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Scripta Materialia 68 (2013) 95–99

Scripta MATERIALIA

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Viewpoint Paper

Critique of mechanisms of formation of deformation, annealing and growth twins: Face-centered cubic metals and alloys

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Available online 28 September 2012

Abstract—The formation of deformation, annealing and growth twins in face-centered cubic materials is discussed. Slip precedes deformation twinning, and twins form from the interaction between primary and secondary slip dislocations having co-planar, but different, Burgers vectors. The influence of several metallurgical variables on twinning can only be rationalized in terms of the model. Annealing twins form due to growth accidents on differently inclined {1 1 1} facets present on a migrating grain boundary. Growth twins also form by growth accidents on the {1 1 1} planes.

Keywords: Deformation twins; Annealing twins; Growth twins; fcc Metals and alloys

1. Introduction

Deformation, annealing, and growth twins in face-centered cubic (fcc) metals and alloys are crystallographically identical. Their coherent twin boundaries (CTBs) lie on the {1 1 1} planes, whereas non-coherent twin boundaries (NCTBs) may or may not exhibit well-defined habit planes and interfacial dislocation structures. These three twin types are observed in a variety of materials, but evolve under dramatically different conditions. The formation of deformation twins certainly requires stresses and appears to involve partial dislocations; annealing twins may need grain boundary migration; and growth accidents are necessary during vapor-to-solid or liquid-to-solid transformations for the formation of growth twins.

The concern of Cottrell and Bilby [1] regarding twinning as a possible deformation mode in fcc metals and alloys has not been borne out. Since the early 1950, numerous observations have been reported in the literature indicating that twins play a significant role in the plasticity of these materials (e.g. [2–6]). Recent studies on Mn-containing steels convincingly demonstrate that twins play a significant role in twinning-induced plasticity [7,8]. The twinning phenomenon is also quite complex and is affected by a number of metallurgical variables [9]. In spite the importance of twinning in crystal plasticity, no attempt has ever been made to critique some of the proposed models [2–6,10–11], and apply them to rationalize the effects of different variables on twinning.

Our understanding of the formation of annealing and growth twins may be better. Certainly, simulations [12,13] have provided some useful information on growth twins, and similar studies may be warranted on annealing twins. Hopefully, this open dialogue would allow researchers to design critical experiments to advance the current knowledge base on the mechanisms that govern twinning.

This Viewpoint paper has two main objectives. We will highlight salient features of some of the models proposed for the formation of deformation, annealing and growth twins; and then rationalize published experimental observations in terms of various proposals.

1.1. Deformation twins

Geometrically, deformation twins can be formed by the passage of a Shockley partial on contiguous {111} planes. The question is: how does the arrangement of Shockley partials required for twinning evolve? There is a consensus that twins form from dislocations. According to Christian and Mahajan [9], the sources can be grouped into two types: prismatic [2] and glide [3–6,10,11]. Prismatic sources refer to those situations where the Burgers vector of the source dislocation does not lie in the twin plane, whereas for glide sources the

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1359-6462/$ - see front matter © 2012 Published by Elsevier Ltd. on behalf of Acta Materialia Inc.
http://dx.doi.org/10.1016/j.scriptamat.2012.09.011

Burgers vector lies in the twin plane. Cottrell and Bilby [1] were the first to consider the role of a prismatic source in fcc twinning and concluded that only single-layer twins may be feasible. This is because Shockley partials cannot double cross slip onto a parallel {1 1 1} to form a two-layer twin. Venables [2] showed that this difficulty can be obviated, and his suggestion is schematically illustrated in Figure 1. We will use Thompson's notation to describe dislocation reactions. A long jog N1N2 in Figure 1a serves as a prismatic source; its Burgers vector is **AC** and does not lie in plane (b). The jog can dissociate into a Frank partial **Aα** that is sessile and a Shockley partial **αC** that is glissile. Under the influence of a stress, the glissile partial **αC** can glide on plane (a), leaving behind an intrinsic fault. Christian and Mahajan [9] discussed in detail how Figures 1c–f develop from Figure 1b, and the reader is referred to their review. Venables suggested that long jogs could be created by intersections between the primary and secondary dislocations. Niewczas and Saada [5] proposed that glissile Shockley partials on the conjugate plane are formed by the interaction of slip dislocations gliding on primary slip planes with Frank faulted dipoles whose segments also lie on the primary plane. In principle, in both models, twins do not lie on the primary slip plane.

Let us now consider some other models involving prismatic sources that assume the Cottrell–Bilby dissociation [1]. Cohen and Weertman [3] suggested that glide dislocations constituting a blocked slip band could dissociate into Frank and Shockley partials, and that the glide of Shockley partials on intersecting {1 1 1} planes could result in overlapping intrinsic faults, leading to twins. Again, twins do not lie on the primary slip plane, and an additional constraint is that glide dislocations must be correctly spaced within the slip band so that the cross-slip of Shockley partials could lead to intrinsic stacking faults on parallel {1 1 1} planes, separated by $a/\sqrt{3}$, where a is the lattice parameter. This is a very difficult situation to achieve given these constraints. The "stair-rod cross-slip model" of Fujita and Mori [4] is conceptually very similar to the model of Cohen and Weertman [3].

There is evidence that twinning in fcc crystals does not begin until the co-planar slip vector is activated on the primary plane [14]. The simplest description to rationalize this observation is that of Mahajan and Chin [10], who considered a reaction between dislocations on the primary system with Burgers vector **BC** and of the co-planar system with vector **DC** to form three Shockley partials according to the following reaction:

$$\mathbf{BC} + \mathbf{DC} \rightarrow 3\alpha\mathbf{C} \tag{1}$$

The above reaction is repulsive in nature. This can be understood by referring to Figure 2. Consider a situation where dislocations **DC** and **BC** gliding on the same plane (a) are dissociated intrinsically into Shockley partials **αC, Dα** and **αC, Bα** as shown in Figure 2a. The above reaction cannot occur because the partial **Bα** of **BC** interacts repulsively with the partial **αC** of **DC**. This implies that reaction (1) could only occur under high stress concentrations [15,16]. However, the reaction appears to take place very readily [17]. Mahajan [17] proposed an elegant solution to resolve this dichotomy. The essential elements of his proposal are schematically illustrated in Figure 2b and c. Imagine a situation where a constriction **DC** is present on the dissociated dislocation **DC**. The constricted segment subsequently dissociates so that the leading and lagging partials swap

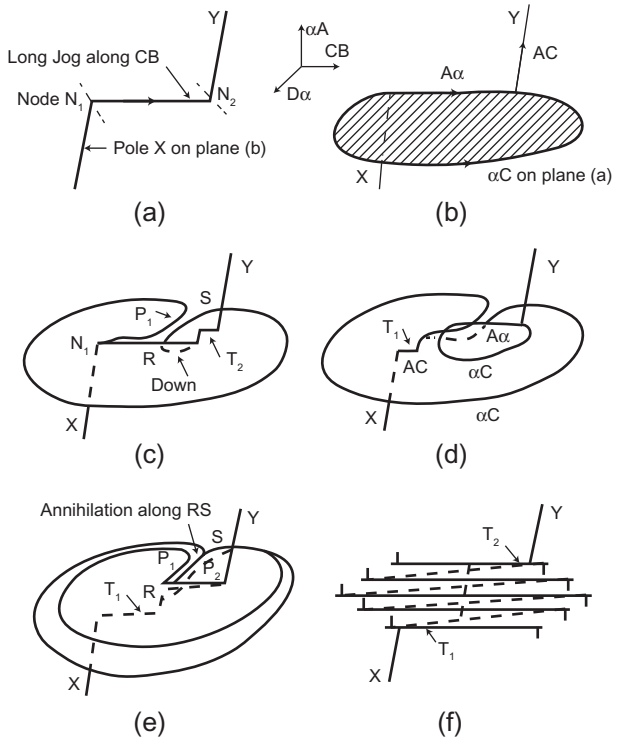

Figure 1. Prismatic glide mechanism for fcc twinning.

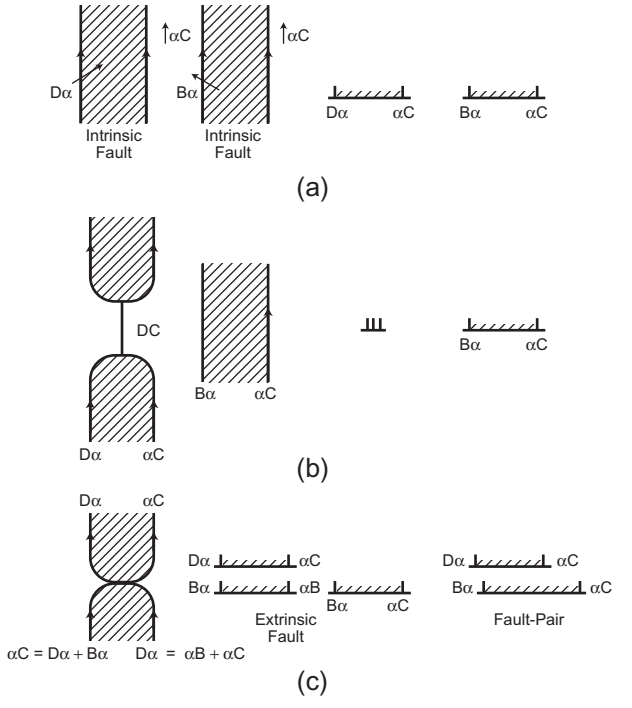

Figure 2. Schematic illustration of the formation of a fault pair in fcc crystals.

positions, and this would result in an anomalous fault. However, the anomalous fault can be converted into an extrinsic fault if the further dissociations $\mathbf{D\alpha} \rightarrow \mathbf{\alpha B} + \mathbf{\alpha C}$ and $\mathbf{\alpha C} \rightarrow \mathbf{D\alpha} + \mathbf{B\alpha}$ are assumed (see Fig. 2c). The partials **αB** and **Bα** annihilate each other, leading to the configuration shown in Figure 2c; the Burgers vectors of partials bounding the left interface add up to **αC**. Gallagher [15,16] was the first to observe such configurations and referred to them as fault-pairs. It is emphasized that the transformation of the anomalous fault into the extrinsic fault entails rearrangement of atoms within the core regions of the dislocations [17]. Initially, Mahajan and Chin [10] suggested that the fault-pairs get converted into three-layer twins, but did not specify a mechanism, and microtwins evolve by the coalescence of the three-layer twins, located at different levels within microslip bands. It is now proposed that there is no need for the transformation; twins could form from fault-pairs as well. Furthermore, in this model, the slip bands and twins lie on the same plane. An interesting, unresolved issue is how fault-pairs and dislocations, located at different levels within a slip band, interact with each other; simulation studies could shed some light on this challenging problem.

There are only two detailed studies in the literature where attempts have been made to present supporting evidence on nucleation and thickening of deformation twins [5,10]. Niewczas and Saada [5] deformed Cu–8 at.% Al single crystals in tension along the [5 4 1] orientation, which is close to the [1 1 0] direction. For this orientation, the primary conjugate planes are, respectively, (1 1 −1) and (1 −1 1). This way they could produce Frank dipoles on the primary planes. The glissile Shockley partials on the conjugate planes could form by the interaction of glide dislocations with the faulted dipoles. The authors certainly observed faulted dipoles in the deformed samples, but evidence on the interaction of the faulted dipoles with dislocations on the primary plane was not obvious. Furthermore, they did not discuss how pole dislocations get incorporated into a growing twin.

Mahajan and Chin [10] correlated the crystallography of slip ahead of the twins, i.e. emissary slip, with that of twins in deformed Co-8 wt.% Fe alloy. This alloy twins readily in spite of the fact that its stacking fault energy (SFE) is not low. Mahajan and Chin showed that: the habit planes of twins and emissary slip were parallel to each other; dislocations needed for reaction (1) were present in the emissary slip bands; and reactions leading to the formation of fault-pairs were seen in the emissary slip bands.

Having critiqued the salient features of different models, let us now apply the Niewczas–Saada and Mahajan–Chin models to rationalize the following well-accepted, experimental observations on twinning: influence of planar and wavy slip; orientation dependence; through-thickness perfection of twins; and influence of grain size. Recent studies on Hadfield steels indicate that planar slip favors deformation twinning [7,8], whereas wavy slip does not. It is not easy to rationalize this observation in terms of the Niewszas–Saada model. Since the Mahajan–Chin mechanism requires coplanar secondary slip on the primary plane, the probability of the occurrence of reaction (1) is much higher if the dislocations are confined to narrow slip bands. Also, planar slip is promoted by decreasing SFE, increasing lattice friction stress and the presence of short-range order [18,19]. That is, there are other factors besides SFE that can produce planar slip. We can thus rationalize the formation of twins in Co–8 wt.% Fe alloy that does not have low SFE.

It is well known that fcc metals and alloys twin when compressed along the [0 0 1] direction, but do not twin in tension. On the other hand, the ⟨1 1 1⟩ oriented crystals twin in tension, but not in compression; whereas the ⟨−1 2 3⟩ crystals do not twin until coplanar secondary slip is activated. To explain these dependences, let us discuss the case of [0 0 1] compression; the ⟨1 1 1⟩ case can be understood in a similar fashion. In response to the imposed shape change, the following slip and twinning systems will be activated: [1 0 −1], [0 1 −1] on (1 1 1); [0 1 −1], [−1 0 −1] on (−1 1 1); [−1 0 1], [0 1 1] on (−1 1 −1); and [0 1 1], [1 0 1] on (1 1 −1); [1 1 −2] (1 1 1); [−1 1 −2] (−1 1 1); [−1 1 −2] (−1 1 −1); and [1 1 2] (1 1 −1); the directionality of twinning was taken into consideration in assigning indices for the four twinning directions. It is clear that twins on the (1 1 1), (−1 1 1), (−1 1 −1) and (1 1 −1) could evolve according to the model of Mahajan and Chin [10] from slip dislocations that are activated concurrently. This may not be possible in terms of the Niewczas–Saada [5] model. Furthermore, Karaman et al. studied the deformation behavior of differently oriented single crystals of Hadfield steel [7,11]. The ⟨0 0 1⟩ and ⟨111⟩ oriented crystals exhibited the expected behavior, but the ⟨123⟩ oriented crystals did not twin up to 50% strain. The authors did not present any evidence as to whether or not the coplanar secondary slip was activated at that strain level. Therefore, it would be difficult to use their results to test the validity of the Mahajan–Chin model. Furthermore, Karaman et al.'s model entails stress-induced separation of leading and lagging Shockley partials, followed by the glide of the leading partial to form a one-layer twin. The absence of twinning for the ⟨1 2 3⟩ orientation is not consistent with their ideas.

Mikkola and Cohen [20] investigated through-thickness perfection of twins in shock-loaded copper single crystals. They found that when twins were examined in edge-on configuration, twinned and matrix regions were interspersed into each other, implying that twins are imperfect. This is a natural consequence of the Mahajan–Chin model, whereas the Niewczas–Saada model predicts highly perfect twins.

Let us now apply the Mahajan–Chin model to rationalize the observed grain size dependence of twinning. Imagine a situation where a nanograin in an fcc metal deforms by single slip, resulting in a slip band that can be likened to a pseudo pile-up. Assume that the grain size is L, then the maximum length of the "pile-up" is L/2. If the number of dislocations in the "pile-up" is N, σ is the applied stress and $|\mathbf{b}|$ is the Burgers vector, then force F acting on the leading dislocation in the "pile-up" is given by: $N\,|\mathbf{b}|\,\sigma\,L$. The force acting on dislocations at yielding is $\frac{YSL^2}{2}$, where YS is the yield strength of the nanomaterial. Equating the two, we can show the following:

$$N = 2\frac{YSL}{\sigma|b|} \quad (2)$$

If we assume that σ is equal to YS and insert appropriate values for various parameters, we obtain N ≈ 30. In addition, N will vary as a function of the applied stress; the lower the value of σ, the higher the value of N. It appears that the computed density of dislocations in the slip band may not be high enough to effect slip-induced lattice rotation where co-planar secondary slip could occur. Therefore, twins may not form according to the Mahajan–Chin model. An alternative mechanism involving the nucleation of Shockley partials from grain boundaries could lead to twinning [21].

1.2. Annealing twins

Carpenter and Tamura [22] were the first to observe annealing twins in a variety of deformed and annealed fcc metals and alloys. Later on, Gertsman et al. [23] showed that annealing twins have a strong influence on the texture of deformed and annealed metals. As the properties of polycrystalline materials are affected by texture, understanding the evolution of annealing twins is important.

Many models have been proposed to rationalize the formation of annealing twins. They can be broadly classified into two groups: (i) growth accidents [24–27], and (ii) nucleation of twins by packets of overlapping stacking faults [28,29]. The suggestions that are conceptually appealing are those of Gleiter [26], Meyers and Murr [28] and Mahajan et al. [27]. Gleiter suggested that grain growth entails the transfer of atoms from a shrinking grain to a growing grain, and this occurs at a grain boundary. By invoking the existence of shallowly inclined {1 1 1} facets on the boundary, he suggested that two-dimensional faults could form through growth accidents as atoms are deposited on the facets during the migration of the boundary. The model is plausible. However, with the exception of twin D in Figure 3, which shows the locations of twins observed in deformed and annealed metals, the formation of twins A, B and C is difficult to rationalize using his model. Meyers and Murr suggested [28] that annealing twins evolve in two stages: initiation and propagation. They proposed that twins "pop out" from grain boundary ledges. The characteristics of the grain boundary regions from which pop-outs occur were not discussed. They also hypothesized that twins propagate by the migration of NCTBs consisting of Shockley partials whose effective Burgers vector is zero. It is not clear what makes this interface move because the force due to stress on the NCTB is zero. Their model also does not require migrating boundaries for the formation of annealing twins. However, Mahajan et al. [27] observed that the frequency of annealing twins in abraded copper surfaces was much higher than that in annealed copper. They attributed this difference to the contribution of slip-induced damage to grain boundary migration in the abraded case.

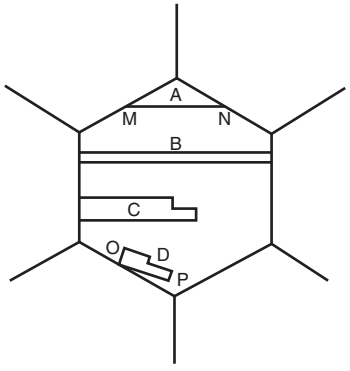

Figure 3. Schematic showing various morphologies of annealing twins observed in fcc crystals.

Mahajan et al. [27] built up on the initial suggestion of Gleiter [26] that grain boundaries have shallowly inclined {1 1 1} facets. They proposed that these facets could have a range of angles with respect to grain boundary habit planes. As suggested by Gleiter, if the angle is shallow, annealing twins labeled D in Figure 3 could evolve. However, it was shown by Mahajan et al. [27] that if the {1 1 1} facet is normal to the boundary habit plane, twins B in Figure 3 could form. If NCTBs are assumed to consist of Shockley partials of the same Burgers vector and sign, then the first partial will be pushed forward by the repulsive force exerted by the partials that subsequently form; B twins could form this way. It is conceivable that as the twin thickens, the net Burgers vector of an NCTB could change to zero. This situation could lead to C-type twins. It is emphasized that grain boundary migration is an essential component of the above model.

1.3. Growth twins

The stacking arrangement of the {1 1 1} planes in the fcc structure is ABCABCABC. It is relatively easy to see that if growth mistakes occur on these planes during vapor-to-solid or solid-to-solid transformations, one-, two-, three-layer and even thicker twins could form. These twins were observed in a variety of semiconducting epitaxial layers and metallic films.

We can mechanistically discuss the formation of growth twins as follows. Assume that gold atoms are arriving on the (1 1 1) gold surface. If the arrival rate is low and the surface temperature is high so that surface atomic mobility is high, the atoms would end up in the correct positions at the surface, and twins will not form. On the other hand, if the arrival of atoms occurs at a high rate and the substrate temperature is low, the arriving atoms will not have sufficient mobility to get to the correct positions, and this would lead to growth twins.

Zhou and Wadley [12] used molecular dynamics to simulate the growth of (1 1 1) copper films as a function of deposition rate and temperature. Simulation results indicated that the expansion of twins in the growth plane occurs at a rate much faster than that of the deposition rate. This is not surprising because the lateral expansion of faults occurs due to repulsive interactions between Shockley partials bounding the faults. Their results also indicated that the formation of twinned structures is difficult to control by changing either the

deposition rate or the processing temperature. Zhang et al. [13] arrived at similar conclusions from their study on sputter-deposited stainless steel.

Lu and co-workers [30] were able to produce a very high density of growth twins in electrodeposited copper by pulsed plating. They observed that these films exhibit high strength, while maintaining good ductility and conductivity. Their results can be understood in terms of the explanations developed by Mahajan and Chin [31]. These authors showed that the motion of dislocations is blocked by twins. Two out three dislocations propagating on a certain glide plane will not be able to propagate across the twin until the slip bands thicken, leading to the development of stress concentration at the slip band–twin intersections. Recent calculations by Mahajan [32] indicated that a slip band consisting of 40 dislocations will provide a stress concentration of adequate magnitude for blocked dislocations to propagate through the twins. This assessment has two ramifications. First, the penetration would add to the ductility of the material because strain will be produced by dislocations having three Burgers vectors in the glide plane instead of one. Second, the separation between twins must exceed a certain value so that slip bands of sufficient lengths can form to provide a stress concentration for dislocations to propagate through the twins.

1.4. Summary

We have critiqued the mechanisms proposed for the formation of deformation, annealing and growth twins in fcc metals and alloys. The highlights of our assessments are as follows:

1. Deformation twins evolve from dislocations. The circumstantial evidence indicates that primary and coplanar secondary slips are involved in the formation. These dislocations interact repulsively, but the reaction can be made attractive by swapping the positions of leading and lagging partials.
2. Annealing twins form by growth accidents on the {1 1 1} facets of a migrating grain boundary; their distribution and configurations are very hard to control.
3. Growth twins also evolve by growth accidents on the {1 1 1} planes during vapor-to-solid or liquid-to-solid transformations; grain boundaries are not involved in their evolution.

Acknowledgements

The author acknowledges stimulating discussions with Professors Enrique Lavernia, John Hirth and Ke Lu.

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