix–A interface. Liu's hypothesis of parallel $\mathbf{K}_1$ planes and $\boldsymbol{\eta}_1$ directions is, however, not generally compatible with the crystallography of twinning, and Cahn's cross-slip case is applicable only to b.c.c. and derived structures.

Complete propagation of a twinning shear across a barrier twin by secondary twinning is usually impossible if the only twins are crystallographically equivalent variants of one mode. It may appear that in cubic compound modes in which $\mathbf{K}_1$ and $\mathbf{K}_2$ are equivalent variants, these two planes could be the $\mathbf{K}_1$ interfaces of the matrix with the A and B twins, and the reflection of the A–matrix interface in the B–matrix interface would then necessarily be (within the twin B) another variant of the same type of plane. However, an analysis by Levasseur[265] and later by Remy[266] shows that the direction of shear which will twin B on this plane has a component normal to the matrix–B interface which is opposite to the component of the twinning direction of A, i.e. the shear produced in the barrier twin would be an anti-twinning rather than a twinning shear.

The b.c.c. structure has the unique feature that three {112} type twins may intersect along a common $\langle 11\bar{1}\rangle$ direction, which is moreover the only possible η_1 direction for all three. This configuration is thus the simplest type of twin–twin interaction. Twinning dislocations in screw orientation on one such plane meeting a barrier twin can, in principle cross-slip on to the interface plane of the barrier twin or on to either of the two {112} planes within the barrier twin. If they form emissary dislocations, they can accommodate the shear of the incident twin by emissary slip on these planes or on any of the three {101} planes in the same zone. The two {112} planes within the barrier twin are respectively the mirror image of the interface between the intersecting twin and the matrix and the plane parallel to their original interface plane.

Such interactions in α-iron were investigated experimentally by Sleeswyk and Helle[267] and Levasseur,[265] and in a Mo–35at%Re alloy by Mahajan.[256] Figure 46 shows two $(\bar{1}\bar{1}2)$ twins, 7A and 7B, interacting with a $(1\bar{2}1)$ twin, 12, in α-iron. It is apparent that 7A and 12 cross each other completely, but the 7B–12 interaction is such that the growing twin appears to end at, or merge into, the obstacle twin. Figure 47 shows a similar interaction in the Mo–Re alloy in which $(\bar{1}21)$ and $(2\bar{1}1)$ twins, T_1 and T_2, merge into each other with little or no deformation of the surrounding matrix. In these 'branching' interactions, it may be seen that both twins cease to widen on the side of the intersection which encloses an obtuse angle, but continue to widen on the side enclosing an acute angle. This effect is another consequence of the unidirectionality of the twinning shear. If the positive direction of shear is taken as $[11\bar{1}]$ for both T_1 and T_2, for example, it follows that the positive plane normals must be $[\bar{1}21]$ and $[2\bar{1}1]$, i.e. the positive normals must enclose an obtuse angle. Consider a (hypothetical) single twinning dislocation, gliding on the $(2\bar{1}1)$ plane until it reaches the barrier interface $(\bar{1}21)$. Instead of crossing the interface, it may cross-slip along it, thus adding an additional layer to part of T_1. The direction of this motion is necessarily that which makes an acute angle with the $(2\bar{1}1)$ matrix plane. A series of such twinning dislocations on successive $(2\bar{1}1)$ planes

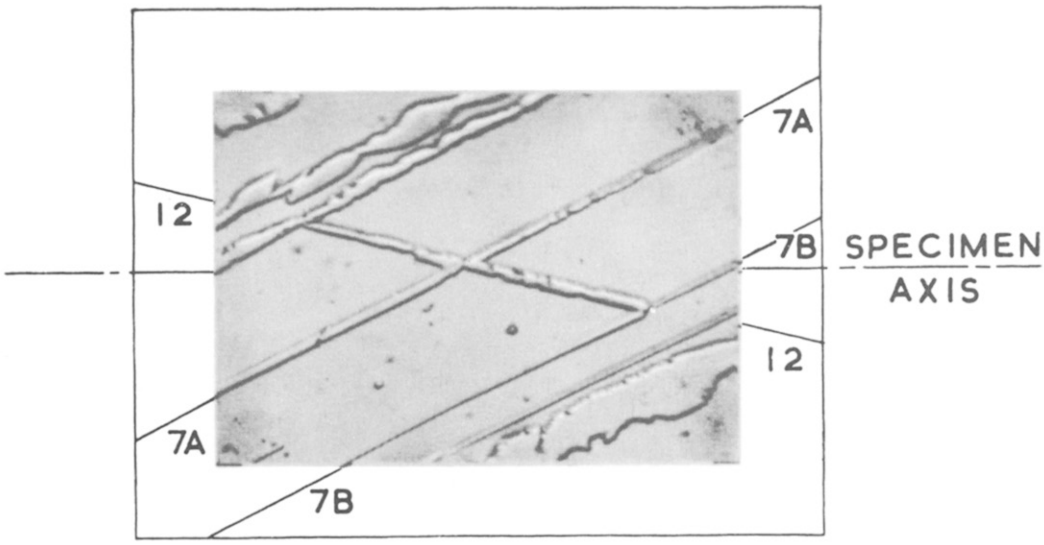

Fig. 46. Micrograph obtained from the surface of an α-Fe specimen after 9.2% deformation in liquid oxygen. Twins 7A and 12 crossed each other completely during the early stage of deformation. Later transverse growth took place only on those sides of the crossing twins which enclose an acute angle. The twin crossing 7B-12 is a branching crossing (after Sleeswyk and Helle[267]).

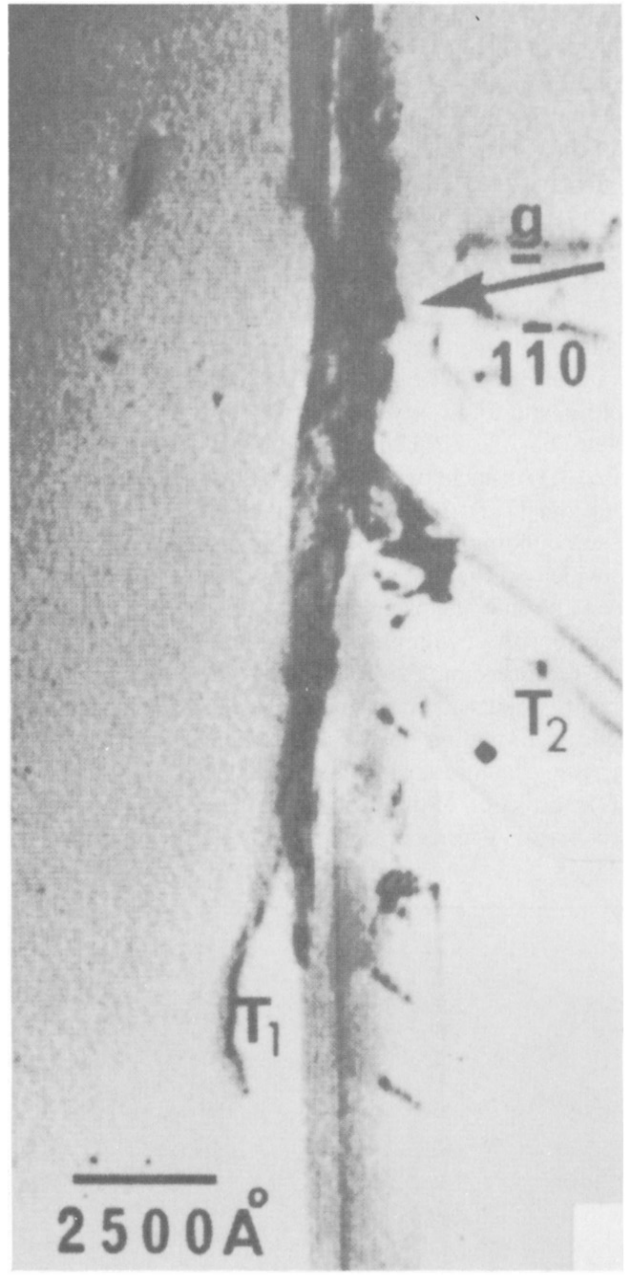

Fig. 47. A ⟨111⟩ twin intersection observed in a deformed Mo–35at%Re alloy specimen (after Mahajan[256]).

will lead to the formation of a twin T_2, and both twins can continue to thicken in this way as a consequence of the compatibility of the atom movements in the acute angle. In the obtuse angle, thickening of T_1 is not compatible with that of T_2.

In Fig. 46, the crossing of the twins 7A and 12 is apparently achieved by emissary slip, i.e. by conversion of the twinning partials of the crossing twin in threes to form slip

dislocations which glide through the crossed twin and then dissociate again in order to continue as a twin on the other side. Sleeswyk and Helle apparently assumed that the slip plane in the twin would be parallel to the composition plane of the crossing twin, since it is also a {112} plane, but as is often the case, it was not possible to determine the slip plane experimentally; indeed, it is frequently not evident from optical or even electron

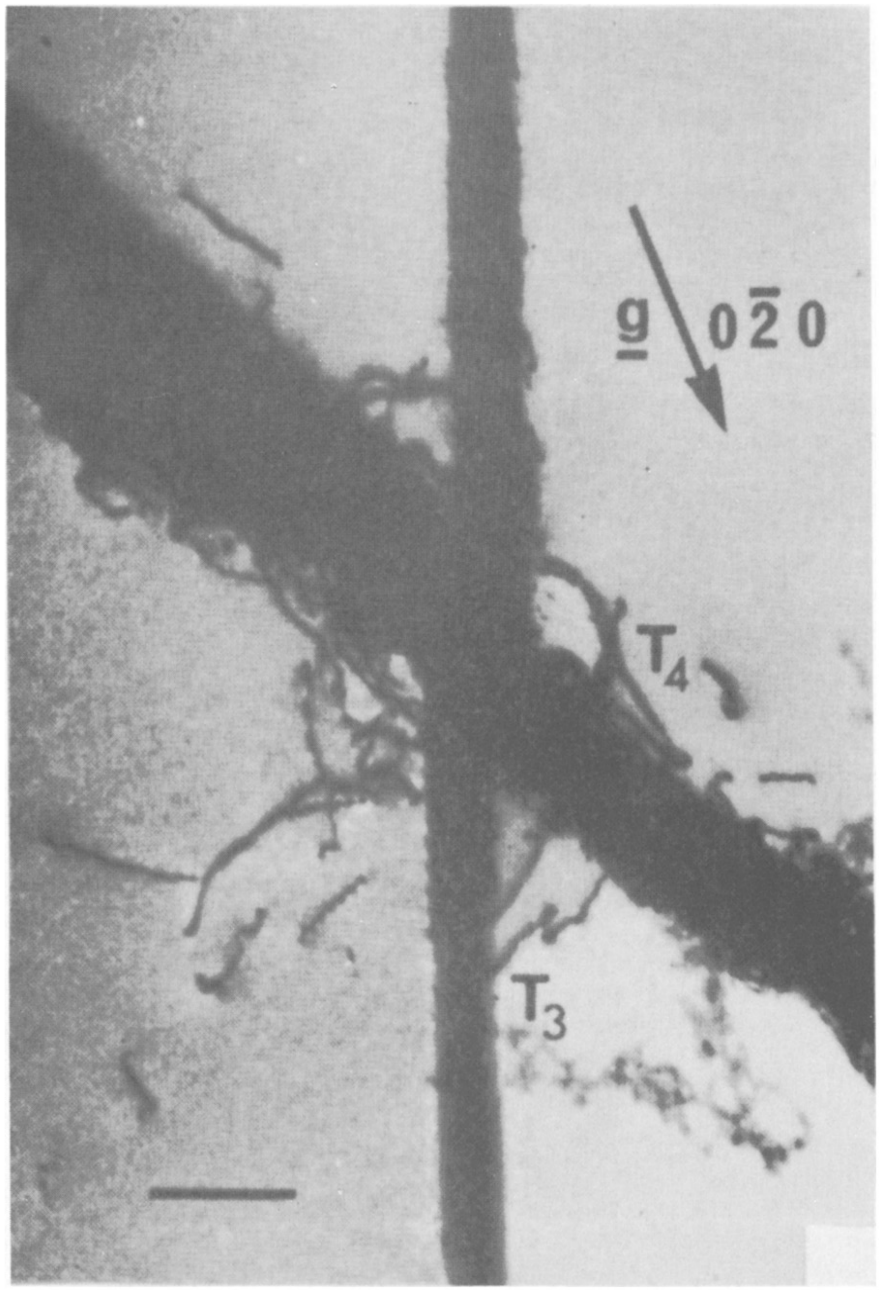

Fig. 48. A ⟨102⟩ twin intersection observed in a deformed Mo–35at%Re alloy sample (after Mahajan[256]).

micrographs which twin is the crossing twin. Levasseur[265] also observed branching interactions from $\langle 11\bar{1}\rangle$ intersections but in addition, he and Kounicky[268] have found evidence for "detwinning" on a plane not parallel to the $\mathbf{K}_1$ plane of the incident twin.

As already noted for the slip–twin interactions, there are several crystallographically distinct intersections between the $\{112\}$ planes, and examples of each configuration have been examined experimentally. Figure 48 shows a $\langle 210\rangle$ type intersection in which the barrier twin (T_3) is $(2\bar{1}1)$ and the crossing twin is (211) so that the twins intersect along $[10\bar{2}]$. Mahajan found the slip plane to be (10,1,5) of the matrix, which is equivalent to $(2\bar{3}1)_T$ of the barrier twin. If the formation of emissary dislocations is assumed, the crystallography is identical with that already discussed for the corresponding interaction of a (211) slip band with a $(2\bar{1}1)$ twin (see eqs (68) and (68a)). This result was later confirmed by Levasseur[265] who also observed that some of the $\frac{1}{2}[111]_T$ dislocations cross-slipped on to a $(1\bar{1}0)_T$ slip plane within the crossed twin. As already mentioned, the observed $(2\bar{3}1)_T$ plane is that one of the possible atomic b.c.c. glide planes which makes the smallest angle with the $\mathbf{K}_1$ plane of the crossing twin, and is thus likely to carry a high resolved shear stress; it also requires a smaller increase in line energy than either of the rival dissociations (69) and (70). The choice of the slip system

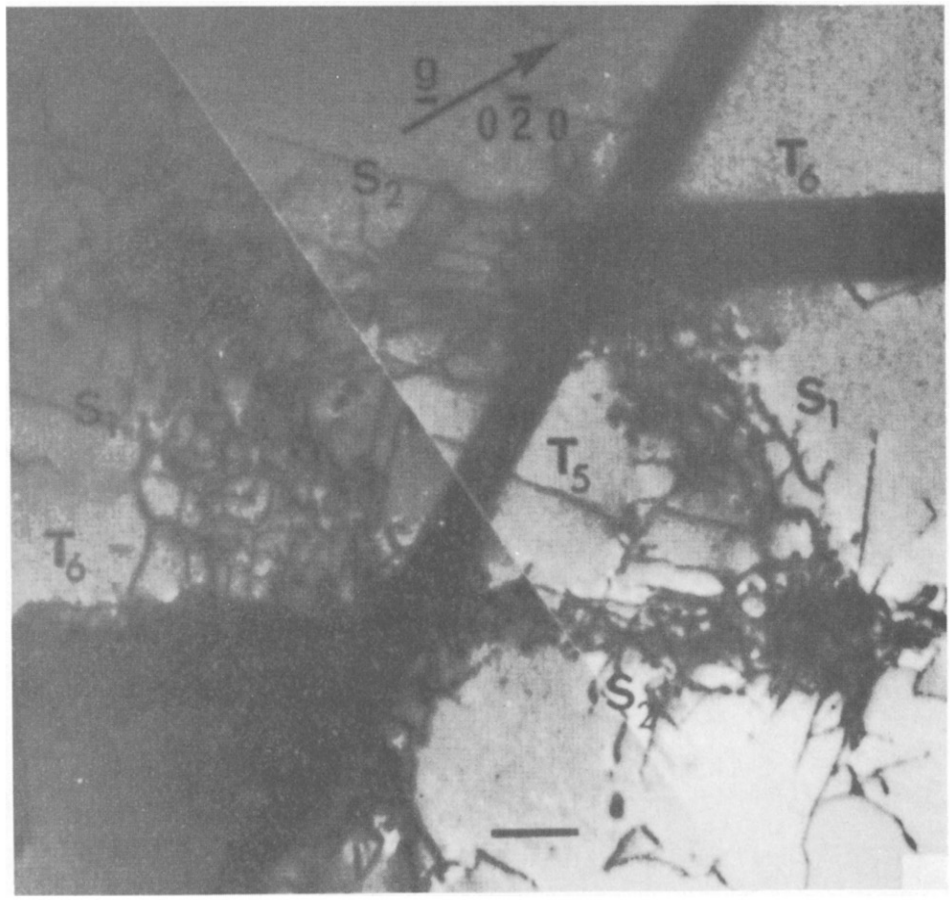

Fig. 49. A $\langle 110\rangle$ twin intersection observed in a deformed Mo–35at%Re alloy sample (after Mahajan[256]).

$\langle 111\rangle_T\{2\bar{3}1\}_T$ thus correlates well with either a maximum driving force (applied stress) or a minimum energy criterion. However, Mahajan also found some small regions of the matrix containing dislocations with Burgers vectors $\frac{1}{2}\langle 111\rangle$ on slip planes $\{2\bar{3}1\}$. These dislocations may be explained formally by a different dissociation of the incident twinning or emissary dislocations as in eqs (69) and (69a). If this is the source of the experimental observation, it implies that transmission of the shear is incomplete. Moreover, the formation of some product dislocations in the matrix causes considerable difficulties.

An experimental investigation of twin intersection along a $\langle 110\rangle$ direction is illustrated in Fig. 49. The twins T_5 and T_6, on (211) and $(\bar{2}11)$ planes, respectively, intersect along $[01\bar{1}]$, and slip bands S_1 and S_2 are also observed. The plane of S_1 is (011), so that the two possible slip directions are $[11\bar{1}]$ and $[1\bar{1}1]$. The trace analysis gives four possibilities, $(\bar{2}11)$, $(\bar{2}13)$, $(2\bar{1}3)$ and $(2\bar{1}1)$, for the plane of S_2. These results are again consistent with the dissociations of the emissary dislocations with Burgers vector $\frac{1}{2}[111]$ formed from three twinning dislocations of the $(\bar{2}11)$ twin. However, it seems unnecessary to include the intermediate formation and dissociation of the emissary dislocations, which may well be an entirely notional rather than a physical process. The two proposed decompositions may then be written more directly as:

$$3 \times \tfrac{1}{6}[111]_{(\bar{2}11)} = \tfrac{1}{6}[15\bar{1}]_{(4\bar{1}\bar{1})} + \tfrac{1}{6}[\bar{1}11]_{(211)} + \tfrac{1}{2}[1\bar{1}1]_{(011)} \tag{76}$$

where (with a type IV orientation relation to define the axes (T) of T_3),

$$\tfrac{1}{6}[15\bar{1}]_{(4\bar{1}\bar{1})} = \tfrac{1}{2}[1\bar{1}1]_{T(011)_T} \tag{76a}$$

and

$$3 \times \tfrac{1}{6}[111]_{(\bar{2}11)} = \tfrac{1}{6}[1\bar{1}5]_{(4\bar{1}\bar{1})} + \tfrac{1}{6}[\bar{1}11]_{(211)} + \tfrac{1}{2}[11\bar{1}]_{(011)} \tag{77}$$

where

$$\tfrac{1}{6}[1\bar{1}5]_{(4\bar{1}\bar{1})} = \tfrac{1}{2}[11\bar{1}]_{T(011)_T} \tag{77a}$$

The S_1 slip bands are produced when the $\frac{1}{2}[1\bar{1}1]$ and/or the $\frac{1}{2}[11\bar{1}]$ dislocations glide on the (011) planes of the matrix away from the line of intersection at which they were formed. Slip is propagated across T_5 on the $(011)_T$ plane, and a twinning dislocation of the T_5 plane glides away along the (211) T_5–matrix interface. The S_2 slip bands could be formed as a consequence of the decomposition of the Burgers vectors $[15\bar{1}] = [1\bar{1}1]_T$ and/or $\frac{1}{6}[1\bar{1}5] = [11\bar{1}]_T$ at the emergent surface to give a rewritten eq. (77) with:

$$\tfrac{1}{6}[15\bar{1}]_{(4\bar{1}\bar{1})} = \tfrac{1}{2}[111]_{(\bar{2}11)} + \tfrac{1}{6}[1\bar{1}\bar{1}]_{(211)} + \tfrac{1}{2}[\bar{1}1\bar{1}]_{(011)} \tag{76b}$$

and there is a corresponding eq. (77b). In principle, the $\frac{1}{2}[111]$ dislocations could each reform as three twinning dislocations, and the twin T_5 would then appear to have crossed T_6 in a similar fashion to that shown in Fig. 48. However, in this example, S_2 slip bands apparently form in preference to the reconstituted twin; it is not known whether or not the two results are characteristic of the usual situation at $\langle 210\rangle$ and $\langle 110\rangle$ intersections, respectively, or whether they just represent alternative possibilities in each case.

The above description implies that the S_2 slip bands are on $(\bar{2}11)$ with a $\frac{1}{2}[111]$ Burgers vector; thus they represent the ultimate emissary dislocations to emerge from the crossing. However, the absence of the S_1 type of band on the exit side of T_5, together with some

experimental evidence of more than one Burgers vector in the bands, led Mahajan to suggest that the $\frac{1}{2}[\bar{1}1\bar{1}]$ and/or the $\frac{1}{2}[\bar{1}\bar{1}1]$ dislocations do not all remain in the (011) plane, but may cross-slip onto the $(\bar{2}13)$ and $(2\bar{1}1)$ planes, respectively, both of which could form part of the S_2 slip bands.

An alternative to the $(011)_T$ slip plane for the propagation of the twinning shear of T_6 into the barrier twin T_5 is the $(\bar{2}11)_T$ plane. This implies, in place of eqs (76) or (77), the dissociation:

$$3 \times \tfrac{1}{6}[111]_{(\bar{2}11)} = \tfrac{1}{6}[511]_{(23\bar{3})} + \tfrac{1}{3}[\bar{1}11]_{(211)} \tag{78}$$

where

$$\tfrac{1}{6}[511]_{(23\bar{3})} = \tfrac{1}{2}[111]_{T(\bar{2}11)_T}. \tag{78a}$$

Mahajan suggested that this reaction may be more probable than (76) and (77) because it requires less energy. The slip plane in the twin unfortunately could not be determined from the experimental data.

In iron crystals deformed at liquid nitrogen temperature, Levasseur observed that microcracks sometimes form at $\langle 011 \rangle$ type twin intersections. He attributed this to a different dissociation which leads to the formation of a $\langle 100 \rangle_T$ dislocation in the barrier twin.

Similar dissociations have been proposed for $\langle 311 \rangle$ intersections[265] and for $\langle 531 \rangle$ intersections[265,256] and have been partly confirmed by experiment, although it was not always possible to determine the slip plane in the twin. In the $\langle 311 \rangle$ intersections, Levasseur found one mechanism involving induced slip on the $\{01\bar{1}\}_T$ plane but experimental evidence again suggested that some of the lattice dislocations cross-slipped within the barrier twin from this plane to a $\{\bar{1}1\bar{2}\}$ plane. For the $\langle 531 \rangle$ intersections, Levasseur distinguished two cases, depending on whether or not the shear direction of the intersecting twin was that of the conjugate mode of the barrier twin. If it is not, slip may be conveyed across the barrier twin on a $\langle \bar{2}31 \rangle_T$ type plane; this prediction is consistent with the experimental results, but the slip plane could not be identified in the experiments. If the $\boldsymbol{\eta}_1$ direction of the incident twin equals $\boldsymbol{\eta}_2$ of the barrier twin, Levasseur concluded that crossing of the two could not be accomplished. Mahajan studied experimentally the intersection of a (211) twin by a $(\bar{1}21)$ twin and found that the shear was transmitted by slip in the (211) twin. The most probable slip plane was deduced to be $(11,\bar{2},1) = (132)_T$, in agreement with the prediction of Levasseur, but this could not be verified. A few dislocations with $\frac{1}{2}[111]$ Burgers vector were also observed, but it is not known how or why they formed.

In f.c.c. and related structures, the $\{111\}$ twinning planes intersect only in $\langle 110 \rangle$ directions so there is no twinning equivalent to the cross-slip of screw dislocations across the twin-matrix interface. The twinning dislocations of a growing deformation twin meet the $\mathbf{K}_1$ interface of a barrier twin either in pure edge configuration or with Burgers vectors at equivalent angles $+30°$ or $-30°$ to their $\langle 110 \rangle$ line direction. In the edge configuration, sometimes termed case I, an intersecting twinning dislocation would create a step of a height equal to two-thirds of the $\{111\}$ interplanar spacing in the $\mathbf{K}_1$ interface of the barrier twin, so that groups of at least three such twinning dislocations are required to give steps with heights which are integral multiples of $2d_{111}$. In terms of the double tetrahedron of Fig. 43 in which the barrier twin is on the plane d, a growing twin on plane c would have a case I intersection if its shear ($\boldsymbol{\eta}_1$) direction were $\gamma\mathbf{D}$. The (case II) 30° twinning dislocations $\gamma\mathbf{A}$ or $\gamma\mathbf{B}$ would produce steps of height $d/3$, so that again groups of three or more are necessary to obtain steps with heights which, in this case, are integral multiples of the unit height, d_{111}.

The motion of any one of the three twinning dislocations in a $\{111\}$ plane of the barrier twin other than the composition plane (d in Fig. 43) produces a secondary (or subsidiary) twin with the same orientation in all three cases. Each of the three possible twinning dislocations in the barrier twin–matrix interface, in principle, returns the barrier twin to the matrix orientation, i.e. they represent detwinning shears. However, if the barrier twin is a deformation twin, full cancellation of its associated shear strain can occur only by the motion of the appropriate barrier twinning dislocation (e.g. $\boldsymbol{\delta'C'}$ if the original twinning dislocations were $\boldsymbol{\delta C}$). In other cases, residual dislocations may form by reaction of the detwinning dislocations ($\boldsymbol{\delta'A'}$ or $\boldsymbol{\delta'B'}$) with any remaining twinning dislocations $\boldsymbol{\delta C}$.

For a type I intersection, several mechanisms have been suggested in which the accommodation shear takes place on the plane of the barrier twin which is the mirror image of the $\mathbf{K}_1$ plane of the intersecting twin; this is the $\mathbf{K}_2$ plane of a possible barrier twin produced by deformation. Mahajan and Chin[259] considered two basic decompositions of three incident edge twinning dislocations on plane $c = (1\bar{1}1)$ which encounter a barrier twin on plane $d = (\bar{1}11)$. In terms of Fig. 43, these decompositions may be written:

$$3 \times \gamma\mathbf{D}_{(c)} = 3 \times \mathbf{D'}\boldsymbol{\gamma'}_{(c')} + 2 \times \boldsymbol{\delta'}\mathbf{C'}_{(d')} \tag{79}$$

and

$$3 \times \gamma\mathbf{D}_{(c)} = 3 \times \mathbf{B'}\boldsymbol{\gamma'}_{(c')} + \mathbf{C'}\boldsymbol{\delta'}_{(d')} + 3 \times \mathbf{AD}_{(c)} \tag{80}$$

or in vector form:

$$3 \times \tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = \tfrac{1}{6}[5\bar{5}\bar{2}]_{(\bar{1}\bar{1}\bar{5})} + 2 \times \tfrac{1}{6}[\bar{1}1\bar{2}]_{(\bar{1}11)} \tag{79a}$$

with (for a type IV orientation relation)

$$\tfrac{1}{6}[5\bar{5}\bar{2}]_{(\bar{1}\bar{1}\bar{5})} = 3 \times \tfrac{1}{6}[1\bar{1}\bar{2}]_{\mathrm{T}(1\bar{1}1)_{\mathrm{T}}} \tag{79b}$$

and

$$3 \times \tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = \tfrac{1}{6}[271]_{(\bar{1}\bar{1}\bar{5})} + \tfrac{1}{6}[1\bar{1}2]_{(\bar{1}11)} + 3 \times \tfrac{1}{2}[0\bar{1}\bar{1}]_{(1\bar{1}1)} \tag{80a}$$

with

$$\tfrac{1}{6}[271]_{(\bar{1}\bar{1}\bar{5})} = 3 \times \tfrac{1}{6}[\bar{2}\bar{1}1]_{\mathrm{T}(1\bar{1}1)_{\mathrm{T}}}. \tag{80b}$$

There is a third possible dissociation of three $\gamma\mathbf{D}$ dislocations but this is just a crystallographically equivalent variant of eq. (80). The only product dislocations of eq. (79) are within the barrier twin and in the barrier twin–matrix interface; note that the latter may be written equivalently as either $\boldsymbol{\delta}\mathbf{C}_{(d)}$ or as $\boldsymbol{\delta'}\mathbf{C'}_{(d')}$. Equation (79) describes a dissociation which allows, in principle, full transmission of the twinning shear, whilst eq. (80) represents only part transmission. The large Burgers vector $\mathbf{AD}$ left on every lattice c plane of the matrix would actually reverse the shear strain due to the incident twin if the dislocations moved back along their slip plane. Clearly, this is impossible if the incident twin is driven by the applied stress, but, as mentioned in relation to eqs (68) and (69), calculations of the stress field of the piled-up twinning dislocations[262] indicate that some limited reverse slip may be driven by the pile-up stresses. Such accommodation slip will presumably cease as a reverse pile-up of the $\mathbf{AD}$ dislocations begins to form. Continued deformation then requires increasing numbers of dislocations in the primary pile-up, and hence increasing applied stress, thus producing work-hardening. The alternative assumption that the matrix dislocations remain in the interface raises many difficulties.

At first sight, both eqs (79) and (80) are able to convert the three incident twinning dislocations into three Shockley partials on the $(1\bar{1}1)_T$ plane of the twin, and thus propagate the twin by formation of a secondary twin. However, the Shockley partials $\mathbf{D'}\gamma'$ and $\mathbf{B'}\gamma'$ are actually anti-twinning dislocations,[266] as shown in the general treatment above. Mahajan and Chin[269] suggested that the resulting A–A stacking could be avoided by dissociation of the anti-twinning dislocation into two twinning dislocations with Burgers vectors at $\pm 60°$ to that of the anti-twinning dislocation. However, this hypothetical dissociation, e.g.

$$\mathbf{D'}\gamma' = \gamma'\mathbf{A'} + \gamma'\mathbf{B'} \tag{81}$$

or

$$\tfrac{1}{6}[5\bar{5}\bar{2}] = \tfrac{1}{6}[72\bar{1}] + \tfrac{1}{6}[\bar{2}\bar{7}\bar{1}] \tag{81a}$$

would not only further increase the already appreciable line energy, but would also result in two Shockleys to each lattice $(1\bar{1}1)_T$ plane. Thus the two component displacements would have to take place consecutively on the same plane, and this would negate any advantage which might otherwise be obtained from the dissociation; in particular, the A–A stacking could not be avoided. A possible mechanism involving secondary twinning is obtained from a dissociation in which only one of the two favourably oriented twinning dislocations on the $(1\bar{1}1)_T$ plane is produced, but this dissociation (described below) is also difficult to envisage.

Alternative dissociations which have been proposed include

$$3 \times \gamma\mathbf{D}_{(c)} = \mathbf{D'A'}_{(c')} + \mathbf{D'B'}_{(c')} + 2 \times \delta\mathbf{'C'}_{(d')} \tag{82}$$

or in vector form

$$3 \times \tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = \tfrac{1}{6}[4\bar{1}\bar{1}]_{(\bar{1}13)} + \tfrac{1}{6}[1\bar{4}\bar{1}]_{(\bar{1}13)} + 2 \times \tfrac{1}{6}[\bar{1}\bar{1}2]_{(\bar{1}11)} \tag{82a}$$

with

$$\tfrac{1}{6}[4\bar{1}\bar{1}]_{(\bar{1}13)} = \tfrac{1}{2}[0\bar{1}\bar{1}]_{T(1\bar{1}1)_T} \text{ and } \tfrac{1}{6}[1\bar{4}\bar{1}]_{(\bar{1}13)} = \tfrac{1}{2}[10\bar{1}]_{T(1\bar{1}1)_T} \tag{82b}$$

and

$$3 \times \gamma\mathbf{D}_{(c)} = \mathbf{D'C'}_{(c')} + \delta\mathbf{C'}_{(d')} + \mathbf{AD}_{(c)} \tag{83}$$

i.e.

$$3 \times \tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = \tfrac{1}{6}[4\bar{1}\bar{1}]_{(\bar{1}13)} + \tfrac{1}{6}[\bar{1}\,1\bar{2}]_{(\bar{1}11)} + \tfrac{1}{2}[0\bar{1}\bar{1}]_{(1\bar{1}1)}. \tag{83a}$$

Dissociation (83) and an equivalent variant, first suggested by Mahajan and Chin,[259] involves slip in the twin and also in the matrix, whereas the slip of equation (82) suggested by Remy,[266] is confined to the twin. Thus eq. (82) gives full shear transmission by slip but eq. (83) does not. Note that eq. (82) may be derived from eq. (80) by the substitution

$$3 \times \mathbf{D'}\gamma' = \mathbf{D'A'} + \mathbf{D'B'} \tag{84}$$

in place of eq. (81). The required anti-twinning shear is thus obtained from the motion of the two perfect dislocations on every three c' planes of the barrier twin.

The interaction is shown[270] schematically in Fig. 50; the obstacle twin has a lattice which is continuous through the intersection region and is undeviated, whilst the lattice of the intersecting twin is discontinuous and its two parts are displaced from each other. The matrix dislocation **AD** of eq. (83) causes similar difficulties to those discussed above in connection with eq. (80); if these dislocations move back along the slip plane (c), they must

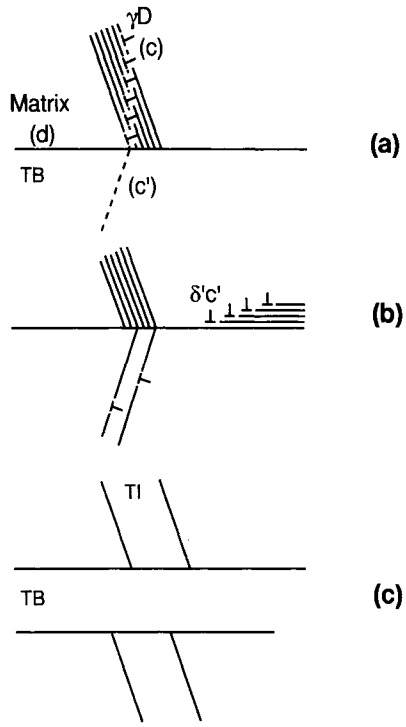

Fig. 50. Schematic illustration of twin intersection in an $L1_0$ structure. The detwinning shear removes the steps in the barrier twin (b). In the final structure the crossed twin appears undeflected and is continuous across the intersection (c) (after Sun *et al.*[271]).

do so against the applied stress; alternatively, they will block the shear transmission and lead to high stress concentrations if they remain in the interface between the matrix and the barrier twin.

Remy[266] has suggested a dissociation which is designed to allow the formation of a secondary twin. The reaction is

$$3 \times \gamma \mathbf{D}_{(c)} = 3 \times \gamma' \mathbf{B}'_{(c')} + \mathbf{B}\mathbf{D}_{(c)} + 2\delta \mathbf{B}_{(d)} \tag{85}$$

which is equivalent to

$$3 \times \tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = \tfrac{1}{6}[\bar{2}\bar{7}\bar{1}]_{(\bar{1}\bar{1}\bar{3})} + \tfrac{1}{2}[10\bar{1}]_{(1\bar{1}1)} + \tfrac{1}{3}[12\bar{1}]_{(\bar{1}11)} \tag{85a}$$

with

$$\tfrac{1}{6}[\bar{2}\bar{7}\bar{1}]_{(\bar{1}\bar{1}\bar{3})} = 3 \times \tfrac{1}{6}[21\bar{1}]_{T_{(1\bar{1}1)_T}}. \tag{85b}$$

There is thus one $\gamma'\mathbf{B}'$ dislocation on each c' plane, and glide of these partial dislocations across the barrier twin will produce a secondary (or subsidiary) twin. Once again, however, the continuity of the shear is not complete because of the matrix dislocations left at the barrier interface.

Instead of secondary twinning of the barrier twin accompanied by reverse shear in the matrix, the possibility of combining slip in the barrier twin with (reverse) twinning of the matrix has also been considered. The following dissociation was first suggested by Mahajan and Chin[259] who identified it, mistakenly, with a similar dissociation proposed previously

by Mahajan *et al.*[103] as an interpretation of experimental results. A variant of the dissociation is:

$$\gamma \mathbf{D}_{(c)} = \mathbf{D}'\mathbf{A}'_{(c')} + \gamma \mathbf{B}_{(c)} + \delta \mathbf{C}_{(d)} \tag{86}$$

which is

$$\tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = \tfrac{1}{6}[4\bar{1}\bar{1}]_{(\bar{1}1\bar{5})} + \tfrac{1}{6}[\bar{2}\bar{1}1]_{(1\bar{1}1)} + \tfrac{1}{6}[\bar{1}1\bar{2}]_{(\bar{1}11)} \tag{86a}$$

with

$$\tfrac{1}{6}[4\bar{1}\bar{1}]_{(\bar{1}1\bar{5})} = \tfrac{1}{2}[0\bar{1}\bar{1}]_{\mathrm{T}(1\bar{1}1)_{\mathrm{T}}} \tag{86b}$$

and there is an equivalent variant which leaves a $\gamma\mathbf{A} = \frac{1}{6}[121]$ partial in the matrix and produces slip dislocations $\mathbf{D}'\mathbf{B}' = \frac{1}{2}[10\bar{1}]_{\mathrm{T}}$ to carry the shear across the barrier twin. These two equations are listed by Remy[260] together with two other similar "mixed" dissociations of $3\gamma\mathbf{D}$ in which the product combinations of twin slip and matrix twinning dislocations are interchanged.

The reaction (86) clearly does not accomplish full shear transmission, and the difficulties now centre on the twinning dislocations with Burgers vector $\gamma\mathbf{B}$ left in the matrix. If these move away from the interface on plane c under the effective stress of the pile-up, they will detwin the incident twin. The detwinning shear direction is at 60° to the twinning direction of the incident twin, so that about one-half of its shear strain is effectively cancelled.

The increases in line energy are even higher in mechanisms involving secondary twinning than in those which depend entirely on slip. The Frank rule estimate[258] gives an energy increase of about 133% and 167% of the initial line energy for slip mechanisms (83) and (82), respectively, and about 233% and 400% for secondary twinning (eq. (85)) and detwinning (eq. (86)), respectively. These figures depend on the assumption that the initial state can be taken as well separated single twinning dislocations. Smaller energy increases (17, 33, 117 and 250%, respectively) are obtained for an initial state consisting of emissary dislocations with Burgers vector $\mathbf{AD} + \mathbf{BD}$ instead of $3\gamma\mathbf{D}$, but this scarcely seems physically realistic. As already remarked, these high energies can only be overcome if appreciable stress concentrations are formed at the head of the incoming slip or twinning dislocations. However, the energy classification gives some indication that accommodation of the incident twinning shear is likely to involve slip rather than secondary twinning.

The above mechanisms all concern case I intersections in which the f.c.c. twinning dislocations meet the $\mathbf{K}_1$ interface in edge orientation. Very little work, either theoretical or experimental, on case II intersections appears to have been published, apart from an early paper by Mahajan *et al.*[103] who investigated the propagation of a thin deformation twin through a thick annealing twin interface in irradiated copper. Some work on case II intersections in superlattice ($L1_0$) structures based on f.c.c., has been published recently and is discussed below, but the available experimental results on f.c.c. intersections are first summarized. Despite a few very careful experiments, it has not been possible to decide the operative mechanism in most individual cases.

Remy[258] reviewed work on f.c.c. structures including his own investigations of twin–twin interactions in cobalt based alloys and in a manganese–chromium steel. He used polycrystalline specimens and concluded in all cases that accommodation was entirely by slip. On the other hand, Mahajan and Chin,[243,259] working with single crystals of Co–8wt%Fe, which had been given a constrained, plane-strain deformation, found examples of shear

propagation by both slip and secondary twinning, with the latter dominating. Figure 51 taken from this work shows an example of slip propagation, and Fig. 52 shows secondary twinning. At high magnifications, very complex structures were observed in conjunction with secondary twinning. As shown in Fig. 53, the matrix is heavily twinned on $(\bar{1}1\bar{1})$ planes, marked T_1 on the micrograph, and the contrast shows that a secondary twin has formed in the barrier twin (T_2) with a habit plane identified as $(1\bar{1}\bar{5}) = (\bar{1}11)_T$. The microstructure also contains (i) some triangular-shaped, striated regions, contiguous to the secondary twins, and (ii) some very small twins within T_1. The striated areas occur mainly on one, but occasionally on both, sides of the secondary twins. These regions may also be subsidiary twins, but the way in which the complex structure has evolved is not known. The choice of accommodation by slip or secondary twinning is probably very dependent both on the ratio of the resolved shear stresses at which slip and twinning can be initiated and on the complex local stresses.

In their investigation of irradiated copper, Mahajan *et al.*[103] studied the penetration of the $(11\bar{1})$ interface of an annealing twin by a thin deformation twin with $\mathbf{K}_1 = (\bar{1}11)$ and $\boldsymbol{\eta}_1 = [\bar{1}1\bar{2}]$. They interpreted their results in terms of a dissociation into a perfect dislocation in the barrier twin and a twinning dislocation in the matrix. Transferring to a variant in which the barrier twin is again $d = \{\bar{1}11\}$ and the plane of the incident twin is c, this dissociation may be written:

$$\gamma \mathbf{B}_{(c)} = \mathbf{A}'\mathbf{D}'_{(c')} + \gamma \mathbf{D}_{(c)} + \mathbf{C}\boldsymbol{\delta}_{(d)} \tag{87}$$

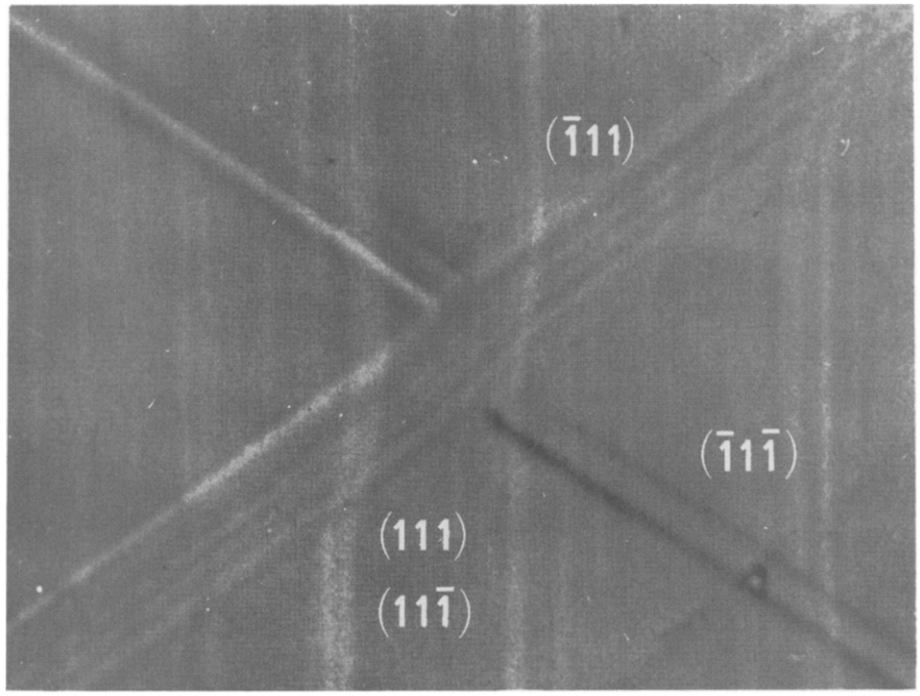

Fig. 51. Optical micrograph illustrating the features of twin–twin intersection involving slip in the cross twin and slip–twin interactions observed in a deformed Co–8wt%Fe alloy single crystal. The plane of the micrograph is (110) (after Mahajan and Chin[259]).

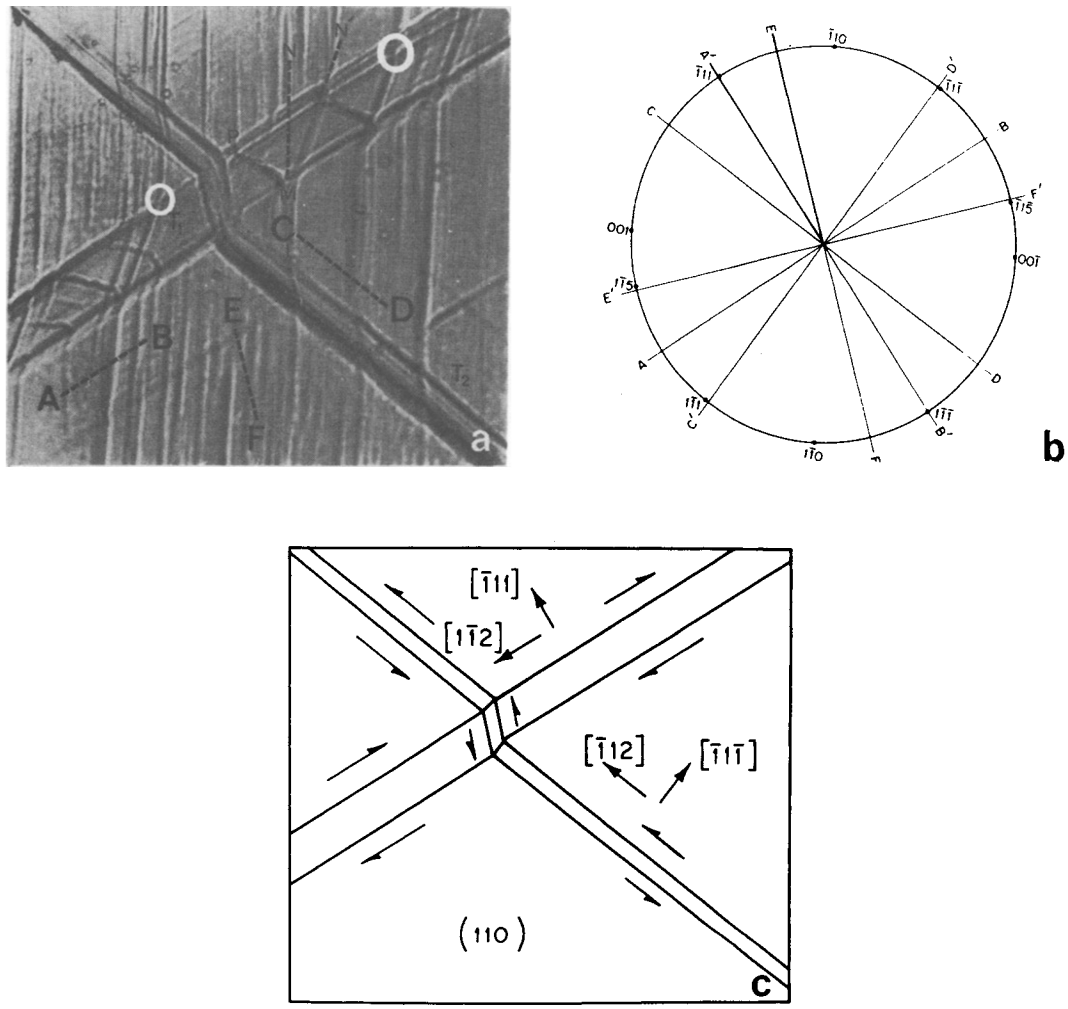

Fig. 52. (a) Micrograph showing twin–twin and slip–twin interactions in a deformed Co–8wt%Fe alloy single crystal. When T_1 propagates through an existing slip trace MN, it is sheared into MN′. (b) Single-surface trace analysis of the observed traces. (c) Schematic diagram of the twin intersection showing the imposed shear stress pattern (after Mahajan and Chin[259]).

i.e.

$$\tfrac{1}{6}[\bar{2}\bar{1}1]_{(1\bar{1}1)} = \tfrac{1}{6}[\bar{4}11]_{(1\bar{1}5)} + \tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} + \tfrac{1}{6}[1\bar{1}2]_{(\bar{1}11)} \tag{87a}$$

with

$$\tfrac{1}{6}[\bar{4}11]_{(1\bar{1}5)} = \tfrac{1}{2}[011]_{T(1\bar{1}1)_T}. \tag{87b}$$

Although eq. (87) resembles eq. (86), the two dissociations are not equivalent since the incident twinning dislocations meet the barrier interface in edge orientation in eq. (86) and in 30° orientation in eq. (87). The dissociation (87) is thus a class II reaction, as pointed out by Sun *et al.*[270] Mahajan *et al.* suggested that the new twinning dislocations in the matrix will produce a new twin within the incident twin; in fact, this new twin represents detwinning of the incident twin to the matrix orientation.

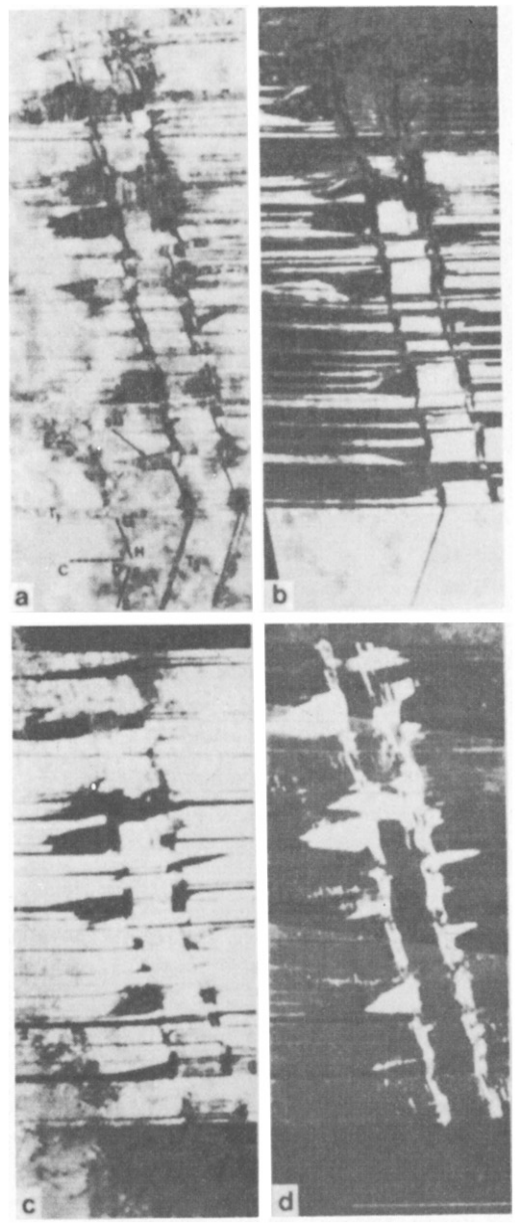

Fig. 53. Twin interactions observed in a Co–8wt%Fe alloy single crystal. The plane of the micrograph in each case is ~(110). Micrographs (b), (c) and (d) show dark-field of the matrix, T_1's and secondary twins, respectively. The traces of $(\bar{1}1\bar{1})$, $(\bar{1}11)$ and $(1\bar{1}\bar{5})$ planes in the (110) plane are identified by CD, EF and GH, respectively. SM refers to the twinned region in the matrix that may have undergone a shear reverse to that of T_2's. The marker represents one micron (after Mahajan and Chin[243]).

In a very recent investigation, Müllner *et al.*[272] studied twin intersection in austenitic steel of low stacking fault energy, under conditions in which twinning is the dominant mode of deformation. They discuss their results in terms of the disclination model of a twin, described above, which they also assume applies to a moving twin. In their analysis (Fig. 54), two

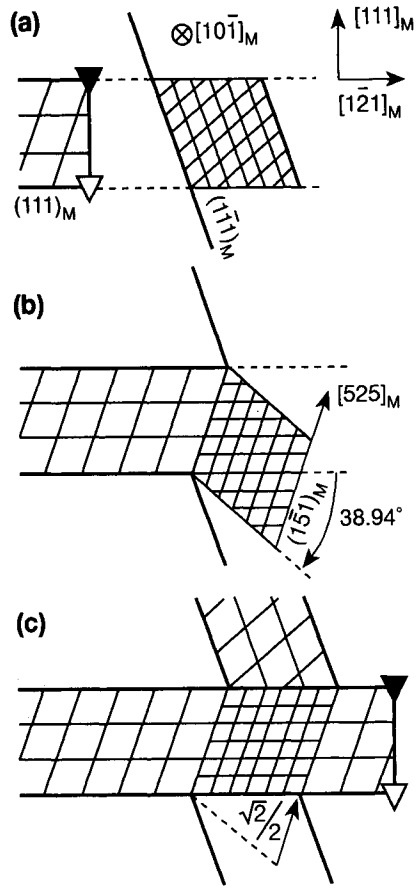

Fig. 54. Separated transformations of twin intersections: (a → b) rotation of −38.94°, (b → c) pseudo-shear of $\sqrt{2}/2$. Asymmetrical Σ9 boundary between the intersecting twins (after Müllner *et al.*[272]).

different kinds of motion of a disclination dipole are considered. In the simplest case, the incomplete dislocation wall migrates normal to itself, and in the other case pairs of oppositely signed dislocations move from the plane midway between the dipole arms out to the two limiting planes. The first kind of motion is representative of the intersecting twin before and after crossing the barrier twin, whereas the second kind represents motion along the {111} plane of the barrier twin which forms the mirror image in its $\mathbf{K}_1$ plane of the $\mathbf{K}_1$ plane of the intersecting twin. As a result of these (simultaneous) processes, the intersected volume undergoes a combined rotation and a pseudo-shear, so called because it is a *lattice invariant deformation* equivalent to the displacement of lattice dislocations and so does not change the crystal orientation. This pseudo shear takes place on the anti-twinning system $\mathbf{D}\gamma_{(c)}$ of eq. (80), the rotation is 38.94° about the normal to the {110} plane of shear, and the pseudo-shear of magnitude $(2)^{-\frac{1}{2}}$ restores the $\mathbf{K}_1$-barrier twin interface plane back to its original orientation, but does not change the rotated lattice. Thus the predicted morphology (Fig. 54d) has an undeviated incident twin which traverses the barrier twin without any change of orientation, and a deviated barrier twin with an interrupted lattice in the intersected region. Other mechanisms which lead to one deviated and one undeviated twin include the dissociations

(79) and (82), and the undeviated slip on $\{\bar{1}1\bar{5}\}_T$, but combined observation of whether one or both twins had reorientated habit planes and/or reorientated lattices should discriminate among the various possibilities.

Some experimental results on an austenitic steel are claimed by the authors to support slightly modified versions of this theoretical description. In one experimental condition, a number of small secondary twins were found in the barrier twin, and it is assumed that these must move to the boundary of the intersection volume to allow penetration to take place. The experiments showed that the intersected volume had the same orientation as the intersecting twin, as predicted by the above theory. In another observed configuration, the intersecting twin was not a single crystal but a 'twin system' consisting of several small twins with an overall shear smaller than the twinning shear of $2^{-\frac{1}{2}}$. This implies a reduction in the rotation of the intersected volume relative to the matrix, so that its final orientation is between the orientations of the barrier and incident twins, and may be predicted if the shear of the imperfect incident twin or twinning system is known. The experimental results for this case showed indeed that the intersected volume had an intermediate orientation, and the measured rotation agreed reasonably well with the predicted value.

There has been much interest in recent years in the mechanical properties of intermetallic superlattice compounds of aluminium, titanium and nickel and Yamaguchi and Umakoshi[273] have recently published a comprehensive review. The mechanical behaviour, and especially the temperature dependence of the stress, is often unusual and attention has focussed mainly on attempts to explain it in terms of dislocation properties in superlattices, but there have also been several recent investigations of twinning.[270,271,274–278] Since the various structures may all be regarded as derived from f.c.c. structures by some form of long-range ordering, the number of true twin modes which correspond directly to f.c.c. modes is zero in cubic superlattice structures and is severely restricted in non-cubic structures, as discussed in Section 2.6. Nevertheless, twinning is an important mode of deformation in superlattices such as TiAl with the tetragonal $L1_0$ structure since the number of available slip systems is similarly restricted.

The double tetrahedron of Fig. 43 may also be used to discuss twinning in $L1_0$, but there is now only one $\frac{1}{6}\langle 112]$ twinning vector to each $\{111\}$ plane. If the twinning direction of the barrier twin is again taken as $\gamma\mathbf{D}$, eq. (79) may be applied directly to the $L1_0$ structure, but eq. (80) is not valid since $\mathbf{B}'\gamma'$ is a vector of type $\frac{1}{6}\langle 121]$ which produces a complex fault, thought to be of high energy. Equations (83) and (84) may also be extended to the superlattice structure, but since two dislocations such as $\mathbf{D}'\mathbf{A}'$ or $\mathbf{D}'\mathbf{B}'$ are needed to form a perfect dislocation of the superlattice, the dissociations have now to be written:

$$6 \times \gamma\mathbf{D}_{(c)} = 2\mathbf{D}'\mathbf{A}'_{(c')} + 2\mathbf{D}'\mathbf{B}'_{(c')} + 4 \times \delta'\mathbf{C}'_{(d')} \tag{83d}$$

and

$$6 \times \gamma\mathbf{D}_{(c)} = 2\mathbf{D}'\mathbf{A}'_{(c')} + 2\delta'\mathbf{C}'_{(d')} + 2\mathbf{A}\mathbf{D}_{(c)}. \tag{84d}$$

Figure 50 shows the dissociation of six elementary twinning dislocations, and thus applies to eq. (83d) as well as to (83).

None of these proposed dissociations is compatible with the latest experimental evidence for TiAl which shows that one twin is undeflected but the lattice is continuous through the deflected twin. Wardle[276] suggested that slip in the barrier twin might take place on the (001) plane rather than on the usual $\{111\}$ plane. This is not generally considered possible in f.c.c. structures, but may well be feasible at fairly high temperatures in $L1_0$ structures, and there

is some recent experimental evidence in support of this hypothesis. Wardle suggested two dissociations involving $(001)_T$ slip, one giving full shear transmission and one giving part transmission. The latter is nevertheless more probable because of the difficulty of avoiding A–A stacking with the full transmission. Wardle's dissociation is:

$$6\gamma \mathbf{D}_{(c)} = 3\mathbf{D'C'}_{(001)_T} + \mathbf{CD}_{(001)} \tag{88}$$

or in vector form

$$6 \times \tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = 3 \times \tfrac{1}{6}[1\bar{1}\bar{4}]_{(\bar{2}2\bar{1})} + \tfrac{1}{2}[1\bar{1}0]_{(001)} \tag{88a}$$

with

$$\tfrac{1}{6}[1\bar{1}\bar{4}]_{(\bar{2}2\bar{1})} = \tfrac{1}{2}[1\bar{1}0]_{T(001)_T}. \tag{88b}$$

The displacements $3\mathbf{D'C'}$ and $\mathbf{CD}$ take place every six atomic (001) planes. Since they form along the direction $\mathbf{AB} = [110]$, they are both initially edge dislocations and could become immobile at low temperatures by forming a Lomer–Cottrell lock.

In addition to shear transmission on $\{111\}$ and (001) planes, experimental results on twin intersections in TiAl have necessitated the consideration of "undeflected" slip, i.e. slip on the plane and direction of the barrier twin which are parallel respectively to the $\mathbf{K}_1$ plane and $\boldsymbol{\eta}_1$ direction of the incident twin. Except for the special case of $\langle 111 \rangle$ slip–twin and twin–twin intersections in b.c.c. structures, where the undeflected plane is a usual $\{112\}$ slip or twinning plane, undeflected transmission of the shear has generally been neglected because of the difficulty in envisaging atomic slip on high-index planes and in high-index directions. Nevertheless the geometrical constraints are sometimes able to force the system to adopt an unusual, undeflected slip system inside a barrier twin, as first noted for zinc by Tomsett and Bevis.[252] The first indication of undeviated shear in f.c.c.-derived materials came in the work of Pirouz *et al.*[173–175,279] and Dahmen *et al.*[280] on silicon and other materials with the diamond cubic structure. The undeviated shear is closely related in the two cases, but produces a different final structure (see below). In the $L1_0$ structure, the undeflected twinning dislocation becomes a new vector given by:

$$\tfrac{1}{6}[1\bar{1}\bar{2}]_{(1\bar{1}1)} = \tfrac{1}{18}[5\bar{5}\bar{2}]_{T(\bar{1}1\bar{5})_T}. \tag{89}$$

If the shear is transmitted homogeneously, there is a zonal displacement of this magnitude every third $(\bar{1}1\bar{5})$ plane. However, this would produce A–A stacking of the $(\bar{1}11)_T$ planes (see Fig. 55), and even if the shear is accompanied by atomic shuffles, these are all likely to require that atoms pass each other at distances corresponding to the small A–A separation. The uniform shear may, in principle, be converted into a lattice-preserving slip shear if a lattice dislocation of type $\frac{1}{2}[5\bar{5}\bar{2}]$ is formed on every 27 $(\bar{1}1\bar{5})$ planes. Although the large magnitude of the Burgers vector (nine times that of an elementary twinning dislocation) implies that a very large stress concentration will be needed to produce this slip, there is nevertheless some good experimental evidence that it is the operative mechanism in TiAl at relatively low temperatures.

As mentioned above, the undeflected mechanism in TiAl is essentially identical with twin–twin interactions in elemental diamond cubic materials and in compounds which are ordered versions of the diamond cubic structure. Twin intersections and secondary twinning in such structures have been investigated in detail by Pirouz and coworkers using

high resolution electron microscopy. They found good evidence for undeflected transmission which in this case, however, results not in emissary slip on the $(11\bar{5})$ plane but in the formation of a new crystal structure, the diamond–hexagonal structure. A possible reason for this is that A–A stacking, or rather shuffles which require atoms to pass at A–A separations, whilst inconceivable in f.c.c. structures might not be so energetically unfavourable in diamond cubic and related structures in which the closest interatomic distance (sometimes described as the length of the covalent bond) is appreciably shorter than the smallest lattice vector.

Figure 55c shows that uniform shear on the $(11\bar{5})$ plane produces the A–A stacking, but Dahmen *et al.*[280] suggested that this could be avoided if the shear were combined with atomic shuffles to change the A–A stacking to the hexagonal-type A–B stacking. The formation of the diamond hexagonal phase with stacking of type ...AαBβ... has been observed by lattice resolution electron microscopy in twin–twin intersections in silicon and germanium (see Fig. 55), and has also been found in the matrix phase of silicon. This latter observation is believed to result from secondary twinning inside previously formed twins, and its subsequent propagation out into the matrix.

Structural changes in twin intersections have not been observed either in pure f.c.c. metals or in ordered compounds. One reason is the stacking difficulty already mentioned, but also in a tetragonal phase such as TiAl, the structure following the shuffles would be (approximately) orthorhombic, or (more strictly) monoclinic.

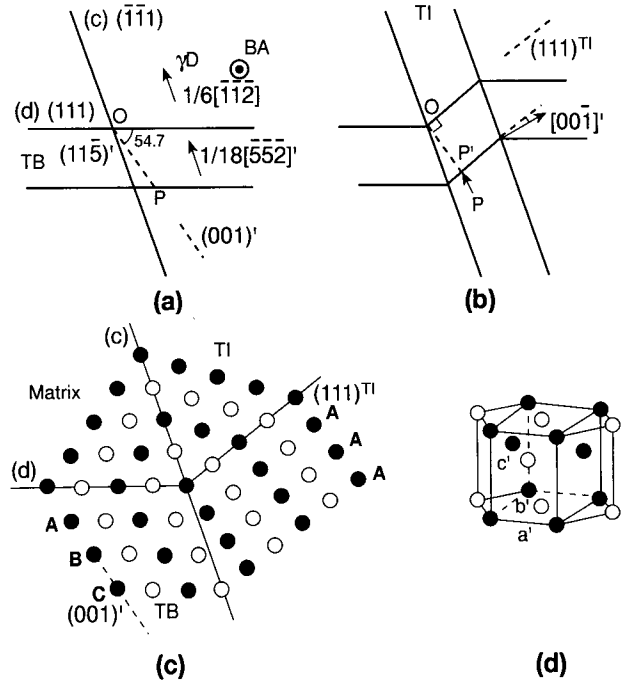

Fig. 55. (a) Schematic illustration showing the structural changes associated with the undeflected penetration. (b) The shear of the incident twin (TI) is $\frac{1}{18}[\bar{5}\bar{5}2]'$ on plane $(11\bar{5})'$ and it transforms the trace of (001)′ OP to OP′ which is normal to the trace of $(111)^{TI}$. (c) Arrangement of atoms around an undeflected intersection in which ...AAA... stacking occurs on plane $(111)^{TI}$; open and solid circles represent respectively Ti and Al atoms which lie on adjacent $(1\bar{1}0)$ planes. (d) Unit cell of an orthorhombic structure of the ...ABAB... stacking (after Sun *et al.*[270]).

Wardle *et al.*[276,278] also considered class II intersections in TiAl in terms of penetration on octahedral planes and they suggested the following two dissociations

$$3 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = 3 \times \boldsymbol{\beta}'\mathbf{A}'_{(b')} + 2\mathbf{DC}_{(b)} + 2\mathbf{C}'\boldsymbol{\delta}'_{(w')} \tag{90}$$

and

$$3 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = 3 \times \boldsymbol{\beta}'\mathbf{A}'_{(b')} + 4 \times \tfrac{1}{3}\mathbf{DC}_{(b)} + \tfrac{1}{2} \times \mathbf{CD/AB}_{(100)} \tag{91}$$

where **CD/AB** means a vector which is twice that joining the mid-points of **CD** and **AB**. In vector form, these equations are

$$3 \times \tfrac{1}{6}[112]_{(11\bar{1})} = \tfrac{1}{6}[7\bar{1}2]_{(\bar{1}31)} + [\bar{1}10]_{(11\bar{1})} + \tfrac{1}{3}[1\bar{1}2]_{(\bar{1}11)} \tag{90a}$$

with

$$\tfrac{1}{6}[7\bar{1}2]_{(\bar{1}31)} = 3 \times \tfrac{1}{6}[\bar{1}\bar{1}\bar{2}]_{T(\bar{1}\bar{1}1)_T} \tag{90b}$$

and

$$3 \times \tfrac{1}{6}[112]_{(11\bar{1})} = \tfrac{1}{6}[7\bar{1}2]_{(\bar{1}31)} + \tfrac{2}{3}[\bar{1}10]_{(11\bar{1})} + [004]_{(100)}. \tag{91a}$$

Both of these proposed dissociations give incomplete shear transmission and leave dislocations with Burgers vector **DC** normal to the shear direction of the incident twin which must move back into the matrix along the twin interface. This effectively fully reverses the component of the twinning shear normal to the intersection line in the mechanism of eq. (90) and partly cancels it in the mechanism of eq. (91), but the displacement parallel to this line is increased. Sun *et al.*[270] give various reasons why these dissociations will probably not operate in practice, especially the inability, in normal circumstances, of the pile-up stresses to drive the new matrix dislocation with Burgers vector **DC** away from the line of intersection.

Four further dissociations suggested by Sun *et al.* are:

$$3 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = \mathbf{C}'\boldsymbol{\delta}'_{(d')} + \mathbf{C}'\mathbf{D}'_{(b')} + \mathbf{B}'\mathbf{A}'_{(d')} \tag{92}$$

$$3 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = 2 \times \mathbf{C}'\mathbf{A}'_{(b')} + \mathbf{DC}_{(b)} \tag{93}$$

$$3 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = 3 \times \boldsymbol{\beta}'\mathbf{A}'_{(b')} + \mathbf{C}'\mathbf{D}'_{(b')} + \mathbf{DC}_{(b)} \tag{94}$$

and

$$3 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = 3 \times \boldsymbol{\beta}'\mathbf{A}'_{(b')} + 3 \times \mathbf{C}'\mathbf{D}'_{(b')}4 + 2\chi\boldsymbol{\delta}'\mathbf{C}'_{(d')} \tag{95}$$

or equivalently

$$3 \times \tfrac{1}{6}[112]_{(11\bar{1})} = \tfrac{1}{6}[1\bar{1}2]_{(\bar{1}11)} + \tfrac{1}{6}[\bar{1}14]_{(\bar{1}31)} + \tfrac{1}{2}[110]_{(\bar{1}11)} \tag{92a}$$

$$3 \times \tfrac{1}{6}[112]_{(11\bar{1})} = [101]_{(11\bar{1})} + \tfrac{1}{2}[\bar{1}10]_{(11\bar{1})} \tag{93a}$$

$$3 \times \tfrac{1}{6}[112]_{(11\bar{1})} = \tfrac{1}{6}[7\bar{1}2]_{(\bar{1}31)} + \tfrac{1}{6}[\bar{1}14]_{(\bar{1}31)} + \tfrac{1}{2}[\bar{1}10]_{(11\bar{1})} \tag{94a}$$

$$3 \times \tfrac{1}{6}[112]_{(11\bar{1})} = \tfrac{1}{6}[7\bar{1}2]_{(\bar{1}31)} + \tfrac{1}{3}[\bar{1}14]_{(\bar{1}31)} + \tfrac{1}{3}[\bar{1}1\bar{2}]_{(\bar{1}11)}. \tag{95a}$$

These mechanisms are all geometrically and crystallographically possible but all have associated physical difficulties, especially with incomplete shear transmission. They fail to agree with the experimental results in various ways. A further suggested dissociation

$$9 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = 3 \times \mathbf{C}'\mathbf{D}'_{(b')} + 2 \times \mathbf{C}'\mathbf{A}'_{(b')} + 2\mathbf{B}'\mathbf{A}'_{(d')} \tag{96}$$

which produces accommodation entirely by slip in the barrier twin is considered by Sun *et al.*[270,271] more probable than any of the above, except that the dislocation $2\mathbf{C'A'}$ is a pure screw superdislocation as it crosses the interface and may thus be locked in $L1_0$ alloys. This suggests that the shear may instead utilize one of the twinning partials, so that eq. (97) is further modified to

$$9 \times \boldsymbol{\beta}\mathbf{A}_{(b)} = 3 \times \boldsymbol{\beta}'\mathbf{A}'_{(b')} + 4 \times \mathbf{C'D'}_{(b')} + 2 \times \mathbf{B'A'}_{(d')} \tag{97}$$

which in vector form is

$$9 \times \tfrac{1}{6}[112]_{(11\bar{1})} = 3 \times \tfrac{1}{6}[7\bar{1}2]_{(\bar{1}\bar{3}1)} + 4 \times \tfrac{1}{6}[\bar{1}14]_{(\bar{1}\bar{3}1)} + 2 \times \tfrac{1}{2}[110]_{(\bar{1}11)}. \tag{97a}$$

This dissociation now has the disadvantage that the three twinning partials of type $\boldsymbol{\beta}'\mathbf{A}'$ have to be distributed over nine planes, so if they are evenly spaced, they will create a large number of stacking faults. However, if they cluster together in groups on successive planes, each such group will be converted into a secondary twin of the barrier twin. One-third of the total volume will be occupied by such twins.

The crystallographic analyses demonstrate clearly that in the simpler crystal structures there are many different geometrically feasible ways of continuing the shear of a moving twin which encounters an obstacle, especially a barrier twin. The conclusion of Sun *et al.*[270,272] was that the main influence on the dislocation emissions comes from the stresses at pile-ups of incident twinning dislocations.

7. TWINNING AND FRACTURE

In many b.c.c. metals and alloys, a ductile–brittle transition is observed at temperatures similar to those at which plastic deformation by twinning becomes more important than slip. The high stress concentrations provided by deformation twins have long been recognized as potentially important in crack nucleation, and there is experimental evidence in some materials that cracks are formed, for example, at twin–twin intersections. Nevertheless, it is necessary to acknowledge at once that twinning and fracture are essentially independent phenomena in the sense that brittle fracture is often observed without any detectable twinning, and that extensive plastic deformation by twinning without cracking is often a feature of tensile or compression tests at extremely low temperatures (see Figs 24 and 25).

There is much evidence available to show that in certain materials, either cracks may induce twins or twins may nucleate cracks. One factor common to both twinning and brittle fracture is the very high growth rate which is often an appreciable fraction of the elastic wave velocity. Thus a rapidly expanding crack which has high shear stresses near its tip produces a very high rate of stressing in the surrounding material, and this high stress rate is a condition likely to favour twinning. In an early paper, Bilby and Bullough[281] showed theoretically that twins may form either side of a moving crack, and this was soon afterwards verified by Derruyterre and Greenough[282] in experiments on zinc. In his comprehensive review of the association of twinning and fracture in b.c.c. metals, published in 1982, Reid[283] attributes the first suggestion of the reverse process, namely that twins induce cracking, to O'Neill[284] in 1926, but it was only in the period from 1945 onwards that this possibility began to be seriously investigated. The pioneering studies of Hull[285–287] and Honda[288] showed examples of twin-induced cracking in iron–silicon single crystals, especially at twin–twin intersections. Hull suggested that when twins with non-parallel shear directions

intersect, microcracks are most likely to form when the resolved normal stress on a {001} potential cleavage plane is large and the line of intersection of the twins is nearly parallel to this plane. It follows that the experimental condition most likely to induce cracking is a tensile test along a ⟨001⟩ axis which could produce (001) cracks at either $\langle 1\bar{1}0\rangle$ intersections of {112} and $\{\bar{1}\bar{1}2\}$ twins or at ⟨110⟩ intersections of $\{1\bar{1}2\}$ and $\{\bar{1}12\}$ twins.

The association of twins and cracks may be tested experimentally either by direct examination of fracture surfaces or by optical or electron metallography. The fracture surface method is valid only for single crystals, where the surface contours ('river lines') generally give a unique indication of the place where the cleavage crack was nucleated. Evidence of a twin pair at or very near to this site thus supports Hull's hypothesis, especially if the twinning systems can be identified. Metallographic evidence of the association of microcracks and twins is less convincing since the origin of either defect is not usually identifiable, thus leaving the 'which came first' problem unsolved.

The early experimental results of Honda[288] and Terasaki[289] on pure iron are consistent with Hull's assessment; they observed an orientation dependence of the mode of stress relief in which cracking was preferred to slip accommodation under appropriate conditions. Edmondson[290] confirmed that cracks form at twin intersections in iron, and they were subsequently observed in molybdenum by Reid *et al.*[291] and in chromium by Marcinkowski and Lipsitt.[210]

There is an apparent contradiction between the experimental work just quoted and the absence of cracking in, for example, the investigations of Mahajan[150,165,256,292] described in Section 6. The difference is probably mainly a chemical effect since both fracture properties and twinning are very sensitive to composition, but in terms of twinning parameters, it may plausibly be linked to the relative growth rates of twins in different materials. Since the dislocation density cannot be increased instantaneously, the sudden imposition of a high stress rate in a localized region requires high dislocation velocities in order to accommodate the field of the twin by slip. In b.c.c. materials, where dislocation velocity is very stress-dependent, this in turn requires high local stresses, which may then exceed the stress required for crack nucleation. This suggests that cracks are more likely to form from twins with high growth velocities at places where the density of mobile dislocations is low, so that the difference in behaviour may be linked to fast twin growth in iron, iron–silicon, chromium, etc. and to much slower growth in molybdenum–rhenium alloys. An alternative description is that the highest stresses develop around a twin which has been prevented from further growth, e.g. by a barrier twin, and the resultant pile-up produces a very high, static stress field which causes cracking.

There are several later reports[293–296] of twin/crack association in b.c.c. metals and alloys, and it is now well established that in many, but not all, such materials, microcracking may be induced by twinning. However, this is by no means the whole story, since the observed microtwins are not necessarily related to the macrocrack which eventually causes failure. The microcracks vary considerably in different experiments, sometimes being located within one or other of the twins rather than in the matrix or along the twin–matrix interface. Microcracks sometimes form at twin–grain boundary interfaces, when they are usually intergranular, or at places where a twin reaches a free surface.

Since the spatial conjunction of a twin and a crack is not sufficient evidence that macroscopic failure is induced by the twin, Williams and Reid[297] attempted to decide whether or not the crack and the twin form at the same time. They used an electromagnetic technique capable of indicating separately the onset of twinning and fracture with a high temporal resolution. With notched samples of coarse-grained silicon iron tested in tension at 77 K,

signals identified as bursts of twins were detected at times of 2–20 μs before the fracture signal, thus indicating that in this case, the twin formation led to both the nucleation and the subsequent growth of the major crack which caused failure. On the other hand, no twinning signal before failure was detectable in similar unnotched specimens. This difference is consistent with earlier indirect attempts to decide on the role of twins by comparing the twinning stress in a compression test with the fracture stress in tension. Reid pointed out that such a comparison is invalid if there is any texture in the material tested (see discussion in Section 5.1). Similar criticism applies to various attempts to test the association of twinning and fracture by comparison of the k_y, k_t and k_f factors derived respectively from Hall–Petch plots of yield, twinning and fracture stresses vs grain size.

As already emphasized, twinning in h.c.p. materials is often a ductilizing rather than an embrittling agent, inasmuch as twin formation helps to compensate for the small number of operative slip systems, and in particular the difficulty of achieving $\mathbf{c} + \mathbf{a}$ slip. The beneficial effect of twinning on ductility is illustrated by the embrittlement of cadmium–magnesium alloys[65] in the composition range where $\{10\bar{1}2\}$ twins are unable to form because of the critical axial ratio of $3^{\frac{1}{2}}$. In general, more than one twinning mode may be required to secure compatible deformation by slip and twinning of polycrystalline material, and it is noteworthy that the very brittle h.c.p. metals (e.g. beryllium or zinc) twin only on $\{10\bar{1}2\}$ whereas the more ductile metals (titanium, zirconium, rhenium) have additional twinning modes. Such correlation is far from perfect; cadmium, for example, has an axial ratio similar to that of zinc and also deforms by twinning only on $\{10\bar{1}2\}$, but is nevertheless appreciably less brittle.

The h.c.p. basal plane is the only cleavage plane for most h.c.p. materials, but in beryllium prismatic cleavage is also observed. There appears to be much evidence[181,244,263,298,299] of plastic accommodation at slip–twin and twin–twin[181,300–302] intersections. Yoo[181] has suggested that twin interfaces are effective sites for nucleation of other twins in materials like titanium, and for cracks in less ductile materials like beryllium, but in contrast to the b.c.c. work, there is little direct evidence of the association of twins with cracks.

Almost all f.c.c. metals and alloys are ductile at all temperatures, but there are exceptions, namely austenitic steels containing about 20% chromium with high manganese and nitrogen contents. Certain alloys of low stacking fault energy undergo ductile–brittle transitions at sub-zero temperatures; the transition temperature is increased by nitrogen and manganese additions (which lower the fault energy) and also by nickel additions. Much of the deformation is produced by twinning, and microcracking has been observed at twin–twin intersections. In a very recent paper, Müllner *et al.*[303] develop a model of crack nucleation in such alloys in terms of the stress field around a blocked twin, modelled as a disclination dipole. In their model which is claimed to give good agreement with experiment, the fracture tendency depends upon the stress field of the blocked twin and the local density of mobile dislocations.

In summary, there is good evidence that blocked twins can nucleate microcracks in some materials and incomplete evidence that these cracks may initiate macroscopic failure. However, brittle failure without detectable twinning appears to occur also in many b.c.c. alloys.

8. ADDENDUM

This review has been written at a time when interest in deformation twinning has risen sharply, largely as a result of its importance in the deformation behaviour of many

intermetallic compounds. The inevitable consequence that some important papers could not be included because they were published after the review was completed would normally have to be accepted, but in one respect 1993 was an unusual year. At the Fall meeting of the Metallurgical Society of AIME, a symposium was organized to discuss all aspects of 'The Twinning of Advanced Materials', and many important papers were presented. A few authors kindly sent preprints in time for their work to be included in the body of this review, but for others the timing made this impossible. However, the majority of the authors whose work concerned deformation twinning and was thus relevant to this review, generously responded to a later request for preprints, and thus facilitated the writing of this Addendum. In addition to those papers presented at the conference, the opportunity has been taken to include a few others which have either been recently published or are soon to be published in the general literature. The topics mentioned in the Addendum will follow, as far as is practicable, the same order as the material in the main text.

In his introductory paper to the twinning symposium, A. G. Crocker[309] described how the definition of a twinning shear as "a homogeneous shear which restores the lattice in a new orientation" led to a generalization of the formal crystallographic theory of deformation twinning, which included the possibility that all four of the crystallographic elements defining a particular mode are irrational. He also discussed the theory of twinning in a four-dimensional space,[310] and its relation to three-dimensional twinning.

A striking new crystallographic result is the report by Baggerly and Williams[311] of an unusual twinning mode in a Ti–6.5at%Mo alloy with a b.c.c. structure. Single crystals of the alloy were quenched from the solid solution region and then tested at temperatures ranging from 77 to 400 K. Deformation was mainly effected by twinning, and the amount of slip was negligible, but the twinning did not utilize the expected $\{112\}\langle\bar{1}\bar{1}1\rangle$ mode. Instead, the $\mathbf{K}_1$ plane was unambiguously identified as $\{33\bar{2}\}$ and the $\boldsymbol{\eta}_1$ direction as $\langle 113\rangle$. As emphasized in Section 2.5, the normal b.c.c. mode is the no shuffle mode of lowest shear. Table 1 shows, however, that the $\{332\}$ mode and its conjugate have one-half of the shear of the usual $\{112\}$ mode, and thus become the modes of lowest shear if up to one-half of the atoms are allowed shuffle displacements relative to the others. The appearance of this mode might therefore not seem so anomalous, were it not that there are no reports of its occurrence in any other alloy system. Excellent agreement was found between the measured shear of 0.35 and the theoretical shear of 0.352. The reason for this unusual mode has yet to be determined.

Goo[312] has reconsidered the problem of twinning in the cubic superlattice structures B2, DO_3 and $L1_2$. He points out that the operative mode in each case may be a pseudomode, a true mode of high shear or a mode requiring atomic shuffles, and he tabulates shear modes of various kinds for each structure when up to 3/4 of the atoms are allowed to shuffle. A survey of the experimental results indicates that pseudotwins are the only shear products formed under stress in any of these structures except for B2 where, as already described in Section 2.6, $\{114\}$ twins have been observed in some alloys.

Goo notes that a $\{104\}$ mode has a smaller shear than the $\{114\}$ mode but in both the B2 and the b.c.c. structures, this mode requires 3/4 of the atoms to shuffle (which is why it is not listed in either Table 1 or Table 2 of the present review). The experimental result indicates that the simpler shuffles of the observed mode are more important than the lower shear of the $\{104\}$ mode. Goo's table for B2 does not include the $\{332\}$ mode, possibly because this mode was not listed in Table 1 of Ref. (35) which gives illustrative examples rather than a complete catalogue. The $\{332\}$ mode has a still lower shear (see above) but also (for B2 but not for b.c.c.) demands that more than half the atoms shuffle.

All the listed modes for the Do_3 structure except the {112} pseudomode derived from the b.c.c. mode, have shears greater than unity, and this is presumably why only pseudotwinning has been observed for this structure. Similarly, only with shuffled atomic fractions of greater than one-half, is it possible to have a twinning shear of less than unity in the $L1_0$ structure. Although the experimental evidence is not very clear, it is believed by most workers in the field that only simple pseudotwins form in this structure.

Values of the Laves shuffle parameter, see p. 34, are listed by Goo, who apparently accepts it as a significant factor in the choice of a twinning mode. However, it is difficult to find any example in which minimizing this parameter is not exactly equivalent to minimizing the fraction of atoms which must shuffle, so that the value of the Laves parameter as a discriminant seems dubious.

Several experimental investigations of the deformation behaviour of Ni_3Al, which has a $L1_2$ structure, have generally failed to find evidence of deformation twinning, except for some two phase $\gamma + \gamma'$ nickel-based superalloys in which microtwinning was observed[313,314] in γ' grains. This microtwinning was attributed to random formation of stacking faults which accumulated to form thin (imperfect) twins. However, Albert and Gray[315] and Gray[316] have recently demonstrated that deformation twinning can occur both in a single phase Ni_3Al alloy containing 0.095at%B and in a two-phase Ni–20at%Al–30at%Fe alloy. The single phase alloy was shock-loaded to a stress of 14 GPa and the two phase alloy was rapidly deformed (strain rate 3,000 s^{-1}) to a total strain of 16%. Twins and stacking faults were observed in some $L1_2$ grains of both alloys, but the other phase of the Ni–Al–Fe alloy which had the B2 structure was apparently untwinned. The twins in each case completely crossed the γ grains in which they were observed, but they were not numerous and it is estimated that those observed contributed little to the overall plastic deformation. In the two phase alloy, for example, extensive planar slip was observed in virtually every grain, but twins were visible in only about 10% of the $L1_2$ grains. No stacking faults were found in the two-phase alloy, possibly because of the higher energy of the fault, or because of the slower strain rate.

Electron microscopic investigation showed the $\mathbf{K}_1$ plane to be {111} but it was not possible to determine whether the product had the $L1_2$ structure or the structure of the pseudotwin. Superlattice spots on electron diffraction patterns were very weak and diffuse, and this is presumably due to the high strain. The authors assume that the final structure is the perfect $L1_2$ and, after dismissing the possibility that the pseudotwinning mode is accompanied by interchange shuffles as being too improbable, they suggest instead that the first no shuffle mode of Table 2 with a shear of $2^{\frac{1}{2}}$ is the operative mode. They concede this has a large shear, but do not give its magnitude, nor do they address the difficulty that atoms must pass one another in A–A configuration to accomplish this shear. On the other hand, the third possibility that pseudotwins form without shuffling is considerably enhanced by the imperfect long range order which must result from the extensive deformation.

Various structures which may conveniently be regarded as differing only in the stacking sequence of equispaced atomic layers can transform into other layer structures or, in some cases, can form deformation twins, by the passage of transformation or twinning dislocations (essentially equivalent to Shockley partials) along the layers; the simplest example is the twinning of f.c.c. crystals. In some crystal structures, however, it may be impossible to effect such a displacement sequentially between pairs of adjacent layers, and it is then necessary to invoke simultaneous displacement of two or more layers in order to avoid intermediate configurations with impossibly close interatomic encounters. Such processes were called 'synchroshear' by Kronberg[317] but appear to have been largely ignored in the subsequent

literature. Hazzledine[18] has recently discussed transformations between, and twinning in, Laves phases from the viewpoint of synchronous shear. All Laves phases consist of alternations of single layers of small atoms which are relatively well separated from closely-spaced triple layers of large–small–large atoms. The triple layers may be in either ABC or ACB configuration, but the layers are so close together that displacement of one relative to the other two is not possible. However, if layer 2 and the crystal above it is displaced in direction $\mathbf{l}_1$ and layer 3 and the crystal above it are simultaneously displaced in direction $\mathbf{l}_2$, an original ABC configuration is converted to ACB. This means that Shockley dislocations with Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ move simultaneously so that the net displacement of the two parts of the crystal is $\mathbf{b}_3 = -(\mathbf{b}_1 + \mathbf{b}_2)$, and the synchroshear may be regarded as the passage of a single Shockley which has, however, a core extended over two planes. Note that a transformation in the case of Laves phases always involves changes in the stacking within triple layers; only in the case of the cubic Laves phase (C15 type) does synchroshear of each triple layer lead to a twin.

There have been further developments in atomistic calculations of the structures and energies of various h.c.p. twin boundaries. Morris *et al.*[319,320] have studied the four $\mathbf{K}_1$ interfaces of Table 5 in the case of zirconium. For the "compression" twins $\{10\bar{1}1\}$ and $\{11\bar{2}2\}$, the relaxed atom sites near to the interface were determined by a combination of molecular dynamics and first principles calculations. In order to implement the molecular dynamics, an empirical many body potential for zirconium was developed using the "embedded atom method" (EAM), and this potential is stated to be similar to the Finnis–Sinclair potential used in the work of Bacon *et al.*[95,97,111] For each twin boundary, a unique, low energy, zero force description was found to be independent of the starting configuration, and a periodic array of twins using the relaxed structure was then used in a first principles calculation of the electronic structure, and hence of the energy. The cell geometry and the atomic positions were finally adjusted to give the minimum energy. These calculations show that mirror symmetry is preserved in both interfaces, and no indication of a previously reported glide displacement for the $\{10\bar{1}1\}$ twin was found; the atomic configurations in the vicinity of the interface are quite similar to those of Bacon *et al.*

The calculated twin boundary energies are shown in Table 6 which also includes a comparison with earlier work. In almost all calculations, the energy of the $\{10\bar{1}1\}$ twin

Table 6. Computed Energies for some h.c.p. Twin Interfaces[320]

	Twin boundary energy (kT_m/α^2)			
Model	$\{10\bar{1}1\}$	$\{11\bar{2}2\}$	$\{10\bar{1}2\}$	$\{11\bar{2}1\}$
Zr first principle[319]	0.28	1.17	—	—
Zr EAM	0.57	0.97	0.86	0.56
Zr FS[360]	0.80	0.87	0.93	0.60
Ti FS[361]	0.60	0.68	0.89	0.49
Mg FS[362]	1.15	1.17	1.52	1.19
na56[97,111]	0.64	0.92	1.15	0.73
LJ56[127]	2.49	0.87	0.95	0.69

Notes—k = Boltzmann's constant, T_m = melting point, α = lattice parameter. EAM = embedded atom method, FS = Finnis–Sinclair potential, na56 = oscillatory long-range potential, originally developed for sodium, LJ = Lennard-Jones simple analytic potential. Since $kT_m \simeq \epsilon$, the energy units are approximately the same as those of column 2, Table 5 which were computed with the na56 potential.

interface is lower than that of the $\{11\bar{2}2\}$ interface, but the difference is much more marked in the first principles calculation of Morris *et al.* than in earlier work with model potentials. The authors point out that the lower energy of the $\{10\bar{1}1\}$ mode implies that conventional nucleation theory cannot explain the preference for the $\{11\bar{2}2\}$ mode at low temperatures.

The first principles calculation necessitated a periodic array of twins, and the resultant error was estimated by calculations of the interface energies for an array and an isolated interface using the empirical (EAM) potential. The results indicated, firstly, that the twin–twin interaction of the array reduces the specific twin interface energy by about 7%, and, secondly, that the ratio of the energy of the $\{10\bar{1}1\}$ boundary to that of the $\{11\bar{2}2\}$ boundary is unchanged in the array configuration. The calculations with the empirical potential give numerical values which, for compression twins, are not in very good agreement with the 'true' values obtained from first principle calculations. Nevertheless, the ratio of the two interfacial energies is appreciably lower than that found in earlier work, although not so low as that derived from the first principles calculation (see Table 6). The similarity of the structures found for the various interfaces when different model potentials are used for the simulations is surprising in view of the wide spread in the compression twin energies, and the authors suggest that this may imply that the structures are determined mainly by the geometry.

First principle calculations are very time consuming and can only be applied to very small atom blocks. Similar calculations are in progress for the tension twins, $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$, but comparable results are not available at the time of writing. However, twin boundary structures and energies have been determined by utilizing the empirical model potential. The structures found are again all very similar to those deduced from earlier work, and in the case of the $\{11\bar{2}1\}$ interface, the atomic arrangement breaks the mirror symmetry across the interface. The energy values are given in Table 6, and in contrast to the behaviour of the compression twins, results obtained with the EAM method now agree remarkably well with previous calculations using potentials appropriate to titanium or zirconium.

Meanwhile, Bacon and Serra[321] have further developed their atomistic simulations of the structures of interfaces and interface dislocations, and have provided the first reported treatment at an atomic level of the interaction between a lattice dislocation in the matrix and a coherent $\mathbf{K}_1$ twin interface. In Section 6, it has been emphasized that the simplest dislocation–interface interactions occur when the interface is planar and the dislocation meets it in screw orientation. This is the condition investigated by Bacon and Serra for $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$ interfaces in titanium. A matrix screw dislocation with Burgers vector $\langle 1\bar{2}10\rangle$ is parallel to both these interfaces and it is known to glide on either basal (i.e. $\{0001\}$) or prism (i.e. $\{10\bar{1}0\}$ planes); these two possibilities will be called BS and PS, respectively. Simple crystallography then allows either type of matrix slip to be continued on either the basal or the appropriate prism plane of the twin. In practice, however, the situation is more complex because calculations indicate that there are two, different, stable core configurations (with similar energies) for the lattice screw dislocation. One structure (BC) approximates to an extended dislocation on the basal plane; the other (PC) is not describable in simple terms, but results from dissociation largely along the prism plane. The PC dislocation moves readily on the prism plane at quite low applied shear strains, but cannot be induced to move on the basal plane; the BC dislocation is relatively immobile on the basal plane up to quite high strains unless other shear strains are imposed.

For a $\{10\bar{1}2\}$ twin, the basal planes of one crystal are at an angle of only 6° to the prism planes of the other, so that cross-slip at the interface on to a different type of slip plane in

the twin is favoured by the applied stress. The calculations show that a PC dislocation moving up to the interface on a prism plane may either cross it on to a basal plane or on to a prism plane of the twin, depending on whether the core centre lies between the widely or the narrowly spaced prism planes which alternate along the twin interface. The BC dislocation transfers from the matrix basal plane to the twin prism plane in both cases. The results show that the $\{10\bar{1}2\}$ boundary acts as a barrier to prism slip and inhibits both the PS–BS and the PS–PS crossing mechanisms.

At the $\{10\bar{1}1\}$ boundary, the basal planes of one crystal are at 32° to the prism planes of the other. This interface also acts as an obstacle to slip, but surprisingly the mechanism found by Bacon and Serra is quite different. In most circumstances, the $\frac{1}{3}\langle 1\bar{2}10\rangle$ screw dislocation does not cross the boundary but dissociates instead into two "twinning dislocations" each with a screw component of $\frac{1}{6}\langle 1\bar{2}10\rangle$ and with small equal and opposite edge components. These dislocations remain in the interface, which is advanced by two lattice planes in the dissociated region between them, but they are clearly not the twinning dislocations which produce the normal deformation twin (see Section 3.2). It is believed, however, that with the edge components they correspond to the twinning dislocations of the transformation twinning $\{10\bar{1}1\}$ mode, which are in fact the most mobile of the possible step defects in this interface. If successive incoming screws are held up at the interface by such a dissociation, the $\{10\bar{1}1\}$ interface must constitute an appreciable obstacle to continued slip.

The results of atomistic simulations of non-screw dislocation interactions with $\mathbf{K}_1$ interfaces must now be awaited with interest. Clearly, however, if the first dislocation is held up at the interface, it is very difficult to simulate the effects of successive dislocations which form pile-ups and thus modify considerably the local stress fields.

Turning next to models of the interfaces of enclosed twins, Mitchell and Hirth[322] have examined a two-dimensional version of Orowan's lenticular twin shown in Fig. 9. Using a method involving Hilbert transforms, they were able to deduce the distribution of straight twinning dislocations normal to the plane of Fig. 9. The details of the distribution, i.e. the position of each dislocation in the array, enables more exact stress calculations to be made. The predicted shape normal to the dislocations is close to a flattened ellipse, except very near to the tip where it deviates in opposite senses for edges and screws. The results thus suggest that the three-dimensional ellipsoid (or oblate spheroidal) model is an adequate approximation to the true shape.

Lee and Yoo[323] have reconsidered the theory of homogeneous nucleation of twins. They first reviewed their previous work on shape bifurcation (see Section 4.1) and extended it to consideration of heterogeneous nucleation on a substrate. They then attempted to simulate twin nucleation in a b.c.c. crystal under stress. The well-known Johnson potential[324] was assumed for the interatomic force law, and the simulation used a modified Monte Carlo technique in which the nearly random displacements of each individual atom are biased in the direction of the net force acting on the particular atom under consideration. The computer "box" was treated either as a crystal with free surfaces or, with periodic boundary conditions, as part of a larger unit, and was stressed by imposing a uniform shear over the whole or over the central part of it. The homogeneous deformation did not produce the anticipated cooperative shearing to a twin nucleus with either the free surface or the periodic boundary assumption. Instead, the structure remained uniform and on removal of stress (i.e. imposed strain), it collapsed back into the b.c.c. form below a threshold value of the imposed strain, and transformed homogeneously into a (metastable) f.c.c. structure above this threshold. The authors attribute the failure to nucleate to the small number of atoms in the computational box, and the relatively high interfacial free energy which results in a large

critical nucleus size. This is undoubtedly true, but it is not obvious that interfacial energy and critical nucleus size are relevant to the homogeneous shear of an isolated crystal. In principle, the whole box can form a twin, not by growth from a small embryo with concomitant strain and interfacial energies, but homogeneously when the uniformly strained lattice reaches a condition of mechanical instability. Since the imposed strain was a simple shear, the collapse to a f.c.c. structure, rather than to a twin, at high imposed strains is remarkable, unless the atomic potential used favoured this structure rather than the initial b.c.c. structure.

Some confusion may be caused by references in this paper to nucleation and it should perhaps be emphasized that a procedure of this type whilst giving a minimum free energy state for given imposed conditions, does not necessarily find the absolute minimum which may require the assembly to pass through intermediate states of higher free energy. Moreover, the relaxation of the structure may both involve procedures not accessible to the real crystal and fail to include real procedures. In particular, the Volmer–Weber–Becker–Dôring type of kinetic process which describes homogeneous nucleation as the result of a series of local fluctuations is very difficult to simulate because of its statistical nature.[20] So-called 'steady state' nucleation is not attained until a quasi-equilibrium distribution of sub-critical embryos of different sizes and shapes has been established, and any successful nucleus must survive many shrinkage fluctuations, the probabilities of which are always higher than those of growth fluctuations, before reaching the saddle point configuration beyond which the probability of growth exceeds that of shrinkage. To simulate such a process would require not only a much larger computational box but also an immense amount of computer time.

When the imposed strain was confined to a central portion of the computer box, interfaces were artificially introduced between the sheared and unsheared regions and their energy was thus available to assist in nucleation. This led to twin formation and in particular to multiple twins, rather than a single twin. This is attributed to free energy minimization; the strain energy of a constrained twin is reduced by dividing it into a number of parallel twins with smaller aspect ratios, but this splitting is opposed by the accompanying increase in surface free energy.

High resolution electron microscopy has been used to verify the fully coherent nature and high state of perfection of $\mathbf{K}_1$ interfaces. Recent examples are lattice images from thin twins and twin–matrix interfaces in TiAl by Wardle *et al.*,[278] by Couret *et al.*,[325] Farenc *et al.*[277,326] and by Appel, Beaven and Wagner.[327–329] Couret *et al.* have also addressed the need for better verification of the magnitude of the shear, mentioned at the end of Section 4.5. They have used electron microscopic methods to measure the total shear across very thin twins and have thus shown that this corresponds to one twinning dislocation having moved through each lattice plane. This is another indication of the perfection of the twin structure which these measurements indicate is within 5%. It should be recalled, however, that in TiAl, the structure permits only one twinning direction to each $\mathbf{K}_1$ plane, so that the probability of occasional faults or defects may be lower than in atomically disordered materials.

Examples of twinning dislocations, i.e. interface steps, have been shown in Figs 13, 14 and 18, for example, and in each case a parallel set of twinning dislocations of the same sign typifies a tapering twin. Measurements by Couret *et al.* on TiAl indicate that the distance between successive twinning dislocations initially increases with distance from the tip in a manner characteristic of that expected from a dislocation pile-up, and then remains approximately constant when the number of twinning dislocations exceeds ~ 15. This is significant evidence relating to the problem of the shape of a twin tip or edge.

Couret and his coworkers[277,325,326] have also carried out deformation experiments *in situ* in the electron microscope, and have thus verified directly that twins form by the motion of twinning dislocations (Shockley partials in this particular case). The observed twin velocities were small and roughly constant, of the order 50 nm s^{-1}, and the separation of the twinning dislocations was unchanged during growth. Backward motion was observed on release of the applied stress. The authors conclude that the growth velocity is governed by a friction force which acts equally on all the twinning dislocations. They also suggest that nucleation simply results from the dissociation of a superdislocation and subsequent interaction of the twinning dislocations with perfect dislocations to form pole sources. Some of their micrographs appear to show such sources.

The distribution of twinning dislocations just described for TiAl and the calculations of Mitchell and Hirth clearly support the lenticular model of an enclosed twin and the pile-up model of a twin tip rather than the disclination model of Müllner and Solenthaler.[238,239] In agreement with this conclusion, there appear to be many published micrographs showing lenticular or tapering twins but few showing blunted twins. Blunted twins were noted by Calais *et al.*[330] in their early work on uranium, but they appeared only during annealing of deformed specimens at temperatures where individual atomic migration was rapid, so that the deformation twin lamellae frequently contracted and eventually disappeared. The authors attributed the blunting to the formation of incoherent interfaces as a result of the enhanced atomic mobility. Similar observations were made by Cahn and Coll.[46]

Müllner and Solenthaler's original argument for a blunted twin depended on the assumption that the leading dislocation is pinned, and this condition has already been discussed in Section 6.1; it clearly does not apply to a freely growing twin. The *in situ* experiments of Couret *et al.* investigated twinning under conditions of very small growth rates, but there is some difficulty in describing, in terms of the motion of individual twinning dislocations, the often observed growth of twins of finite thickness at velocities approaching the speed of sound. The difficulty arises from the relatively slow growth normal to the interface predicted by the pole mechanism or by a spontaneous nucleation mechanism. To avoid this difficulty, Hirth[331] has proposed that fast growth might be due to a preformed dislocation wall (or 'square') interface, the constituent (edge-type) twinning dislocations of which could move together at near-sonic velocities. Such a twin may be formed by the bowing out and breakaway of a segment of a symmetrical tilt boundary (or the tilt component of a more general grain boundary), in a similar fashion to that described by Olson and Cohen[332] for the nucleation of martensite. The problem of slow normal growth is thus avoided by setting this growth rate to zero and utilizing a nucleus which already has the final thickness. One objection is that, except for b.c.c. structures, the Burgers vectors of the interface dislocations will not readily convert into those of twinning dislocations, nor will they have the correct density to produce just the required number of twinning dislocations. Another is that the model applies only to that part of the periphery of a plate where the twinning dislocations have edge orientation. Finally, an Orowan type bow-out would probably lead to a moving interface which is not flat but has the shape of a circular or elliptic cylinder. In any event, a fixed array of twinning dislocations, whether representative of a tapering (lenticular), a hemicylindrical or a flat square interface, must presumably be able to migrate parallel to K_1 with high velocity.

There are many recent papers proposing twinning mechanisms, most of them for specific structures. However, a paper by Basinski *et al.*,[333] although formulated with reference especially to the f.c.c. structure, essentially deals more generally with the relation between pole and ratchet mechanisms. The authors show that if a long jog initially dissociates to

form a ratchet-type source (i.e. an antigenerating node), the two opposite partials which meet on adjacent planes after the first turn may, in principle, glide past each other so that each attaches itself to the opposite node and both recombine with the sessile dislocation along the original superjog to form a new dislocation with the Burgers vector required by the pole mechanism. (In the Venables mechanism, each segment recombines separately with part of the sessile dislocation, and the cross-slip effects the interchange necessary for "node conversion".) The adjacent elements of twinning dislocation can now rotate about the two nodes in the opposite sense to that of the first turn, and the configuration has become a true pole.

In terms of the f.c.c. structure, the reaction involved in the conversion is simply:

$$\tfrac{1}{3}\langle 111\rangle + 2 \times \tfrac{1}{6}\langle \bar{1}\bar{1}2\rangle = \langle 001\rangle,$$

(see eq. 52). However, this ingenious proposal has the same difficulty as the monolayer true pole mechanism, namely the necessity for elements of twinning dislocation to pass each other on adjacent lattice planes. In fact, since both pole and ratchet form from the same lattice dislocation, there must be other (virtual) processes linking the two. The simplest, but physically least probable, conversion requires $\mathbf{b}_B^*$ to emit two twinning dislocations which glide away from it on opposite sides. One of these can then eliminate the fault left by the original dissociation, and ultimately the twinning dislocation (with Burgers vector $-\mathbf{b}_T$) bounding it, whilst the other trails a new fault of the same type on the opposite side of $\mathbf{b}_B^*$.

A model for b.c.c. twinning described by Lagerlöf[334] is a ratchet mechanism closely similar to the Pirouz model for semiconductor materials. Lagerlöf assumes that a short screw segment of a lattice dislocation lying between pinning points in its glide plane dissociates into three $\frac{1}{6}\langle 111\rangle$ dislocations which are assumed to lie on successive lattice planes of type $\{11\bar{2}\}$. The group of three twinning dislocations bows out under an applied stress and rotates about the pinning points in a manner equivalent to that of a Frank–Read source, to give a closed loop of a three-layer fault or thin twin. After one turn, the screw dislocation is regenerated and then undergoes double cross-slip onto the next three $\{11\bar{2}\}$ planes on which it blows out another loop of three-layer faults. The twin is thus assumed to grow by alternating double cross-slips.

This theory is essentially a combination of earlier theories which depend on the dissociation of screw dislocations with the simple ratchet mechanism of Venables[144] and Pirouz.[173–175] There are the difficulties already noted that the postulated dissociation of the screw dislocation is more usually described as a spreading of the core, and the intimate double cross-slip is also essentially a core effect rather than genuine cross-slip. The repeated alternation of the dissociation, bowing out fine cross-slip and recombination needed to produce a twin of adequate thickness appears somewhat improbable, but Pirouz emphasizes in relation to his own theory that "although the term 'double cross-slip' is used . . . what is really happening is just a rearrangement of the dislocation cores from one plane to the next".

Pirouz[335] has reviewed his own theory as applied to bulk semiconductors in both elemental and compound form. His description, as already noted, depends on a large difference in the mobilities of the two Shockley partials into which a lattice dislocation dissociates, and the periodic cross-slip is to the immediately accessible next lattice plane.

A matter of considerable practical importance is the formation of deformation twins in coherent epitaxial films which have been deposited on a slightly misfitting substrate. When

the thickness of the film exceeds a critical value, its large elastic strains begin to be reduced by nucleation of dislocation loops at the free surface of the film and their subsequent spread to the substrate–film interface where they become misfit dislocations. The elastic coherency strains may also be relieved by twinning, and Pirouz[33] envisages that this occurs by nucleation of a twinning dislocation rather than a lattice dislocation at the surface of the film, followed by subsequent nucleation and spreading of further loops on immediately adjacent planes. This accommodation twinning may be regarded as a special kind of deformation twinning.

When the misfit is sufficiently small, surface nucleation may not be needed since misfit dislocations may be generated by the glide of threading dislocations. An alternative mechanism for twin formation might be the dissociation of threading dislocations into Shockley partials and subsequent glide of one of the partials under the influence of a misfit-induced stress.

Twinning in semiconducting materials usually occurs more readily at low temperatures where there is little intrinsic ductility. Deformation twins may produce some plasticity either around a microindentation of the specimen or in a specimen subjected to a uniaxial compressive stress superimposed on a uniform hydrostatic pressure. The strong covalent bonds in semiconductors lead to high lattice friction and twinning dislocations tend to lie along ⟨110⟩ Peierls valleys with Burgers vectors at 30° or 90° to the line direction; in addition, straight ⟨112⟩ (screw or 60°) dislocation segments have also been identified. *In situ* experiments on silicon or GaAs at temperatures where twinning is the dominant mechanism of plastic deformation are very difficult because of the presence of microcracks. However, Vanderschaeve and coworkers[336,337] have recently found that twins form in thin foils of some III–V compounds during *in situ* deformation at elevated temperatures where deformation is primarily by dislocation glide. Thus in GaAs, no twins appear to form in foils deformed in tension in the medium temperature range of 443–543 K, but at 573 K, twins were found in the vicinity of crack tips. The nucleation of these twins is suggested to occur only above the brittle–ductile transition, which would thus be placed for these specimens somewhere in the range 543–573 K.

The motion of the twinning dislocations appeared to be smooth and continuous, and this is taken as an indication that they are subject to a high lattice friction (Peierls–Nabarro) stress even at this relatively high temperature. Growing twins frequently appeared to have a few groups of 3–4 twinning dislocations moving ahead of a procession of a large number of twinning dislocations. In each group, the leading dislocation had an angular appearance with segments of nearly screw and 60° orientations, whilst the following dislocations were smoothly rounded. The tentative explanation of these observations is that in addition to the forces which act on all the twinning dislocations, the leading dislocation experiences an additional retarding force per unit length equal to the magnitude of the stacking fault energy per unit area. The angular shape is attributed to this extra term, whilst a smoothly curved shape is taken to indicate that the net stacking fault stress is zero since any new faulted area extended behind a following dislocation is balanced by an equal reduction in fault area ahead of it. Vanderschaeve and Caillard[337] argue that their observations indicate that these twins are not 'regular' (i.e. perfect) since if a twinning dislocation moves on every plane, there would be only one angular dislocation leading each twin. The angular dislocations were initially formed as 30° dislocations, and there was a gradual transition to the kinked screw-60° character; this is attributed to greater mobility of 90° kinks than of 30° kinks.

A recent *in situ* investigation by Vanderschaeve *et al.*[336] of twins forming at crack tips in InP crystals deformed in tension at 623 K came to similar conclusions, notably that the mobility of the 90° partial is greater than that of the 30° partial in this structure also. The asymmetry is probably a consequence of the different core structures. However, Azzaz *et al.*[338] in a recent investigation of the deformation of undoped InP crystals deformed in compression at low strain rates ($2 \times 10^{-5}\,s^{-1}$) found extended stacking faults, both intrinsic and extrinsic, but no evidence of twinning. The authors suggest without detailed justification that extrinsic faults have lower energy than intrinsic faults in this and other III–V compounds, but the partials bounding them have very small mobilities.

In situ studies of the nucleation and propagation of deformation twins which form during slow deformation (and even, remarkably, during creep) of TiAl crystals at low and intermediate temperatures have recently been reported by Jin and Bieler.[339-341] The experiments are clearly similar to those of Vanderschaeve *et al.* on semiconducting materials, and more especially those of Couret *et al.* on TiAl, described above, but were for an alloy of composition Ti–48at%Al–2at%Nb–2at%Cr which had a two phase $\gamma + \alpha_2$ lamellar microstructure. High resolution electron microscopy has been used in very detailed investigations by Appel *et al.*[327-329] of the structure of the interfaces in similar two-phase alloys with compositions Ti–48.5at%Al–12.5at%Mn and Ti–48at%Al–2at%Cr. The microstructure of these alloys consists of equiaxed γ (TiAl) grains and colonies of thin parallel lamellae of α_2 (Ti_3Al). In the alloys of Appel and Wagner,[328] the volume fraction of α_2 lamellae was less than 5% and the lamellar thickness was typically 10 nm–1 μm. With appropriate heat treatment, crystals of the γ phase may consist of alternating lamellae in true twin orientation, a structure which Yamaguchi and Umakoshi[273] refer to as polysynthetically twinned (PST) crystals since this term is used in mineralogy. PST is evidently a form of transformation twinning, and as discussed briefly in Section 2.7, arrays of twins formed in this way can be very effective in inducing ductility.

Yamaguchi and Inui[342] showed that the γ phase in such lamellar structures is inherently ductile in contrast to the single γ phase structures with more than 50at%Al studied by Couret *et al.* which are brittle up to quite high temperatures. The ductility is however, very anisotropic and Yamaguchi and his coworkers have shown[273] that the lamellar structure is 'hard' when shear has to cross the lamellar interfaces (e.g. when an axis of compression is parallel or normal to the lamellae) and 'easy' when shear is parallel to the interfaces which may then be displaced to produce the required strain. However, there are contradictory reports in the recent literature about the effects on deformation twinning of varying the composition in the approximate range 48–52at%Al. Huang and Hall[343] reported that the tendency to twin was much higher in the two-phase (48at%Al) than in the single phase (52at%Al) alloy, but Sriram *et al.*[344] found that at room temperature and above, twinning occurs readily at all aluminium levels in this range. Increase in deformation temperature above room temperature led to increased twinning in all alloys, and this was often manifested by the formation of thicker twins rather than by an increase in their number density. The number density was higher in γ foils from the two-phase 48at%Al alloy than in foils from the 52at%Al alloy, but Sriram *et al.* suggest this may be due to the finer grain size in the two-phase (titanium-rich) alloys, rather than to any intrinsic effect of the change in composition. The finer grain size, especially in the alloys with a lamellar microstructure, provides more grains with favourable Schmid factors for twinning, and the authors point out that this is consistent with the results of Sun *et al.*[270,271] who showed that the operative slip systems agree with predictions based on Schmid value calculations. A second suggested effect of a fine grain size is that it leads to more intense regions of inhomogeneous strain which

Sriram *et al.* suggest is needed for the grain boundary nucleation. The difference in twinning behaviour in the experiments of Huang and Hall[343] on the one hand and Sriram *et al.*[344] on the other is then attributed to the much finer lamellae in the specimens examined by Huang and Hall. An alternative reason for the anisotropy is the orientation dependence of the slip modes in the α_2 (Ti_3Al) phase.

Jin and Bieler suggested that the observations of Farenc *et al.* and Coujet *et al.* may not apply directly to twinning in the less brittle two-phase alloy, and indeed their *in situ* observations in some ways correspond more to the semiconductor results of Vanderschaeve *et al.* than to those of Farenc *et al.*[326] Although no angular dislocations were observed in TiAl, Jin and Bieler also observed that the twins appeared to grow by successive formation and bowing out of twinning dislocations from grain boundary regions on to adjacent lattice planes of the γ matrix. The leading dislocation, or sometimes the leading pair, moved slowly and eventually came to a halt in the interior of the parent grain. Once formed, the next dislocation moved relatively rapidly to the vicinity of the lead dislocation, and apparently pushed it a little further into the grain before itself coming to a halt a very short distance behind its leader. Repetition of this event then produced a microtwin. The formation at the grain boundary of half-loops of interface single steps (elementary twinning dislocations) on successive $\mathbf{K}_1$ planes is thus the operative nucleation mechanism in most of the single twins observed, but the exact interactions which produce the half-loops are not yet known. It is intriguing to note that most of the twins were highly regular, possibly suggesting either sympathetic nucleation of successive layers or some form of grain boundary pole mechanism.

Occasionally, with relatively thick foils, twins appeared to nucleate from the grain interiors, as in the experiments of Coujet and his coworkers. However, a strong counter example is provided by a remarkable micrograph by Appel *et al.*[328] showing twins nucleating on individual misfit dislocations of a semi-coherent γ–γ boundary (see Fig. 56). At this point, the customary, but necessary reservation must be emphasized; these thin foil experiments may not be at all representative of the twinning process in bulk material. Nevertheless, the evidence for grain and/or interphase boundary nucleation in the two-phase alloys seems fairly convincing.

Jin and Bieler observed that the twinning dislocations near the tip of a twin were closer together than those remote from the tip, and they made a qualitative comparison with the results of Marcinkowski and Sree Harsha, but not with those of Mitchell and Hirth. However, this work provides further confirmation of the lenticular model, at least in cases of slow growth. In further experiments, the actual distribution of twinning dislocations along a thin semi-lenticular twin of the plano-convex type illustrated in Fig. 38 was measured and the results used to calculate the back stress acting along the twin interface.[345] As expected, the back stress was very high near the tip but fell off rapidly with distance back along the twin.

The absence of agreement on the value of a twinning stess in many metals and alloys despite very careful experiments has been addressed by Embury *et al.*[346] They investigated in detail the effects of chemical composition, specimen orientation and test temperature on the twinning stress of Cu–Al single crystals tested in tension. After analyzing a large amount of data, they propose a criterion for twinning in these alloys as follows. "Two conditions must be satisfied simultaneously if twinning is to occur. (i) The onset of twinning occurs only when there is a change in the dominant slip system, and (ii) a minimum stress, τ_N, is required." In a tensile test, the change in orientation of the specimen eventually forces (with usually some 'overshoot') the primary system to become less active than the conjugate system. The

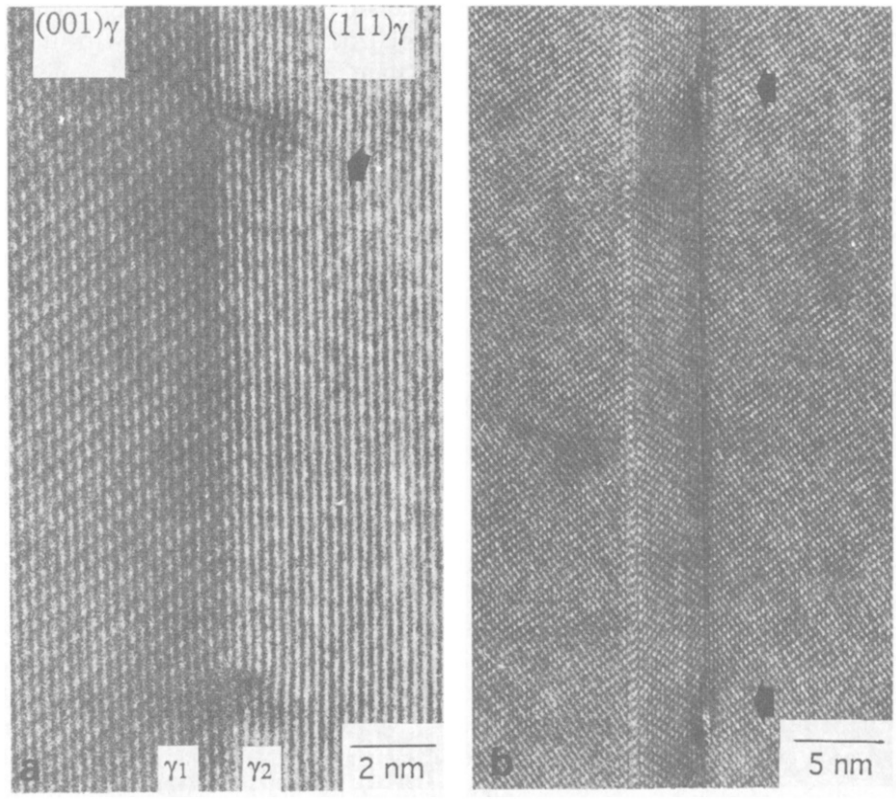

Fig. 56. High resolution electron micrograph of deformation twin nucleated at a γ–γ (TiAl) interface. The interface is semicoherent and the twin (arrowed in (a)) has been nucleated on one of the two misfit dislocations visible in (b). The specimen was deformed to failure (10.2% strain) at 800°C. (After Appel *et al.*[328].

meaning of the proposed criterion is that if the applied stress at this point exceeds τ_N, twinning will begin and that applied shear stress will be the twinning stress. If, however, the second part of the criterion is not met, slip will continue on the conjugate system until, after possibly a second overshoot, the primary system becomes dominant again. At this point, there is a second opportunity for twinning to begin, and this will again depend on whether or not the current applied (shear stress) level exceeds τ_N.

If τ is less than τ_N and the ductility is adequate, the cycle can then be repeated. According to the hypothesis, a high work-hardening rate clearly favours early twinning, but although there is a convincing weight of experimental evidence the proposed criterion is entirely empirical as propounded. If it becomes established, it will no doubt influence the development of theories of twinning in f.c.c. crystals and other materials which twin only after appreciable deformation by slip.

Most of the recent work on twinning in intermetallic compounds has been concerned with TiAl, but there have been a few investigations on other 'advanced materials', including that already described for Ni_3Al with the $L1_0$ structure. Kumar and Vasudevan[347] investigated twinning in a Ni–25at%Mo–8at%Cr alloy after ageing in the temperature range 650–700°C. The short range order of the solid solution is thereby converted into a structure in which there is a high density of long range ordered Ni_2Mo precipitate particles with the Pt_2Mo structure. At room temperature, the tensile strength of the alloy is almost trebled by this heat treatment, whilst the ductility decreases from 70% to 56% and 36% after 10 h at 650 and

700°C, respectively; a further slight reduction was observed after longer ageing times at 650°C but the ductility remained high after all such treatments. The solution treated material deformed entirely by dislocation glide, but in the aged samples, microtwinning was the major contributor to the plasticity. The $\mathbf{K}_1$ plane was found to be the f.c.c. $\{111\}$ plane for both the ordered precipitates and the matrix, and the authors' preliminary observations suggest that the initial formation of the twins may be attributed to the overlapping of stacking faults.

The slip in the solution treated material is very planar, and this probably applies also to the initial deformation of the aged material. The authors suggest that the dissociation of slip dislocations into partials takes place when the slip is arrested by the long-range ordered precipitates. This is consistent with the observation that the majority of the twins are observed to be within the precipitates. Six orientation variants of the long-range ordered phase within a matrix grain were all identified, and the availability of these various deformation modes is probably responsible for the ductility remaining high despite the inhibition of slip. In this case, increasing plastic deformation at fixed temperature was apparently accomplished mainly by thickening of existing twins rather than by an increase in the number of twins. Although it is easy to understand that the high density of ordered precipitates will cause the large increase in flow stress, it is not obvious why the deformation mechanism changes from slip to twinning since both processes are inhibited by long range order.

A different strengthening mechanism also involving twinning as the principal mode of deformation is observed in some solid-solutions. Yang and Vasudevan[348] have recently examined supersaturated solid solutions containing 10–16at%Al in Nb. These solutions exhibit imperfect B2 type ordering, the extent of which increases with aluminium content, as does the microhardness at room temperature. The microstructures examined after cold rolling to 25% reduction in the 10at%Al alloy and 5% reduction in the 13 and 16at%Al alloys were found to contain many twins with $\mathbf{K}_1$ planes of $\{112\}$ type. Although, a positive identification of the twinning mode was not made, the presumption is that it is the usual b.c.c. mode which is a pseudo mode of the B2 structure. In these alloys, the effects of the incomplete B2 ordering in inhibiting twinning is apparently outweighed by that of the aluminium solute in promoting twinning.

Further investigations of the propagation of either slip bands or deformation twins through other (obstacle) twins have been reported, especially for TiAl. Jin and Beeler[339,340] observed twin–twin intersections by electron microscopy during *in situ* deformation of a Ti–Al–Nb–Cr alloy. They observed a type I intersection in which two thin twins succeeded in propagating across a thin barrier twin whilst two others were halted by the barrier. However the lattice in the intersected region was not changed in orientation and no dislocations were seen to cross it. The mechanism seemed to be simply that a pile-up of twinning dislocations at the barrier twin eventually led to the nucleation of two new twinning dislocations on the far side of the barrier twin. These glided a little way into the matrix and then halted until they were pushed further by the nucleation and emission of more dislocations from the farther twin interface. Thus there is formally a glide discontinuity which is presumably taken elastically across the barrier twin. The authors relate this mechanism to their back stress measurements,[345] but it is not clear whether the mechanism is confined to very thin obstacle twins only.

Rather similar conclusions could be derived from some of the micrographs of slip–twin and twin–twin intersections obtained by Appel *et al.*[327,328] They examined both semi-coherent γ–γ boundaries and fully coherent $\mathbf{K}_1$ twin interfaces as obstacles. The semi-coherent interfaces have high residual stresses despite the misfit dislocations and this

leads to generation of high densities of glissile dislocations and small twins. Shear strains are more readily translated across fully coherent interfaces; the main mechanism is not known in detail but again may involve the nucleation of new dislocations rather than the incorporation processes discussed previously.

Most work on deformation twinning has examined twins formed at relatively slow strain rates of the order 10^{-5}–$10^{-4}\,s^{-1}$, but it has long been recognized that twinning is very sensitive to strain rate, and in many materials, it is promoted by high strain rates and low temperatures. Recent work shows that, in some cases, the same rules apply to ordered phases and intermetallic compounds, namely that deformation at high strain rates, and especially under shock loading conditions, tends to suppress slip and to promote twinning. One much quoted explanation rests on the postulate that dislocation glide is thermally activated so that the stress to sustain a given mean dislocation velocity, and hence a given strain rate, increases at low temperatures and/or high strain rates. The twinning stress, in contrast, is considered to be relatively insensitive to temperature or strain rate, so that when the stress reaches a critical level, twinning takes over from slip the task of maintaining the imposed strain rate. As mentioned in Section 5.3, with the very high strain rates obtained in shock loading, twinning may even be induced in f.c.c. alloys of aluminium with very high stacking fault energies.

In a survey of the influence of strain rate on twinning, Gray[316] points out that some intermetallic compounds, e.g. those based on Ti_3Al, usually do not twin even under shock loading conditions, whereas others, e.g. Al_3Ti, twin readily. Recent experiments have shown that shock loading induces twinning in polycrystalline Ni_3Al, in the B_4C component of an Al–B_4C cermet and in a Ti–48at%Al compound with additions of vanadium, chromium and/or niobium. Compounds based on TiAl, however, not only form deformation twins under shock loading, but also, as described above, deform by twinning at slow or even creep strain rates, and the amount of twinning increases with increasing temperature. This anomalous behaviour leads Gray to suggest that different twinning mechanisms may be responsible for twinning in TiAl at very fast and slow strain rates, respectively.

The phenomenon of elastic twinning was discovered by Garber 56 years ago, but is still the subject of active research. A model of an elastic twin as a planar pile-up of continuously distributed twinning dislocations has given a fairly full description of elastic twinning under quasi-static conditions, but recent work has been directed towards dynamical descriptions of elastic twinning. In the theoretical description given by Boyco *et al.*[349] the (twinning) dislocation motion is assumed to be thermally activated at low velocities and viscous at the high initial velocities. A non-linear set of equations describing the dynamics of a thin elastic twin is developed and solved with suitable approximations to give the various stages in the transition from a thin elastic twin to a residual twin lamella, and finally thickening of this lamella. Various predictions were checked against new experiments on elastic twinning in calcite crystals and good agreement is claimed. The possibility of obtaining elastic twinning in advanced materials has also been considered. Elastic twinning as a stage of mechanical twinning can be obtained if a concentrated load is used and if the twin which appears satisfies a criterion which depends on the friction force. The authors predict that the high temperature superconductor $Y_2a_2Cu_3O_{7-x}$ and the ferroelastic $Gd_2(MoO_4)_3$ should exhibit elastic twinning. Finally, the publication[350] by the American Institute of Physics of an English translation of a Russian book by Boyko, Garber and Kossevich dealing with elastic twinning should be noted.

In another recent paper, Boyco and Beshers[351] consider the possibility of using acoustic emission to estimate the twin velocity. Investigation of the acoustic emission associated with

elastic twinning has enabled the physical origins of the emission to be identified, and the application of acoustic methods to the study of twinning kinetics is discussed.

Kriven[352] has given a very informative survey of recent work on twinning in structural ceramic materials. Much work in this area is concerned not with deformation twinning in the strict sense but with transformation twinning resulting from martensitic transformation in materials like zirconia or from ferroelastic materials. As first noted in Section 2.7 in connection with hexagonal $\{10\bar{1}1\}$ twinning, and also as discussed above in relation to PST crystals of TiAl, arrays of twins formed in this way can nevertheless act as deformation twins if the product phase is subsequently stressed, and Kriven gives many examples of this kind of behaviour. Ferroelastic domains, like twins in martensitic transformations, are generated from mirror planes or two-fold axes of symmetry in the parent phase and are then in twin relation in the product. Growth of some domains and shrinkage of others is a mode of plastic deformation which may require much less stress than normal deformation twinning since the twins are preformed. Kriven, following Wadhawan and Boulesteix[353] refers to this as pseudoplasticity. Whatever the merits of this name, which is not generally used, there is no doubt that the modification of the twin structure by the tensile stress field of a propagating crack can give a two–three-fold increase in the toughness of ceramics of type (3Y-TZP), based on single phase zirconia, and (GMO), based on gadolinium molybdate.

Rabenberg and Kim[354] have examined the twin interfaces in monoclinic zirconia martensitically transformed from the tetragonal phase. Their specimens were partially reduced zirconia which gave an exceptionally high density of twin interfaces, together with stacking faults and dislocation-like defects; the twins were almost all of type (100)[001]. Steps parallel to the [001] twinning direction were visible in the interfaces when thin foils were examined by conventional TEM but $\mathbf{g} \cdot \mathbf{b}$ analysis failed to give consistent results for the Burgers vectors of these steps. However, lattice imaging is a powerful technique for studying interface structure, and it showed that the steps have screw character, i.e. the effective Burgers vector is parallel to the step, and that they are three unit cells in height. A structural model of the boundary incorporates a relative translation $\mathbf{t} = \frac{1}{2}\mathbf{c}$ away from the mirror symmetry atomic arrangement in order to reduce the misfit. The existence of this relative translation has been verified by comparison of actual lattice images with computer simulations of these images.

The misfit, i.e. the effective Burgers vector, of the rather high interface steps would be very large if each were composed entirely of elementary twinning dislocations, but if such a step is combined with a lattice [001] dislocation of opposite sign, this vector has the small magnitude of $c - 2[3a \sin(\beta\text{-}90°)] \simeq 0.074\ c$. Motion of these steps would thus produce a shear of magnitude $s = 0.074c/3a \simeq 0.025$, whereas the shear of the (100)[001] twinning modes has the much larger value of 0.328. Whilst neither the Burgers vector nor the shear could be measured directly, the contrast experiments showed that it was very small. The observed steps are thus analogous to the b.c.c. dislocations discussed and enumerated by Bristowe and Crocker;[93] they are allowable defects, but they do not produce the observed deformation twin. They have presumably formed as a result of accommodation stresses producing cancellation effects equivalent to emissary slip.

Genuine deformation twinning, as distinct from the motion of transformation twins, was first investigated in thin film specimens of zirconia by Bailey[355] who measured the shear displacements and thus tabulated all the twinning elements for various modes, the most important of which have $\mathbf{K}_1$, η_1 and s parameters of (100), [001], 0.328 and (110), $[1\bar{1}8]$, 0.228, respectively. Recently First and Heuer[356,357] have investigated the twins formed around a diamond indentation (or indent) produced by a Vickers hardness test on a single

crystal of zirconia. The complex stress field was approximated as a number of in-plane compression axes and the Schmid factors for various possible twins evaluated. The observed twins were predominantly of (110) type and these were also the most favourably orientated twins.

Sapphire and ruby gemstones and the mineral corundum are all essentially α-Al_2O_3 and are isostructural with haemetite (α-Fe_2O_3). The structure is rhombohedral, but since the oxygen ions are in a slightly distorted h.c.p. packing and the aluminium cations occupy two-thirds of the octahedral interstices in a highly ordered fashion, it is convenient to use hexagonal rather than rhombohedral indices in describing the crystallography. In both haematite[358] and corundum,[359] some deformation twins (referred to as rhombohedral twins) have been identified with the following 'macroscopic' mode:

$$\mathbf{K}_1 = \{01\bar{1}2\} \quad \mathbf{K}_2 = \{0\bar{1}14\} \quad \boldsymbol{\eta}_1 = \langle 0\bar{1}11\rangle \quad \boldsymbol{\eta}_2 = \langle 02\bar{2}1\rangle$$

Geipel *et al.*[360] have recently used high resolution electron microscopy to examine the interface structure of a deformation twin in sapphire, and have obtained results in good agreement with the earlier study by Bursill and Lin[361] of the interface structure and the 'micro' twinning elements in haematite. They describe the twin as a 'screw twin'; i.e. the atom sites in the two crystals are related not solely by a 180° rotation about $\boldsymbol{\eta}_1 = \langle 0\bar{1}11\rangle$ (as in a classical type II twin) but also by a translation $\mathbf{t} = \frac{1}{6}\langle 0\bar{1}11\rangle$ parallel to this axis. Thus the two-fold pseudo-symmetry axis of classical theory is actually a two-fold screw pseudo-symmetry axis relating the atom sites of the two crystals. [A similar situation occurs in the isosceles model of a b.c.c. $\mathbf{K}_1$ interface, see Fig. 8(b)]. Geipel *et al.* propose that the twins form by double cross-slip of a zonal twinning dislocation, a mechanism analogous to that suggested by Pirouz[14,173–175] for semiconducting materials.

In a separate paper, Lagerlof *et al.*[362] describe a model for basal twinning in sapphire; this type of twinning becomes more important than slip as a deformation mode below about 1000°C and has the following macroscopic crystallography (Kronberg[363]:

$$\mathbf{K}_1 = \{0001\} \quad \mathbf{K}_2 = \{10\bar{1}1\} \quad \boldsymbol{\eta}_1 = \langle 10\bar{1}0\rangle \quad \boldsymbol{\eta}_2 = \langle \bar{1}012\rangle$$

The mechanism proposed is the dissociation of a basal plane slip dislocation of type $\frac{1}{3}\langle 11\bar{2}0\rangle$ into a leading partial $\frac{1}{3}\langle 10\bar{1}0\rangle$ and a trailing partial $\frac{1}{3}\langle 01\bar{1}0\rangle$. The motion of the leading partial will create a two-layer microtwin, and this partial is assumed to rotate independently about pinning points and then to reunite with the trailing partial. The recombined lattice dislocation is then supposed to cross-slip up or down two planes and finally to redissociate and repeat the cycle. Thus the Piroux mechanism is again invoked to give layer by layer growth. However, the recent proliferation of models using this ratchet-type mechanism may be misleading since they mainly originate from one group, and it should be emphasized again that there is, at present, little or no direct evidence to support it.

Since much of the emphasis of this review has been on crystallinity, it is appropriate to conclude by drawing attention to the fact that deformation twinning can be obtained in materials which are non-crystalline. Twins were found in a cast Al–Cu–Fe icosahedral quasicrystal by Dai and Urban[358] who suggested the crystallographic parameters of a possible deformation mode which could produce the observed orientation relation. However, the origin of this twin is not known it could well have arisen from a growth accident, so the possibility of deformation twinning of a quasicrystal remained open until the recent experiments of Shield and Kramer.[359] They deformed an alloy of nominal composition $Al_{65}Cu_{23}Fe_{12}$ by high temperature creep in compression to a total strain of more than 30%.

The specimens prepared by powder metallurgical techniques were about 70% face-centred icosahedral quasicrystals and 30% Al_7Cu_2Fe and this phase structure was apparently unaffected by the large deformation. Electron microscopy of the deformed specimens showed numerous twinned regions of quasicrystal superimposed on a structure of finer (possibly slip?) bands. Analysis of the electron diffraction data leads to the conclusion that both $\mathbf{K}_1$ and $\mathbf{K}_2$ are five-fold planes whilst $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$ are midway between two two-fold axes of the quasicrystal. In terms of the coordinate axes and indexing scheme of Cahn *et al.*, the twinning elements may be written $\mathbf{K}_1 = \{1/0\ 0/1\ 0/0\}$, $\mathbf{K}_2 = \{0/1\ 0/0\ 1/0\}$, $\boldsymbol{\eta}_1 = \langle 1/2\ 1/1\ 2/1\rangle$ and $\boldsymbol{\eta}_2 = \langle 1/2\ 1/1\ 1/0\rangle$ and the twinning shear is $s = 1.02$. This mode is identical to that found by Dai and Urban and it is interesting to note that it is the equivalent of a compound mode since all the twinning elements are rational.

SUMMARY

The concepts of twinning shears and twinning modes are introduced. The early attempts to predict these features are presented. This is followed by a detailed discussion of the formal theories of Bilby and Crocker and Bevis and Crocker for predicting these elements. Their formalisms are applied to predict twinning modes in single lattice structures, superlattices, hexagonal close packed structure and other double lattice structures. Wherever possible the predicted modes are compared with those observed.

The description of fully coherent, rational twin interfaces is presented, and the concepts of elementary, zonal, complementary and partial twinning dislocations are discussed. It is suggested that the irrational K_1 twin interfaces may be faceted on the microscopic scale, and these facets may be coherent.

Homogeneous and heterogeneous nucleation of twins are discussed. The growth of twins by the nucleation of twinning dislocations on planes parallel and contiguous to the coherent twin boundary is considered. Various dislocation models proposed for the formation of twins in b.c.c., f.c.c., diamond cubic, zinc-blende and h.c.p. structures are critically reviewed. In some cases the supporting experimental evidence is presented. Additionally, the effects of deformation temperature, imposed strain-rate, alloying and doping, prestrain, precipitates and second phase disperions on deformation twinning are discussed.

Mechanistic details regarding the accommodation processes occurring at twins terminating within a crystal, slip–twin, twin–slip and twin–twin intersections are reviewed and are compared with the experimental results. The role of twins in the nucleation of fracture in materials is also considered.

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