DEFORMATION TWINNING

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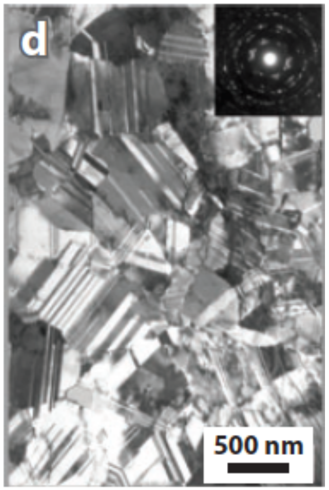
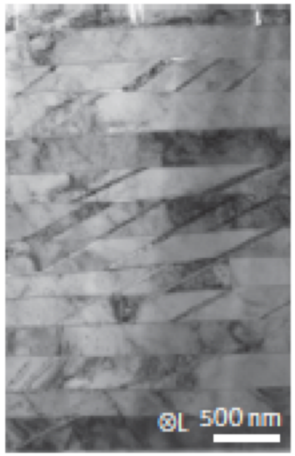
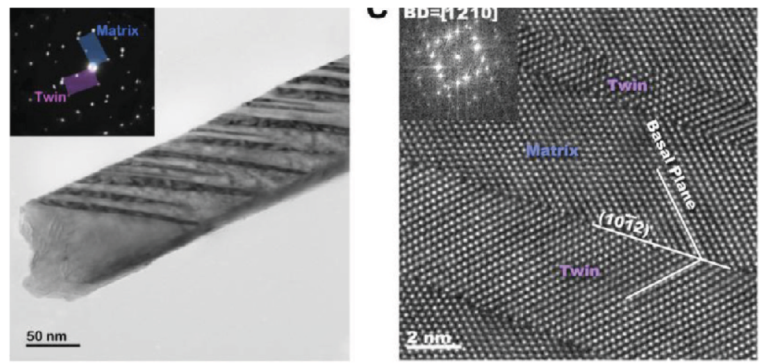
Twinning in materials



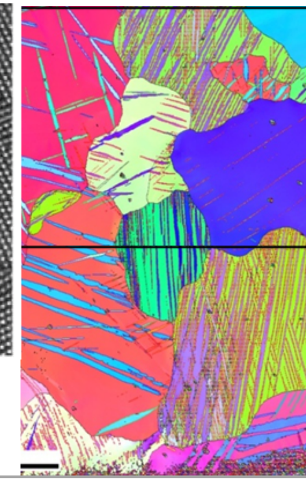
Nanotwinned Cu,
L. Lu et al., *Science, 2004*



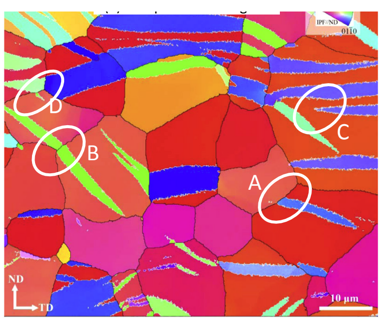
Bio-exoskeleton,
Nat. Mater, 2014



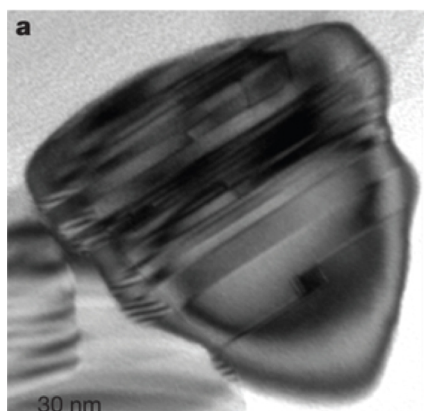
Magnesium, Yu et al. Nano Lett, 2012



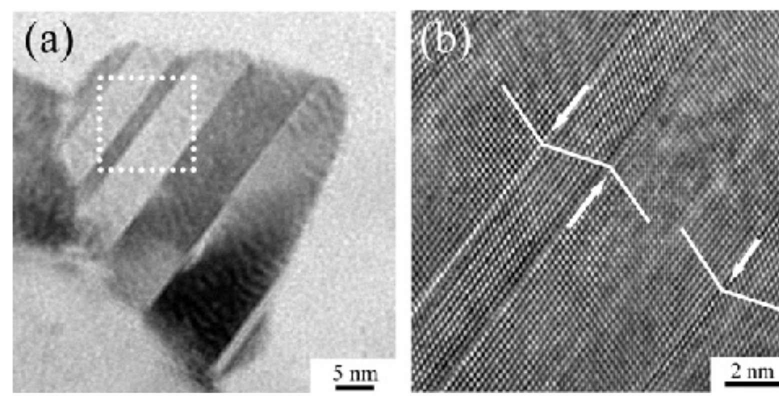
Uranium,
Courtesy of McCabe



Magnesium
M. Arul Kumar, LANL



Boron Nitride,
Tian et al. *Nature* 2013



Nanocrystalline metals,
Ma and Zhu, *Ref Mod Mat Sci Mat Engng*, 2016

Basics

- Deformation or in growth (we focus on deformation here)
- Different crystal structures (fcc, bcc, hcp, orthorhombic, B2)
- Different metals and alloys (brass vs Ti64)
- Amounts are sensitive to strain level, direction of straining, alloying, temperature, and strain rate

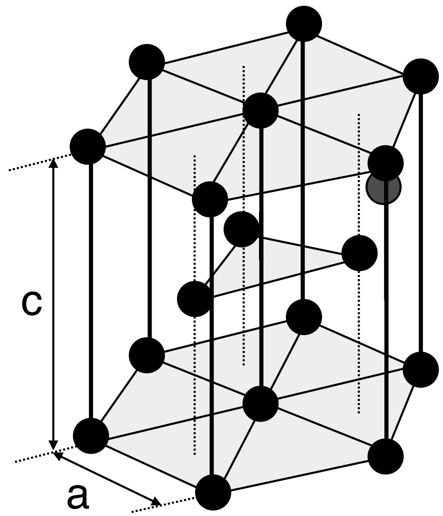
- Common features
  - Manifests as a domain within a crystal
  - Introduces a subcrystalline boundary or boundaries
  - Theoretical twin/matrix misorientation
  - Crystallographic planes are sheared a finite amount

- For this lecture, we will consider twinning in HCP metals

HCP METALS AND ALLOYS

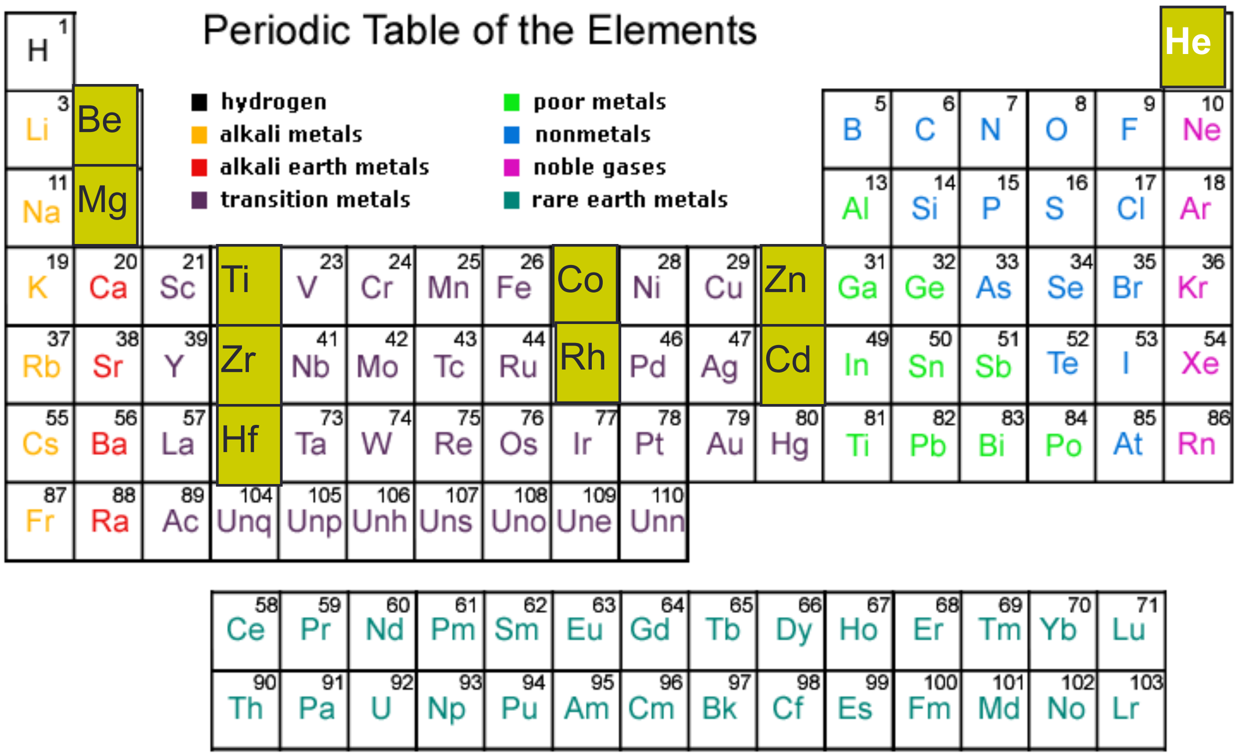
Hexagonal close packed (HCP) metals:

HEXAGONAL CLOSE PACKED



c/a = 1.56 – 1.89

c/a ratio:
Mg: 1.624
Zr: 1.593
Ti: 1.587



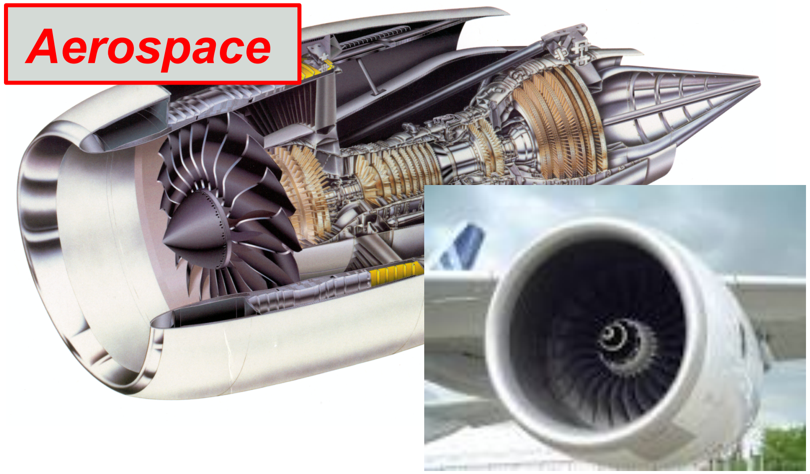
HCP metals and their alloys

High strength to weight, biocompatibility, fatigue resistance, radiation resistance

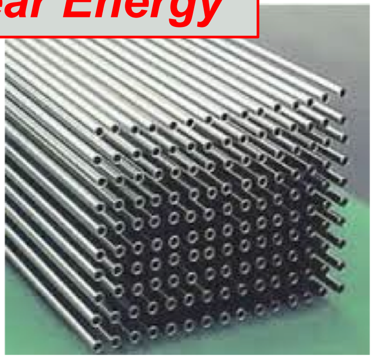
Automotive

Armor

Aerospace



Nuclear Energy

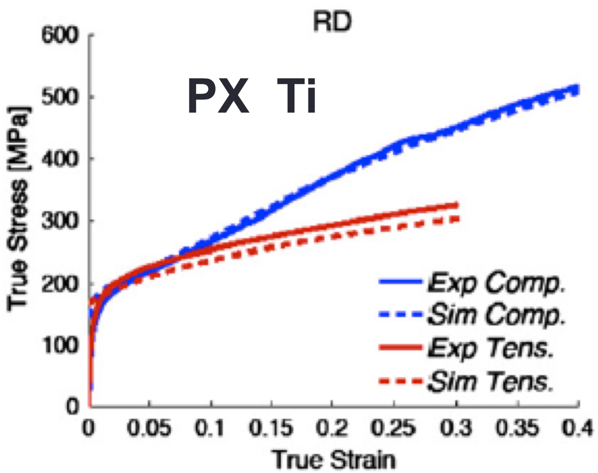


Biomedical

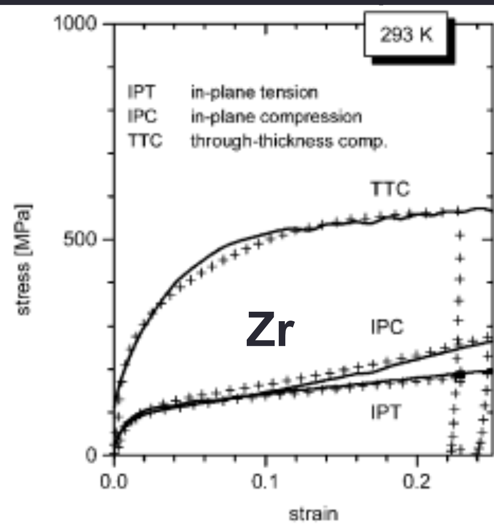
Aircraft

Deformation behavior of hcp metals

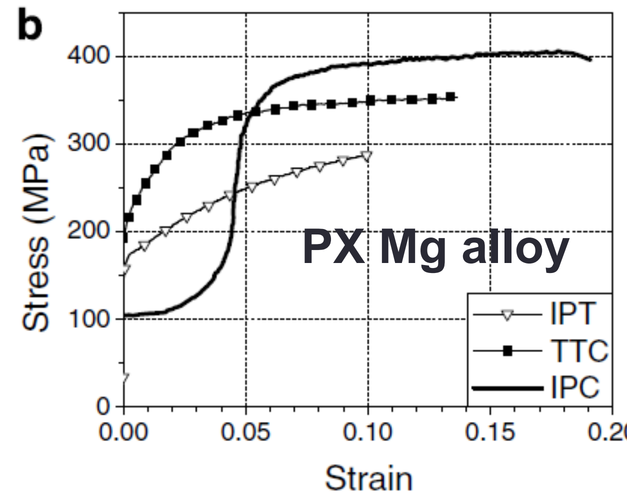
- <u>Significantly depends on direction (plastic anisotropy)</u>



Knezevic et al., MSE-A 2013

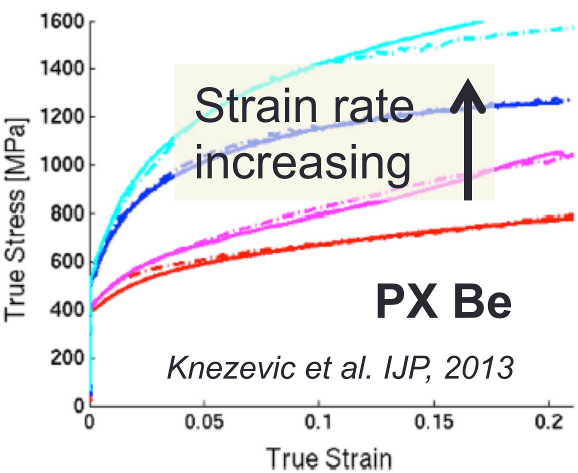


Tome et al. Acta Mater 2001

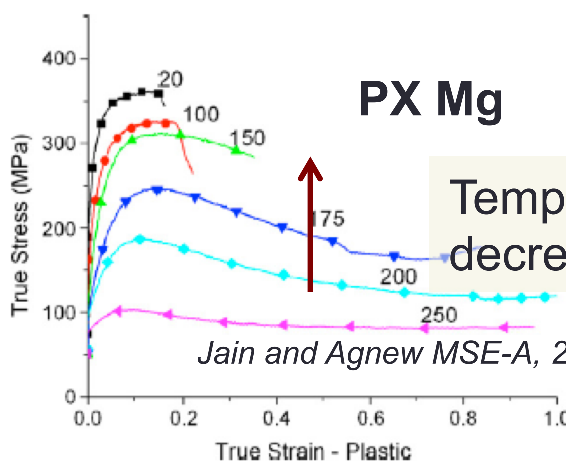


Proust et al. Acta Mater 2007

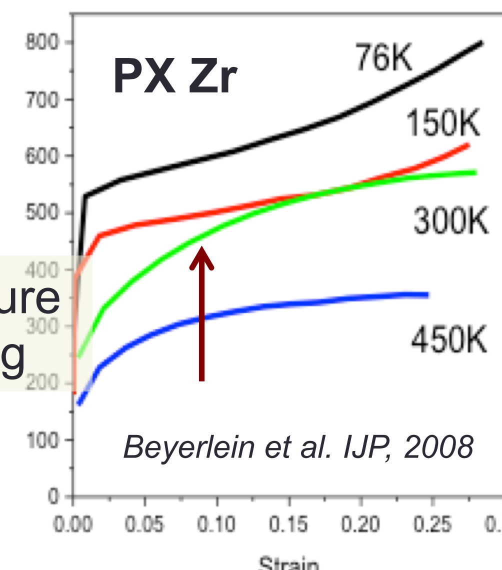
- <u>Significantly depends on conditions</u>



Knezevic et al. IJP, 2013

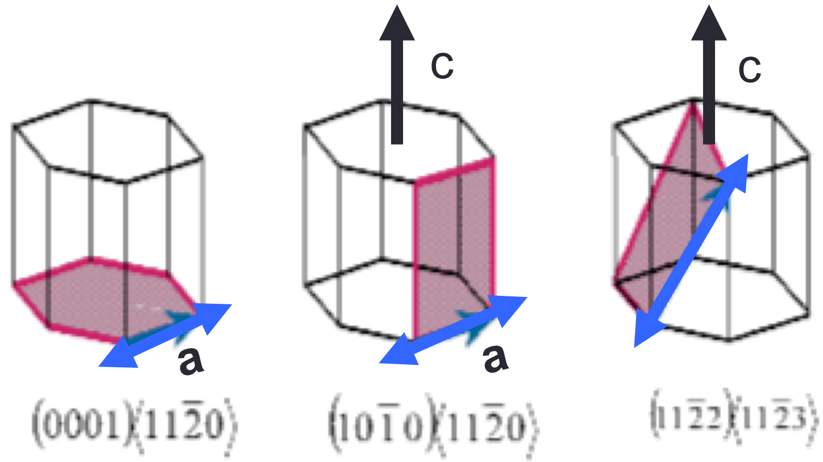


Jain and Agnew MSE-A, 2007



Beyerlein et al. IJP, 2008

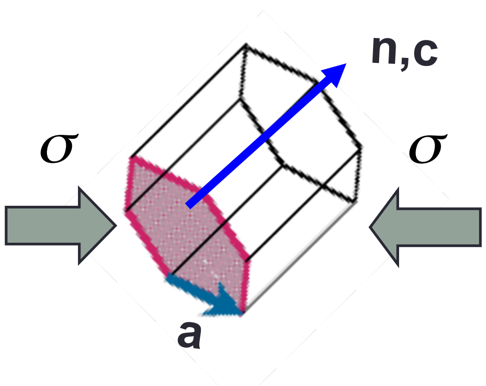
hcp metals can exhibit large differences in CRSS

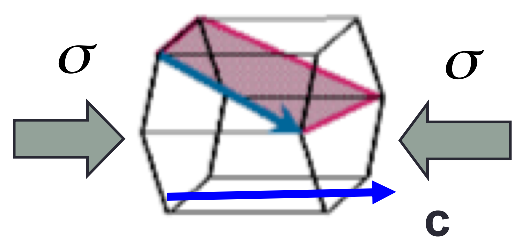


Basal slip | Prismatic slip | Pyramidal slip

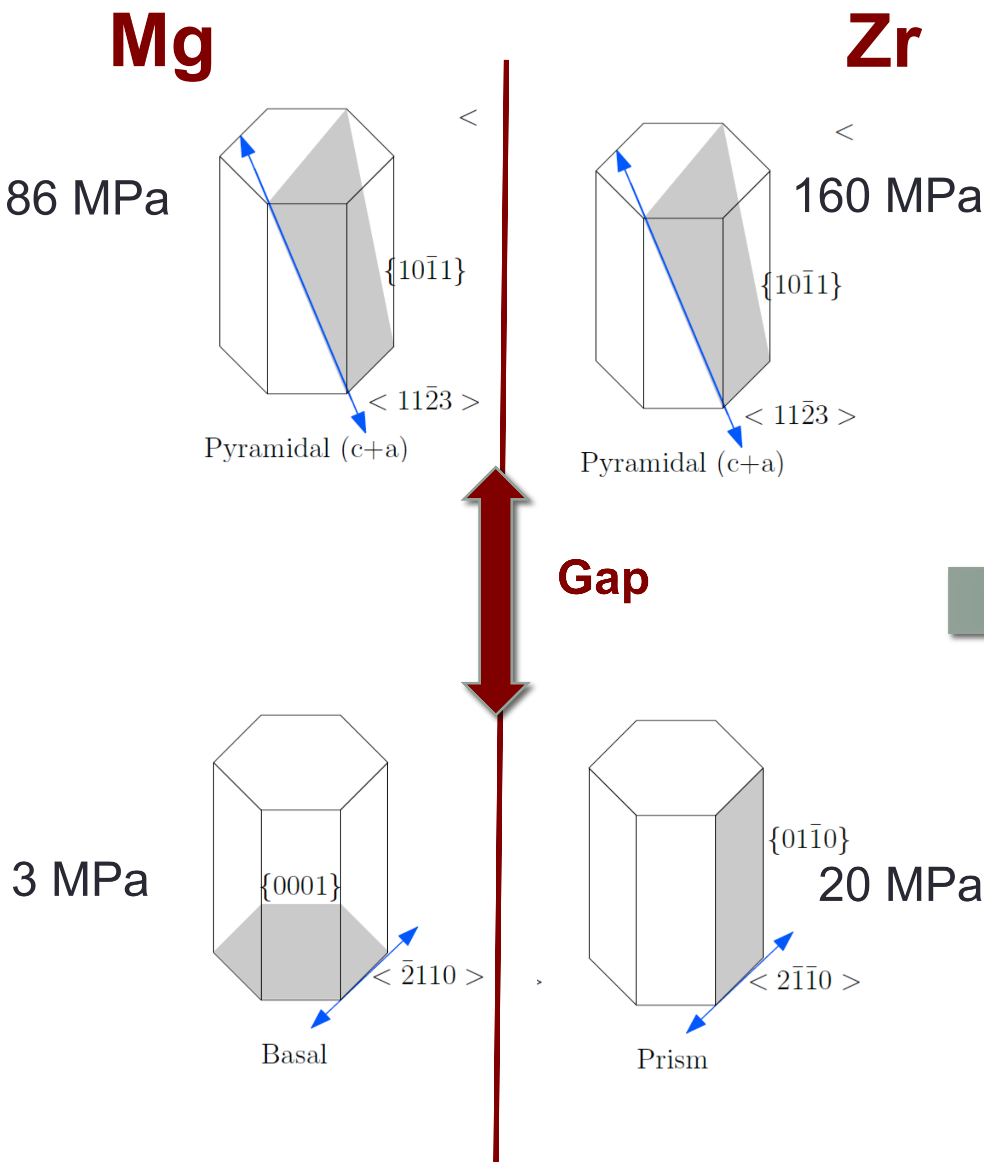
Usually large CRSS differences

$CRSS_{pyram}$ >> $CRSS_{basal}$ and $CRSS_{prism}$

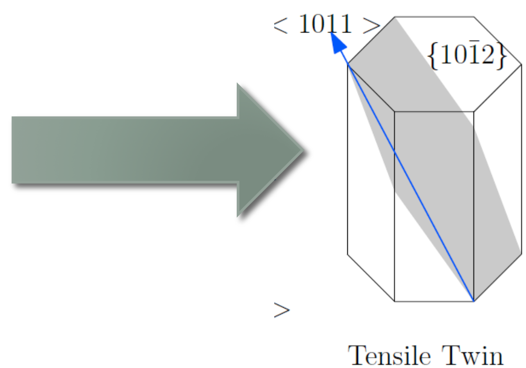




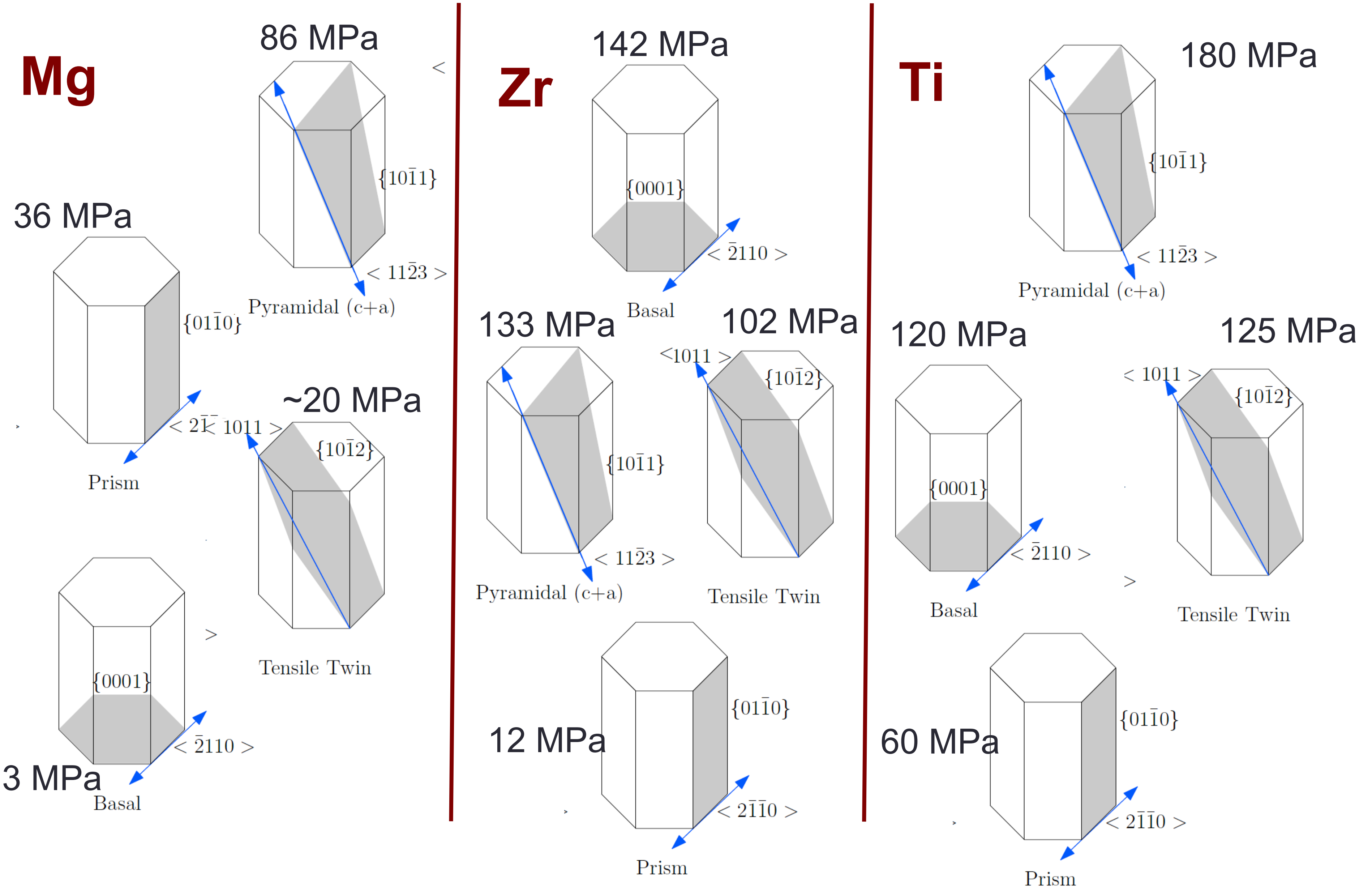
Hcp crystals have a high propensity for twinning



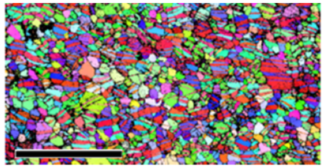
"Extension Twin"
Accommodates extension along the c-axis

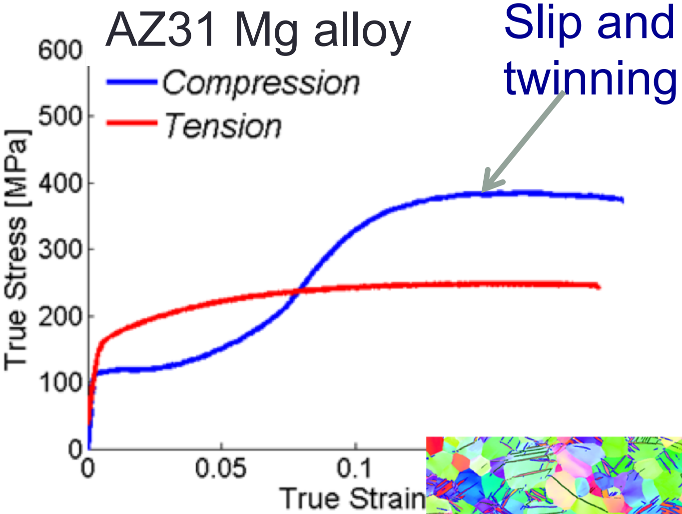


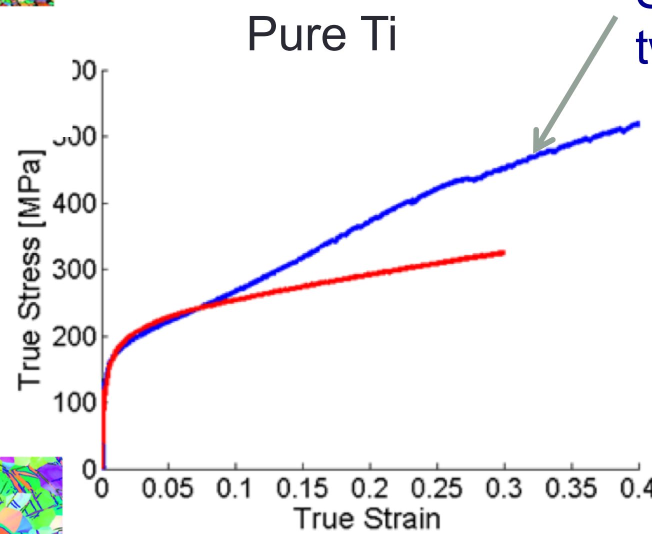
Mesoscopic CRSS values for slip

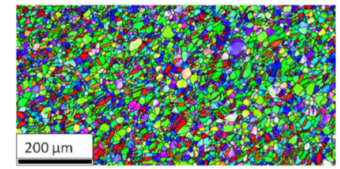


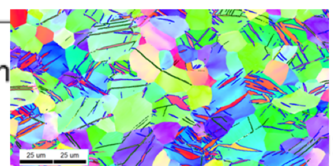
Slip and twinning affect stress-strain response

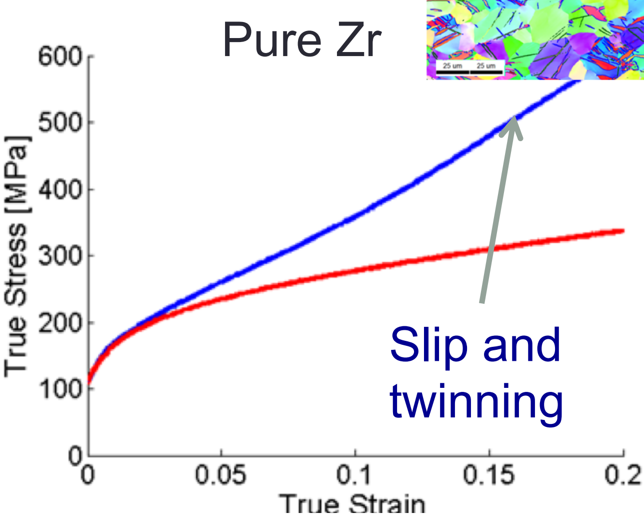


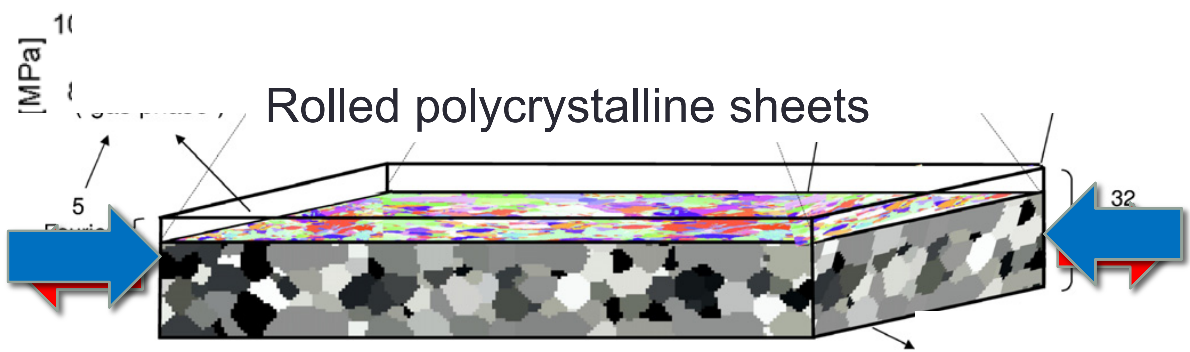








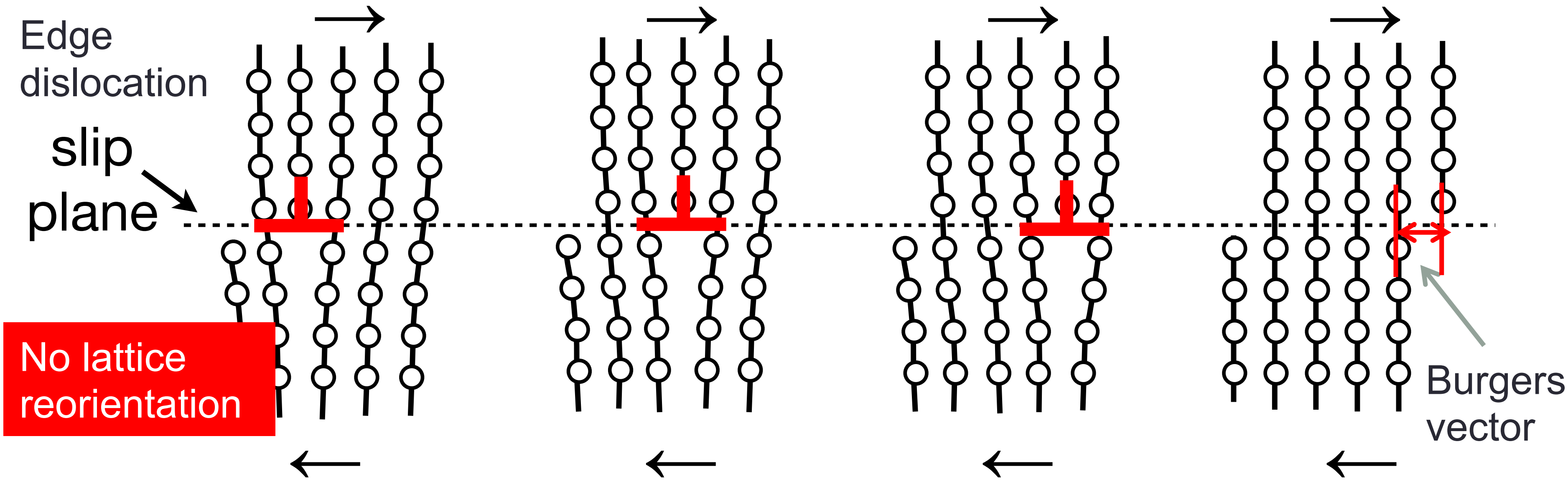




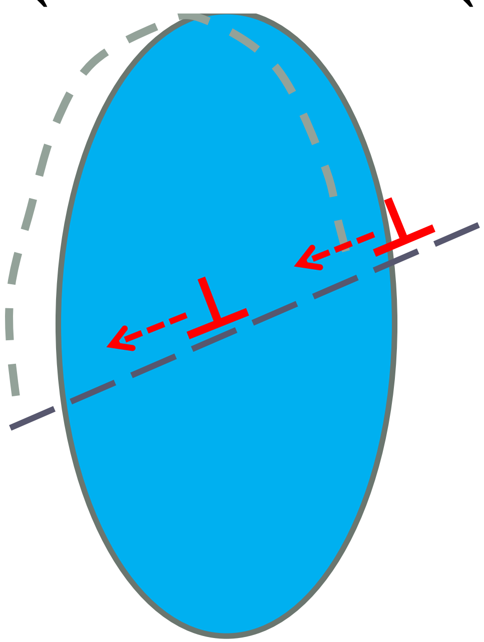
Knezevic et al. Scripta Mater 2016

BASICS OF DEFORMATION TWINS

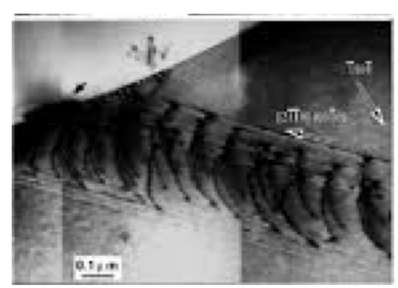
Lattice dislocation (slip)

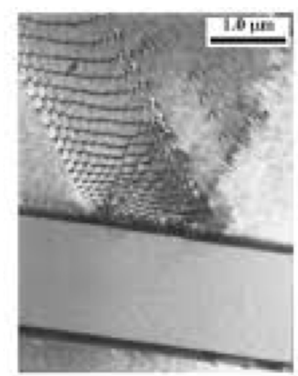


R. LeSar; Computational Materials Science



Dislocation arrays and pile ups

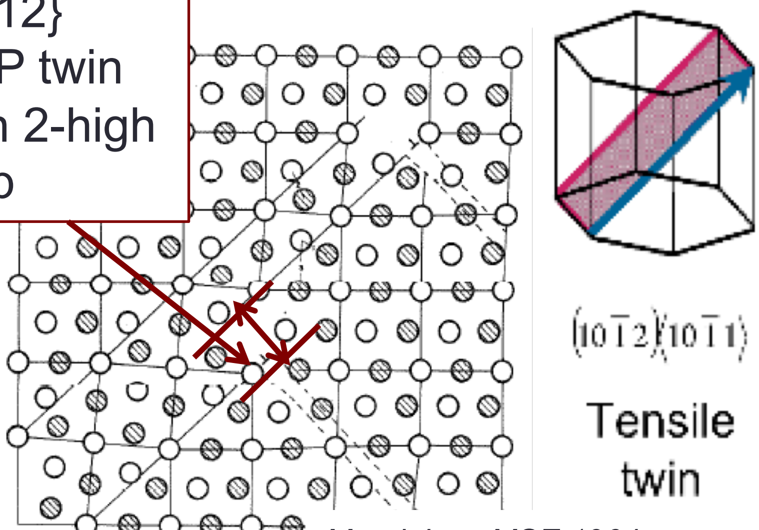




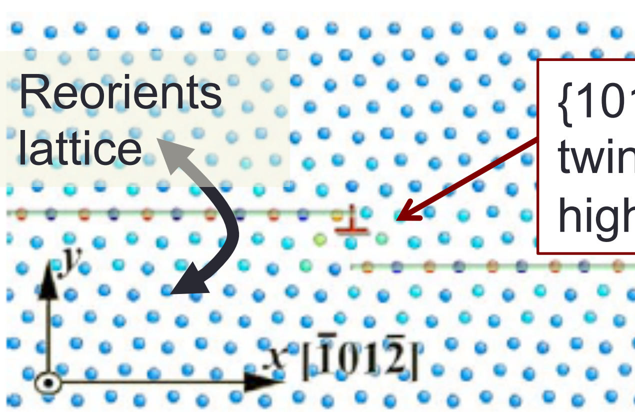
Twinning dislocations

. . . have a Burgers vector and step height

{1012} HCP twin with 2-high step

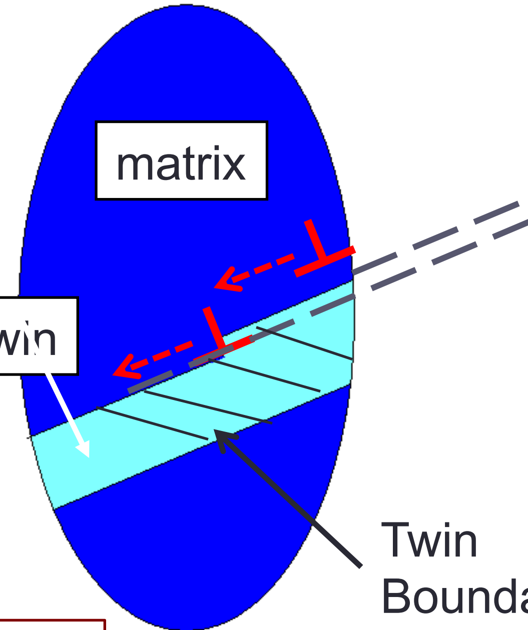


Mendelson MSE 1964

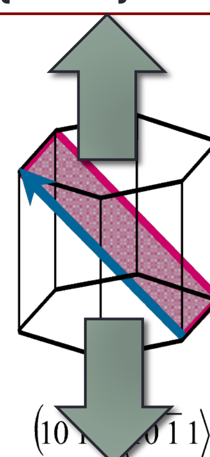


{1011} HCP twin with 2-high step

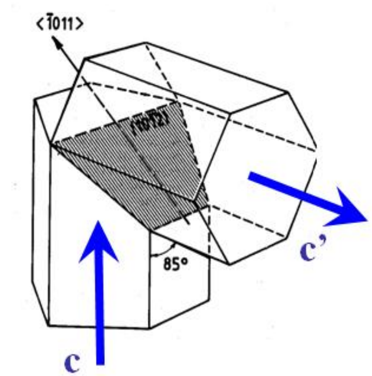
Wang, Beyerlein, Hirth, Tome, Acta Mater 2011



{1012} twin



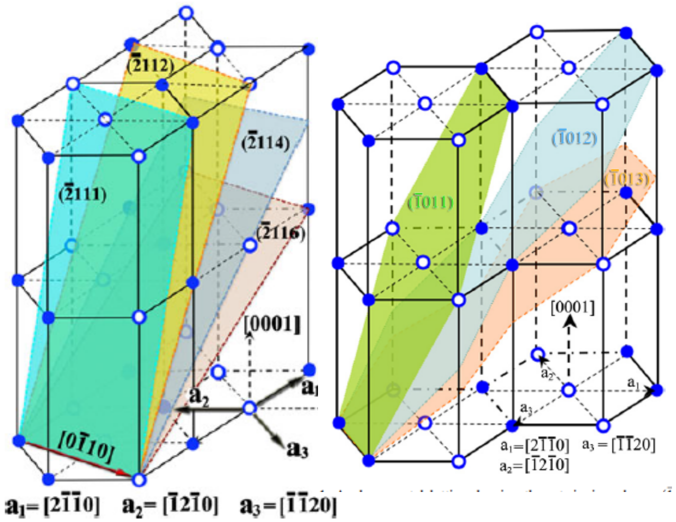
Tensile twin



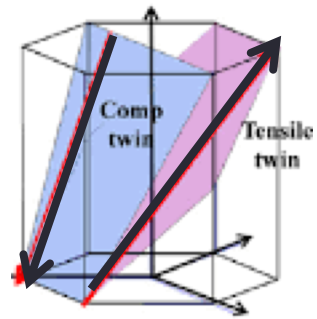
- **Reorients the lattice**
- **Forms a boundary**
- **Shears the material**

Twin modes

7 observed twin planes

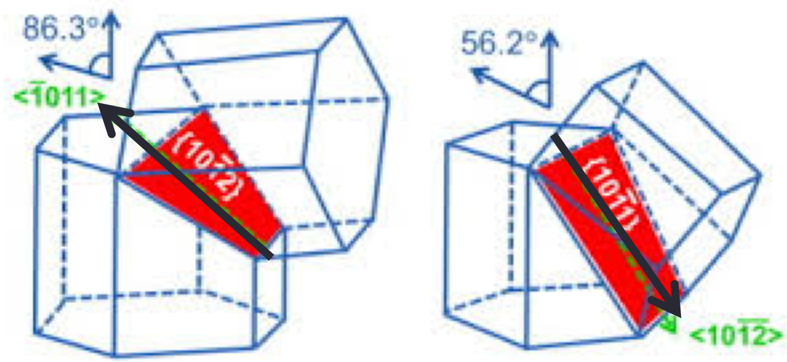


Wang et al. MSMSE 2011



Characteristic shear of the (1012) twin
Mg: 12.9%

Characteristic shear of the (1011) twin
Mg: 40.4%

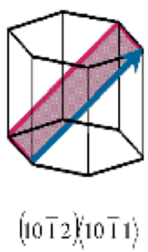


Distinct properties:

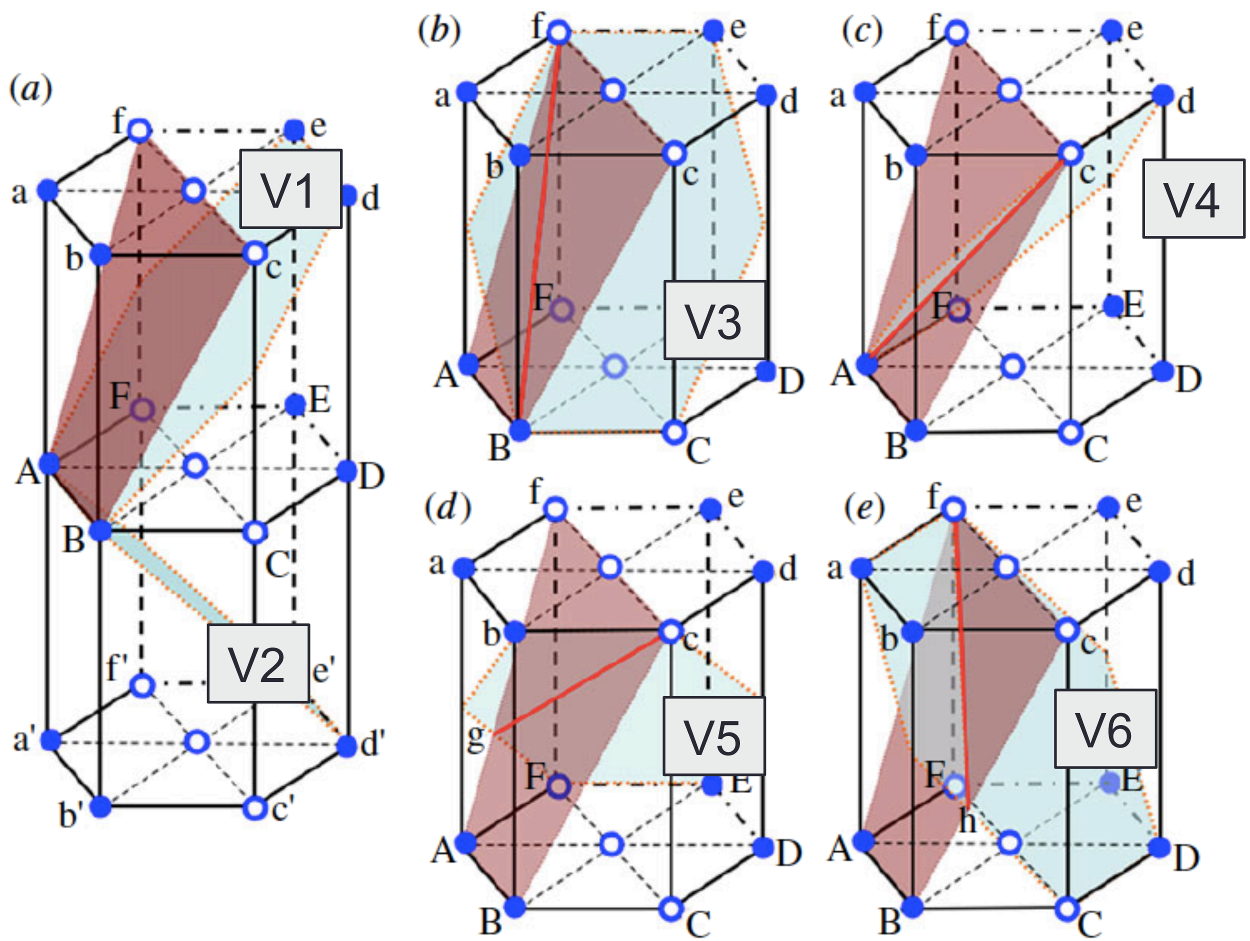
- **Twinning plane**
- **Twinning direction**
- **Characteristic twin shear**
- **Step height on twinning partial**
- **Consequently,**
  - **different twin/matrix orientation relationship**
  - **shear zone axis**
  - **accommodates c-axis contraction or extension**

Twin variants

Dark red plane is a {1011} type plane



Tensile twin



There are six variants $\nu^{(i)}$

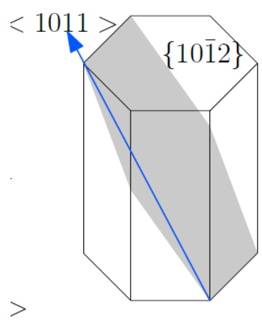
Independently oriented

Twins are mesoscale structures

1) Reoriented 3D domains, V
2) Provide unidirectional shear, γ
3) Limited amounts of shear; fixed *twin shear* S
4) Shear rate limited by boundary migration
5) Two latent effects on slip

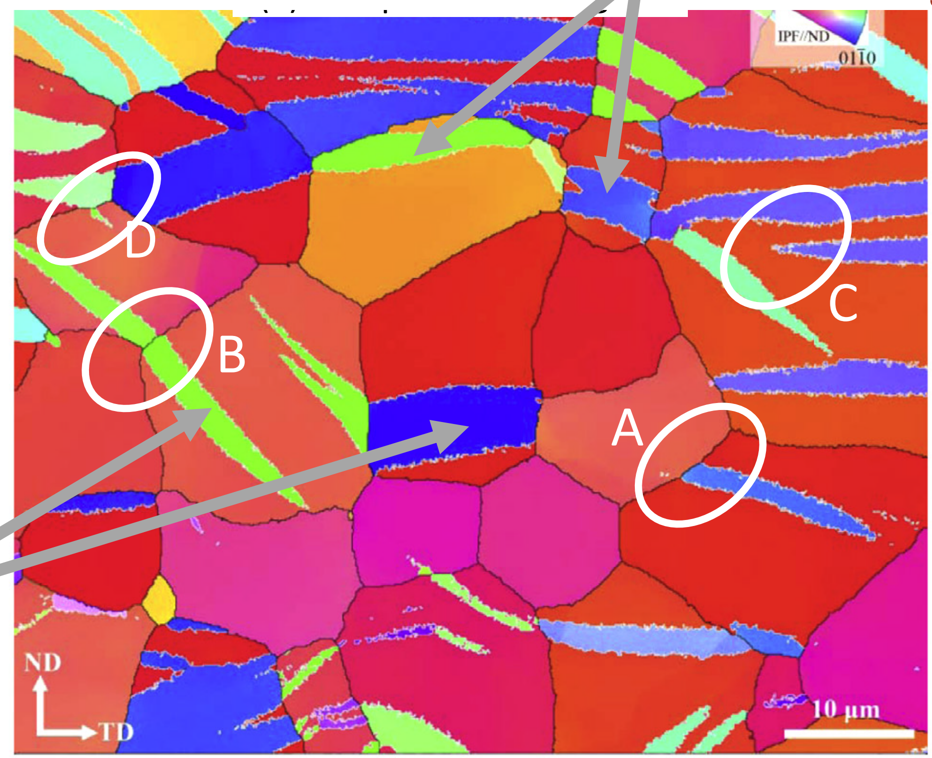
$$\gamma = SV,$$

$$\dot{\gamma} = S\dot{V},$$



Tensile Twin

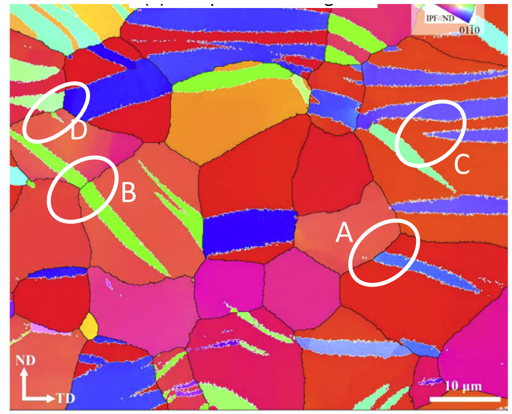
Boundary is a barrier for slip and twinning



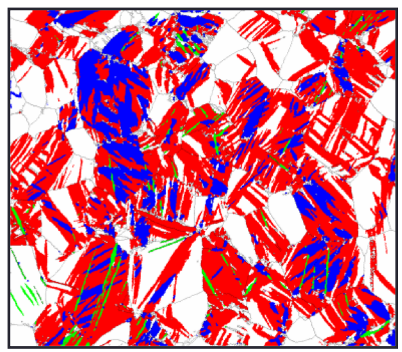
Domain for new slip or twinning activity

Manifestations of twinning in hcp metals

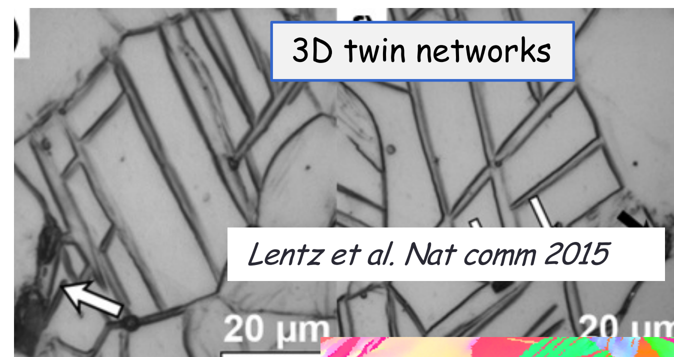
- Can be identified by OIM
  - Shape (thickness, volume)
  - mode
  - variant within type
- Can take on many configurations:
  - Twin intersections,
  - Many parallel twins
  - double twinning,
  - twin chains
- If the applied load were to be reversed, detwinning has been reported to happen.



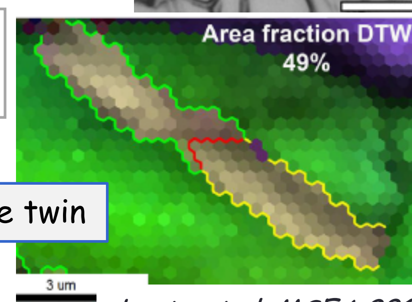
Beyerlein et al. Phil Mag 2008



Secondary blue twins in red twins

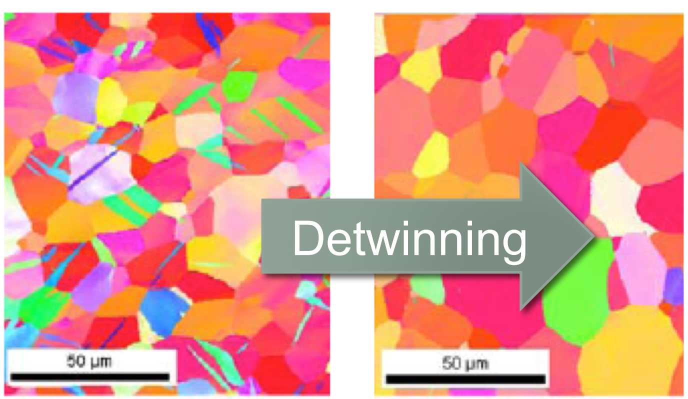


Lentz et al. Nat comm 2015



Double twin

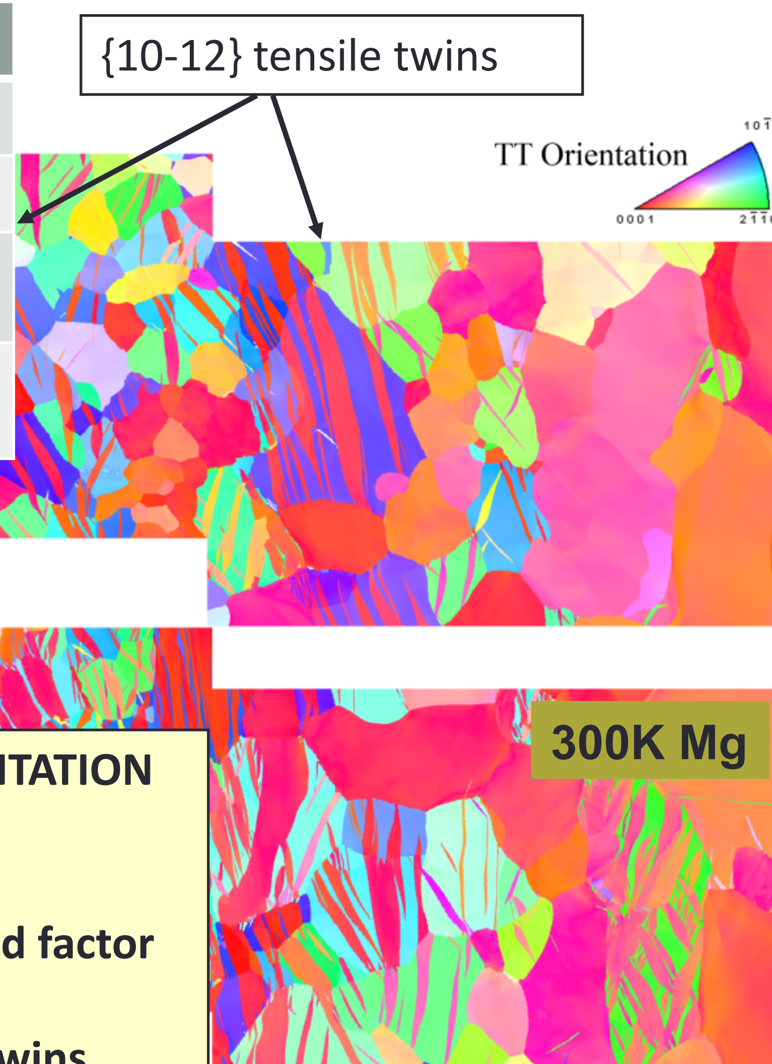
Lentz et al. MSEA 2014



Proust, Beyerlein et al., Expt Mech 2006
Knezevic, Beyerlein et al., IJP, 2013

Twinning is statistical in nature

FEATURE	Mg 3%
# of grains	2340
# of twins	8550
# of twinned grains	1534
# of grain boundaries	11698



GRAIN AREA, GRAIN ORIENTATION, GRAIN ORIENTATION

- Not all favorably oriented grains twin
- Some not favorably oriented grains twin
- Only 40% of twin variants have highest Schmid factor
- Not all grains of the same orientation twin
- Twinned grains contain variable numbers of twins
- Not all grains of the same size twin
- Twins have variable thickness

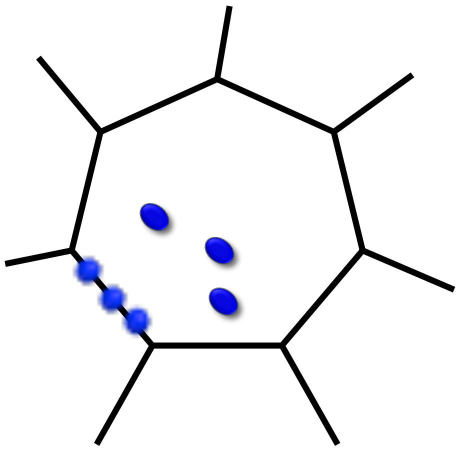
Beyerlein et al., Phil Mag 2010

STAGES OF GROWTH OF TWINNING UNDER DEFORMATION

Multiscale stages in twin development

Stage 1: Formation
Embryo

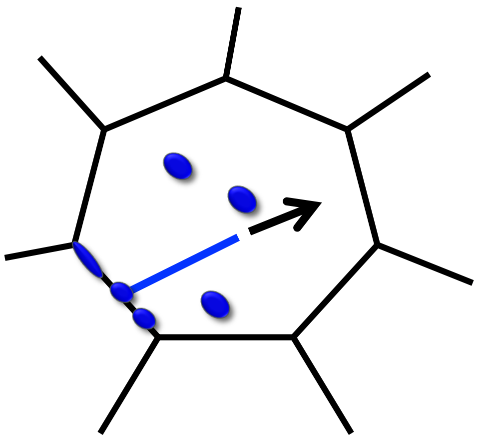
1) NUCLEATION



ATOMIC TO NANOSCALE

Stage 2: Propagation
Embryo->Lamella

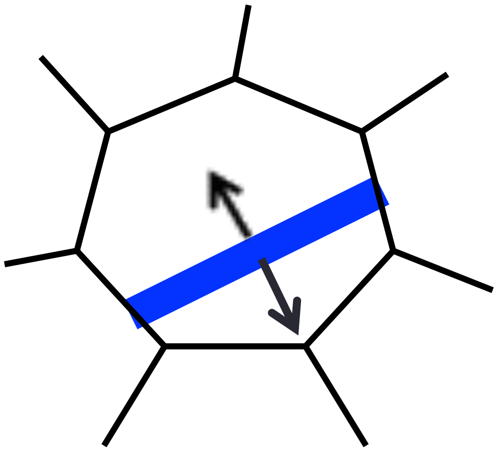
2) EXPANSION: PROPAGATION



NANOSCALE TO SUBMICRON

Stage 3: Expansion
Lamellae

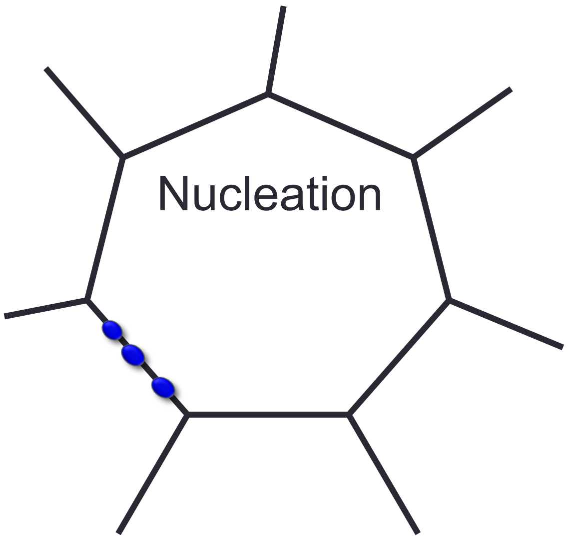
3) EXPANSION: THICKENING

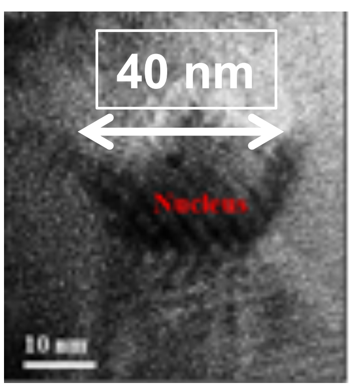


SUBMICRON TO MICRON SCALE

Observations

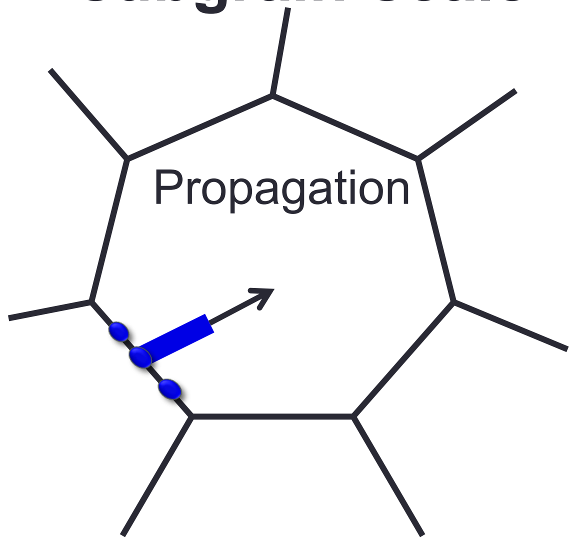
Atomic to dislocation-scale

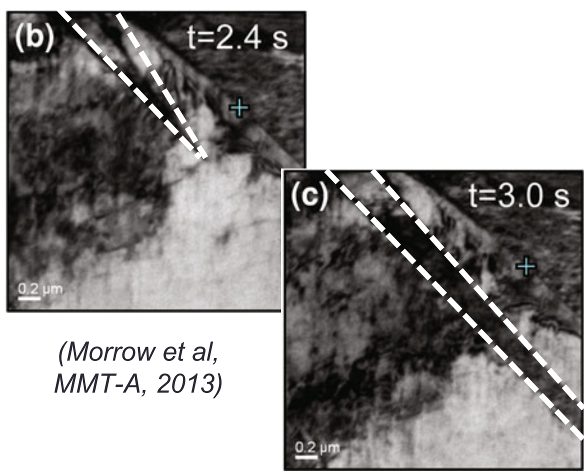




Courtesy of Lin Jiang, UC-Irvine

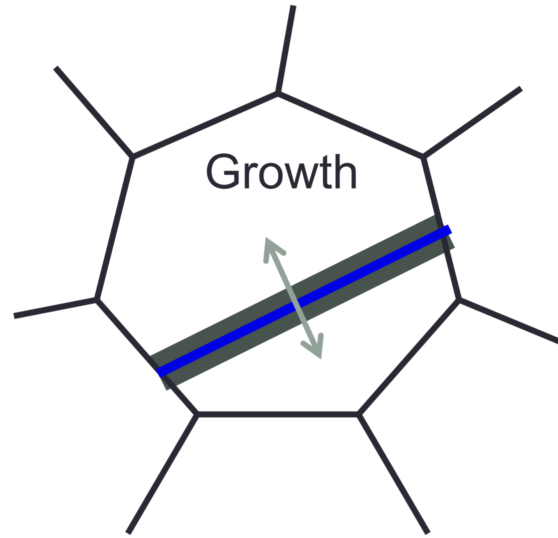
Substructure-subgrain-scale

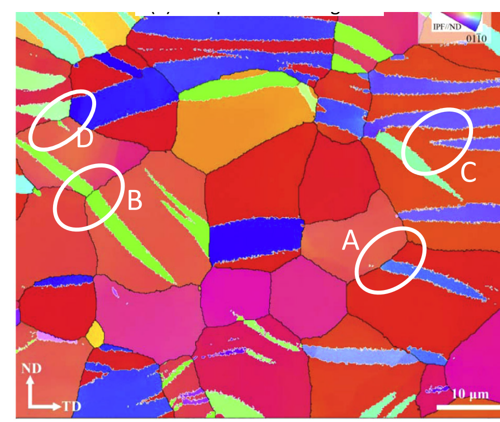




(Morrow et al, MMT-A, 2013)

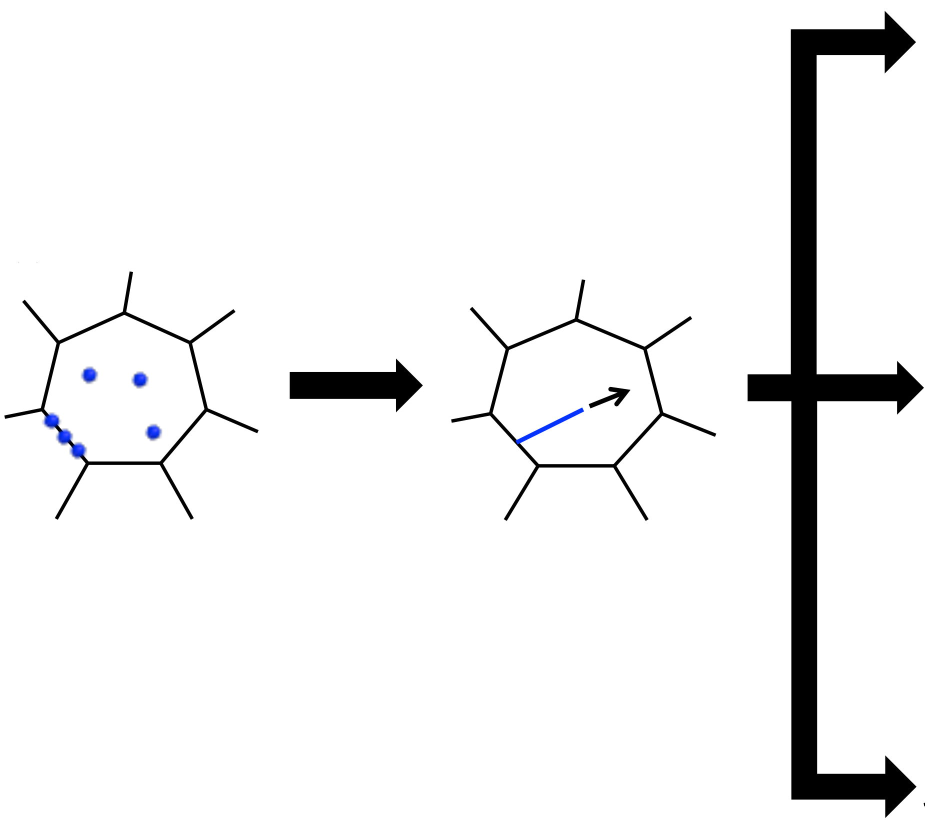
Grain-scale Plasticity

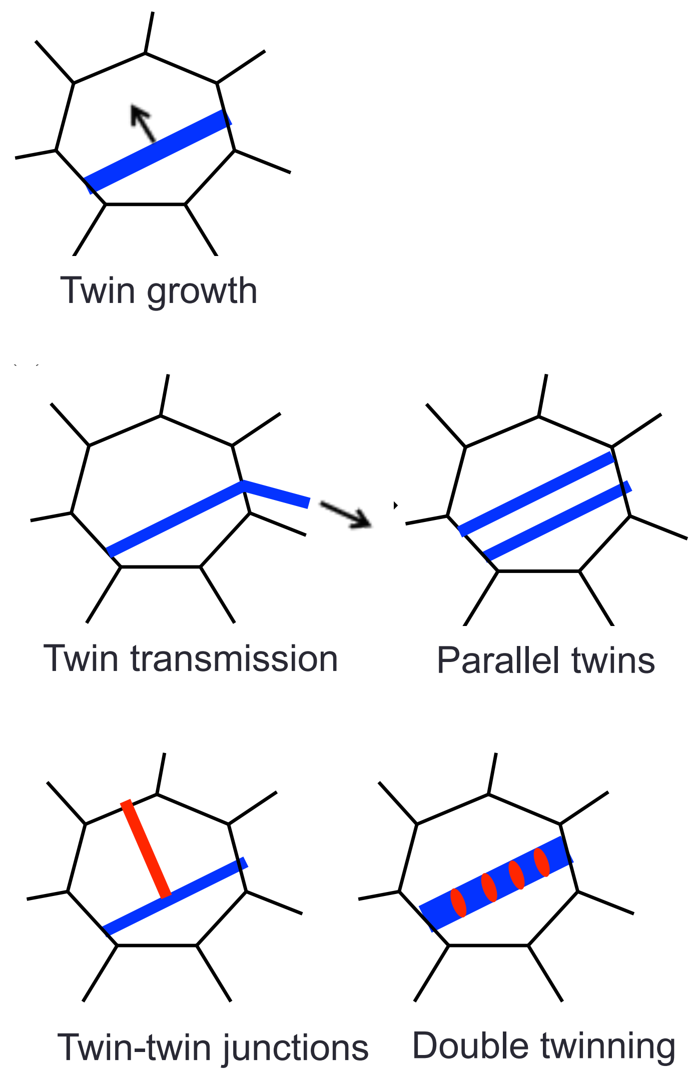




Courtesy of Arul Kumar LANL

Other variants of growth at the mesoscale



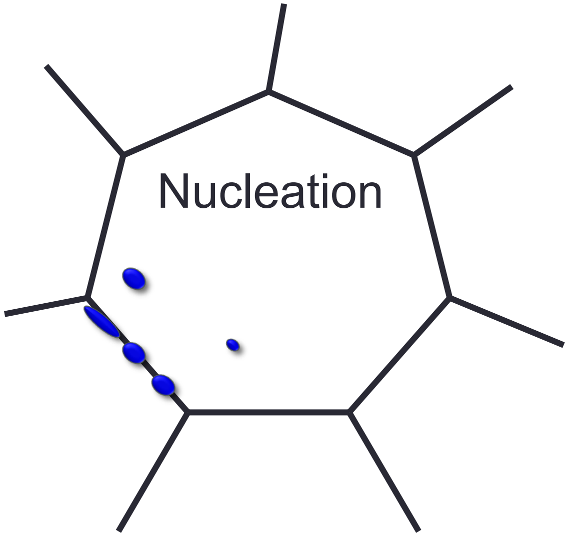


SEVERAL DISTINCTIVELY DIFFERENT RESPONSES ARE POSSIBLE

- How are these accomplished?
- What drives them?

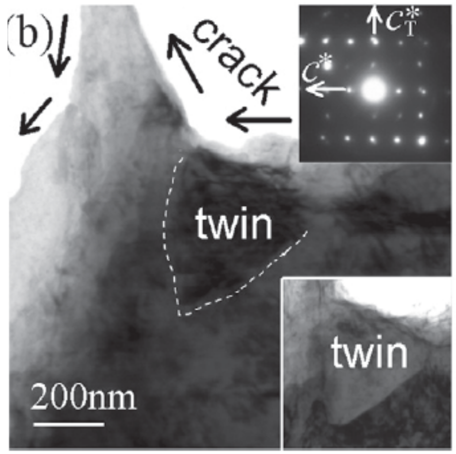
NUCLEATION

Twin embryos



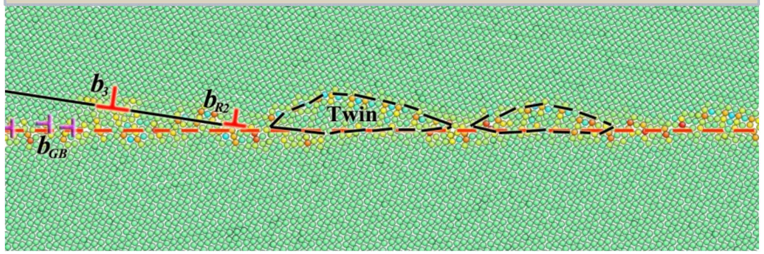
Embryos take on a seed-like or ellipsoidal shape

At a crack surface



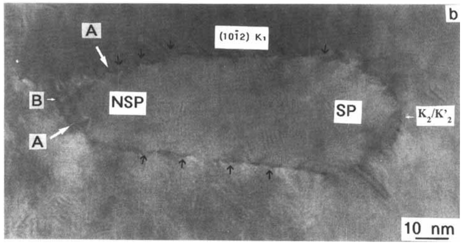
Basha et al. 2018

MD: in a low angle boundary



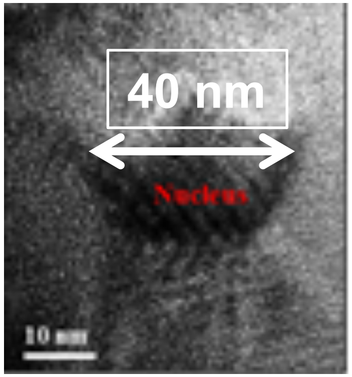
Wang and Beyerlein MSMSE 2012

Inside a Zn crystal



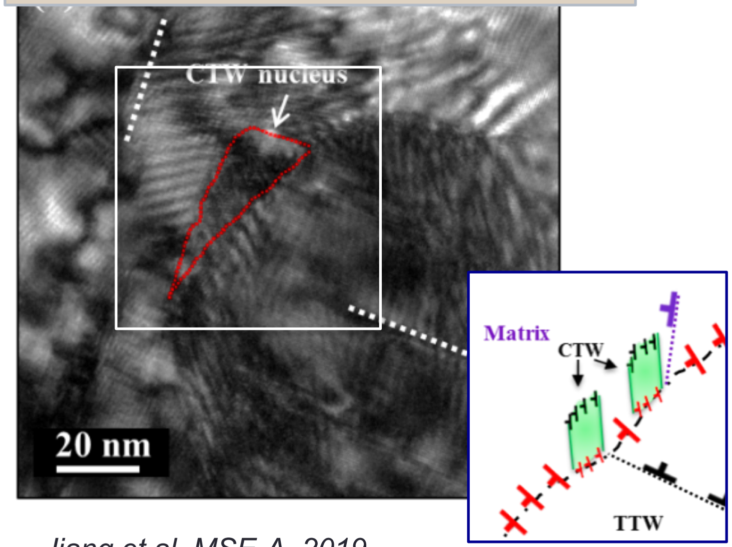
Braisaz et al. 1997

Single crystal Mg pillar

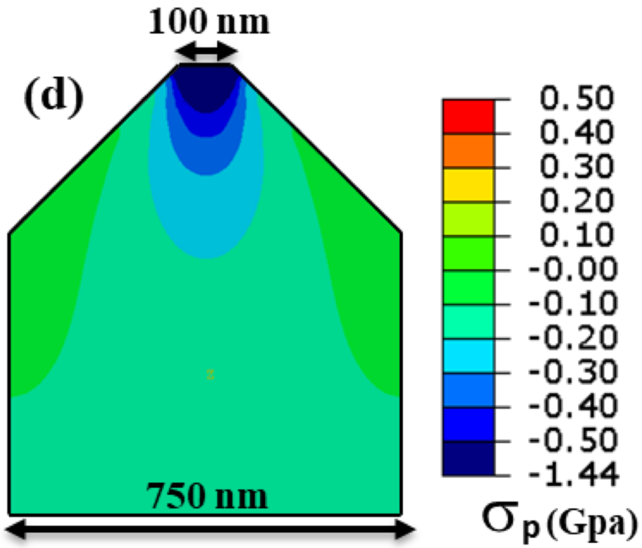


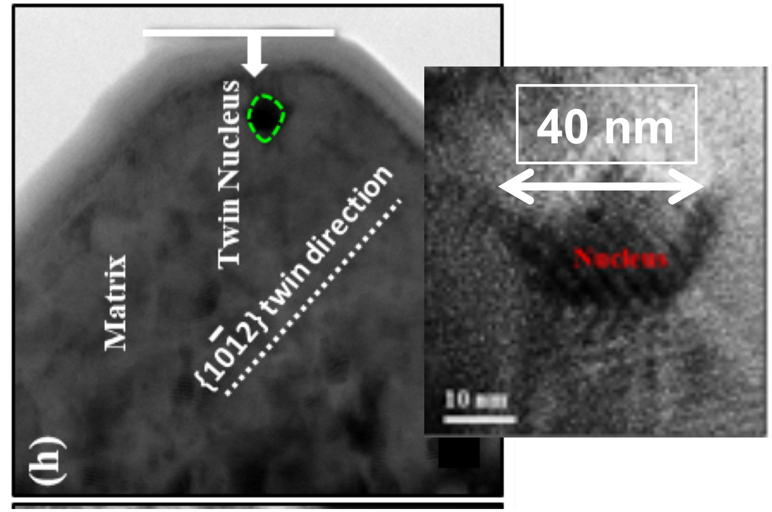
Courtesy of Lin Jiang, UC-Irvine

At a {1012} twin boundary

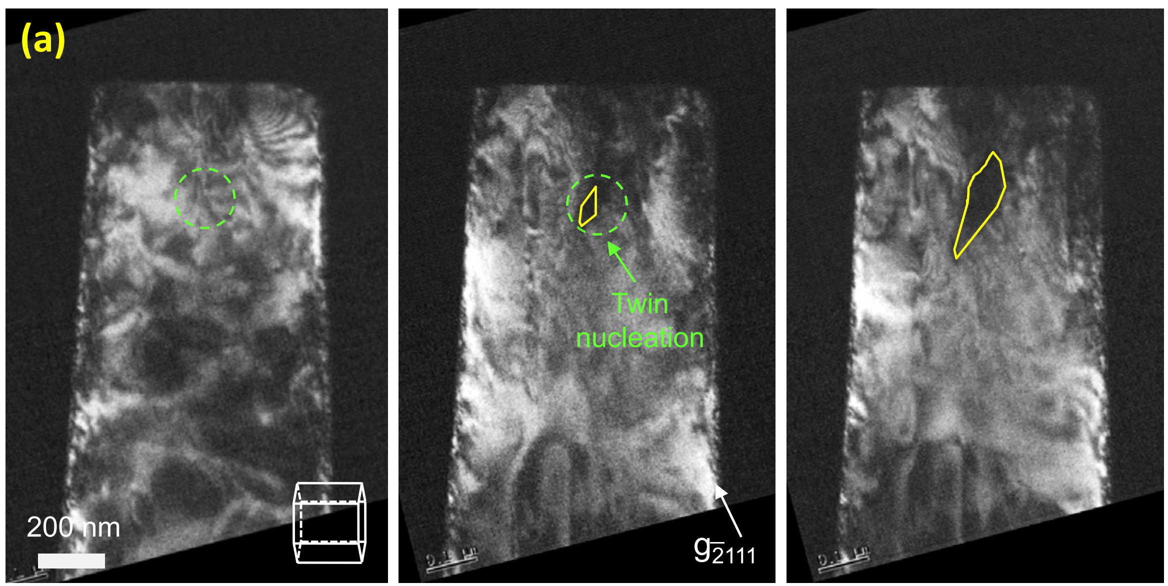


Jiang et al. MSE-A, 2019





Jiang et al. unpublished



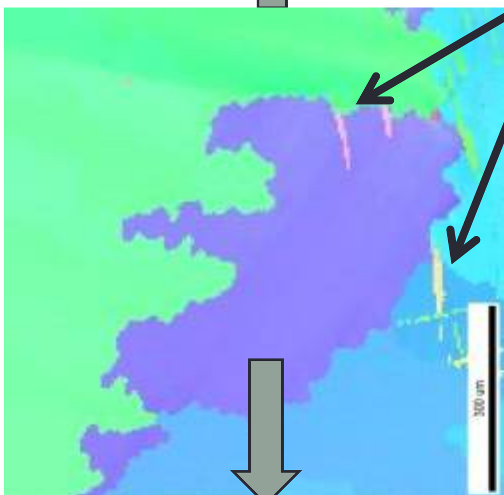
Jeong et al. Acta Mater 2018

Twin nucleation at grain boundaries

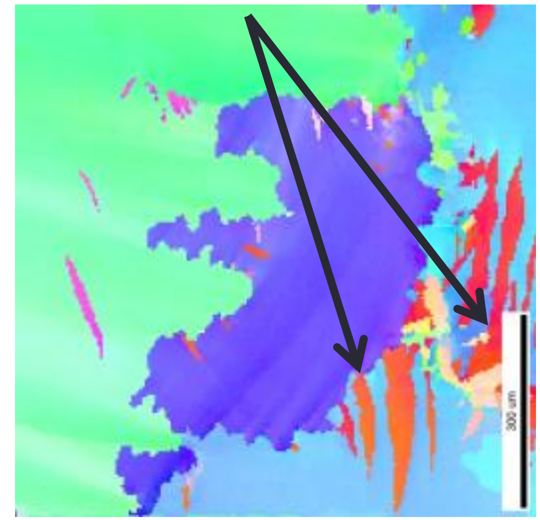
Load Direction

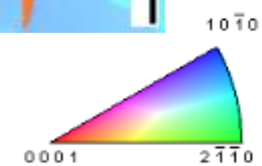
Twin nucleation from boundaries

Another new set of twins from other boundaries



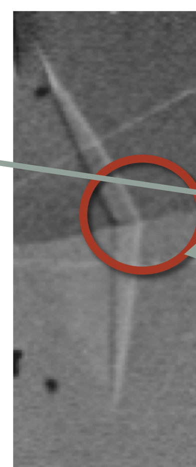
New twins from other boundaries





Mg-Ce, B. Adams et al. Mat. Sci. Forum 2012

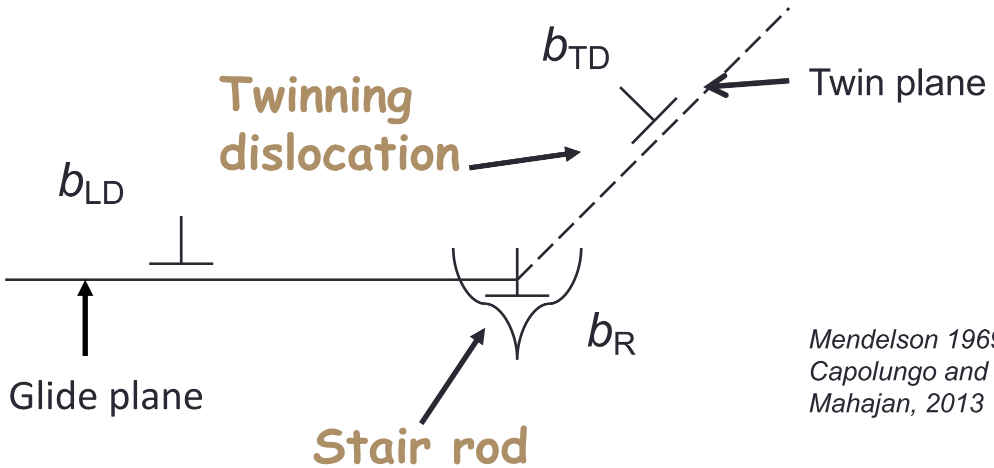
Zr: Courtesy of Ellen Cerreta



Ti, from L. Wang et al. 2010, Scripta Mater

Heterogeneous activation
Driven by GBs and neighborhood
Small scale process

Twin nucleation in hcp metals



Mendelson 1969, 1970
Capolungo and Beyerlein 2008 (3D)
Mahajan, 2013

Conservation of the Burgers vector

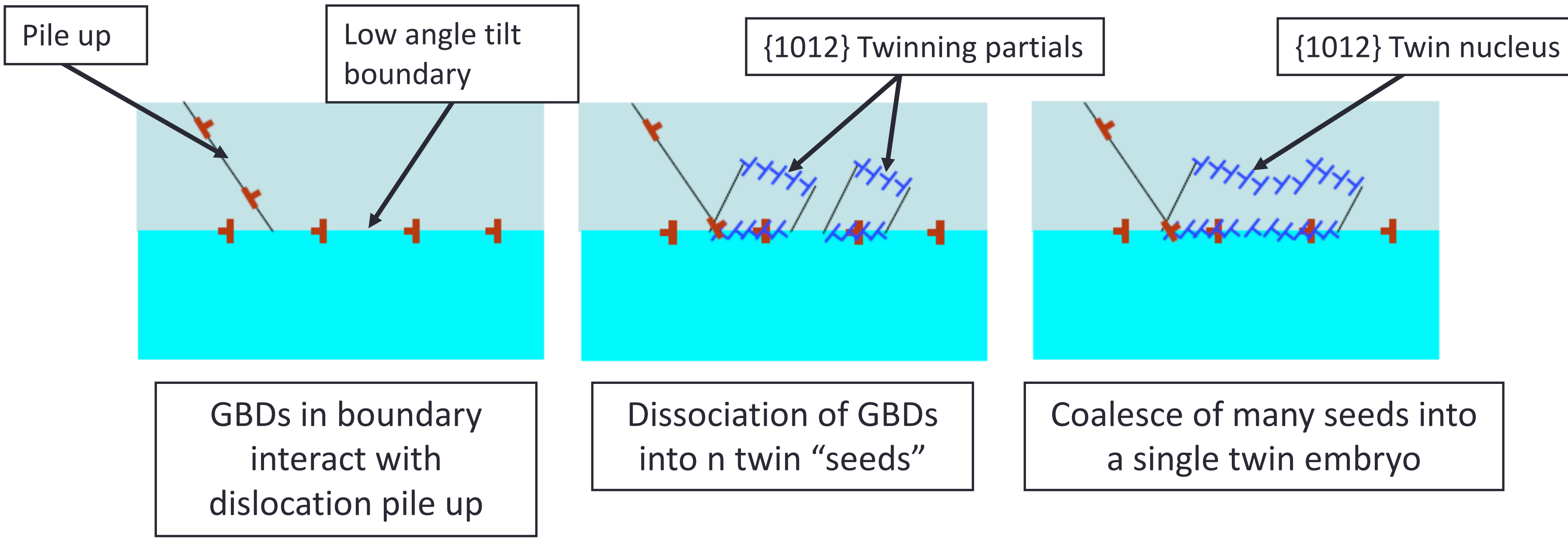
$$b_{LD} \Rightarrow b_R + nb_{TD}$$

Energy

$$\Delta W = W_{core} - \Sigma W_{\text{int}} + \gamma r - W_{work}$$

Capolungo and Beyerlein 2008 (3D)

A possible grain boundary mechanism for twin nucleation



Beyerlein and Tome, Proc. Roy. Soc. A, 2010

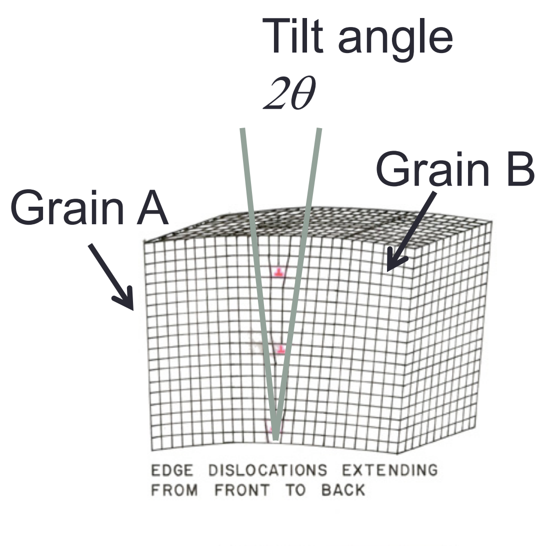
Conservation of the Burgers vector

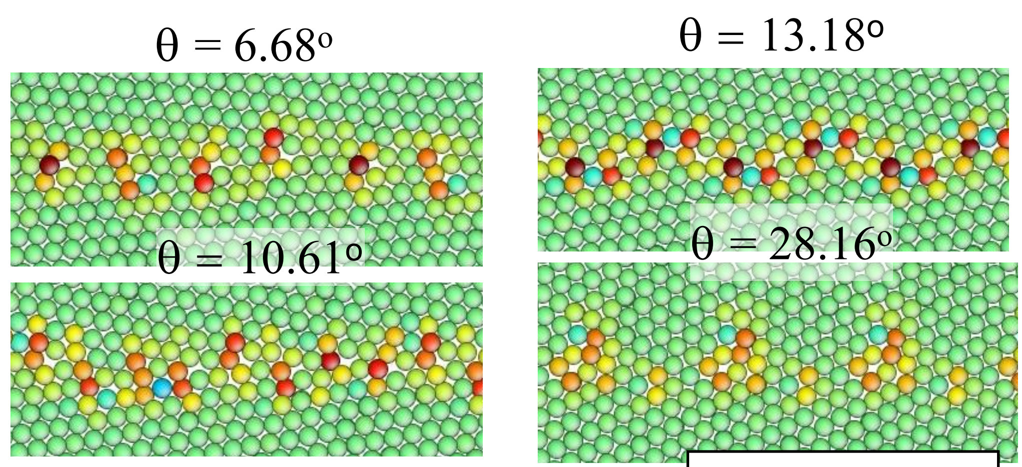
$$b \Rightarrow b_R + nb_{TD}$$

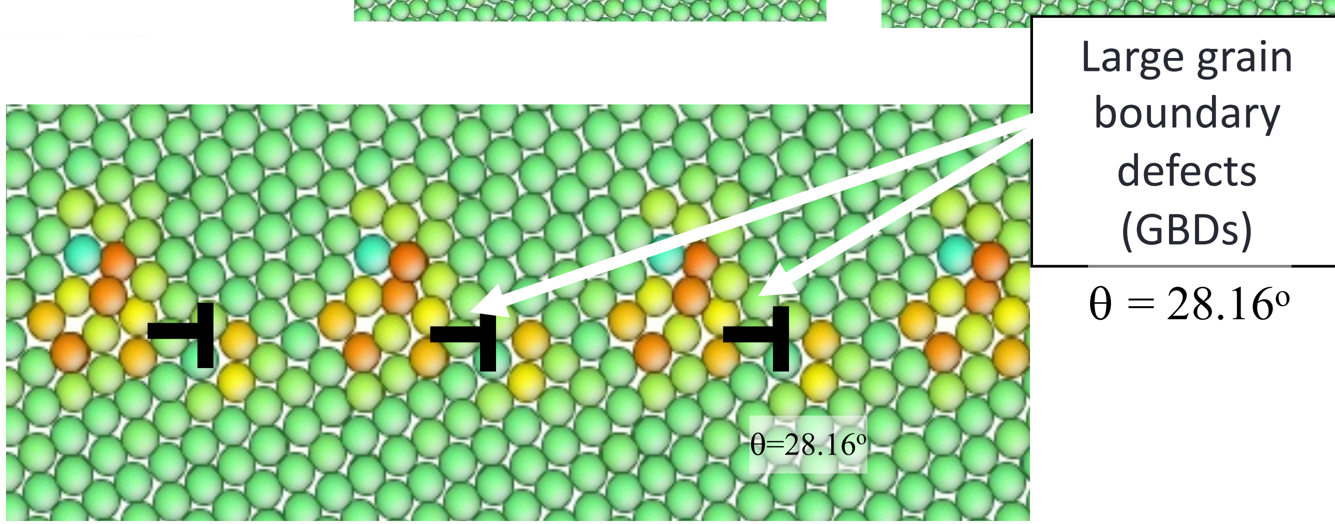
Energy

$$\Delta W = W_{core} - \Sigma W_{\mathrm{int}} + \gamma r - W_{work}$$

MD simulation: Symmetric tilt boundaries contain defects with large Burgers vectors

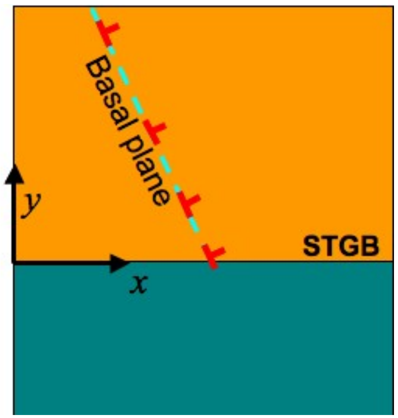




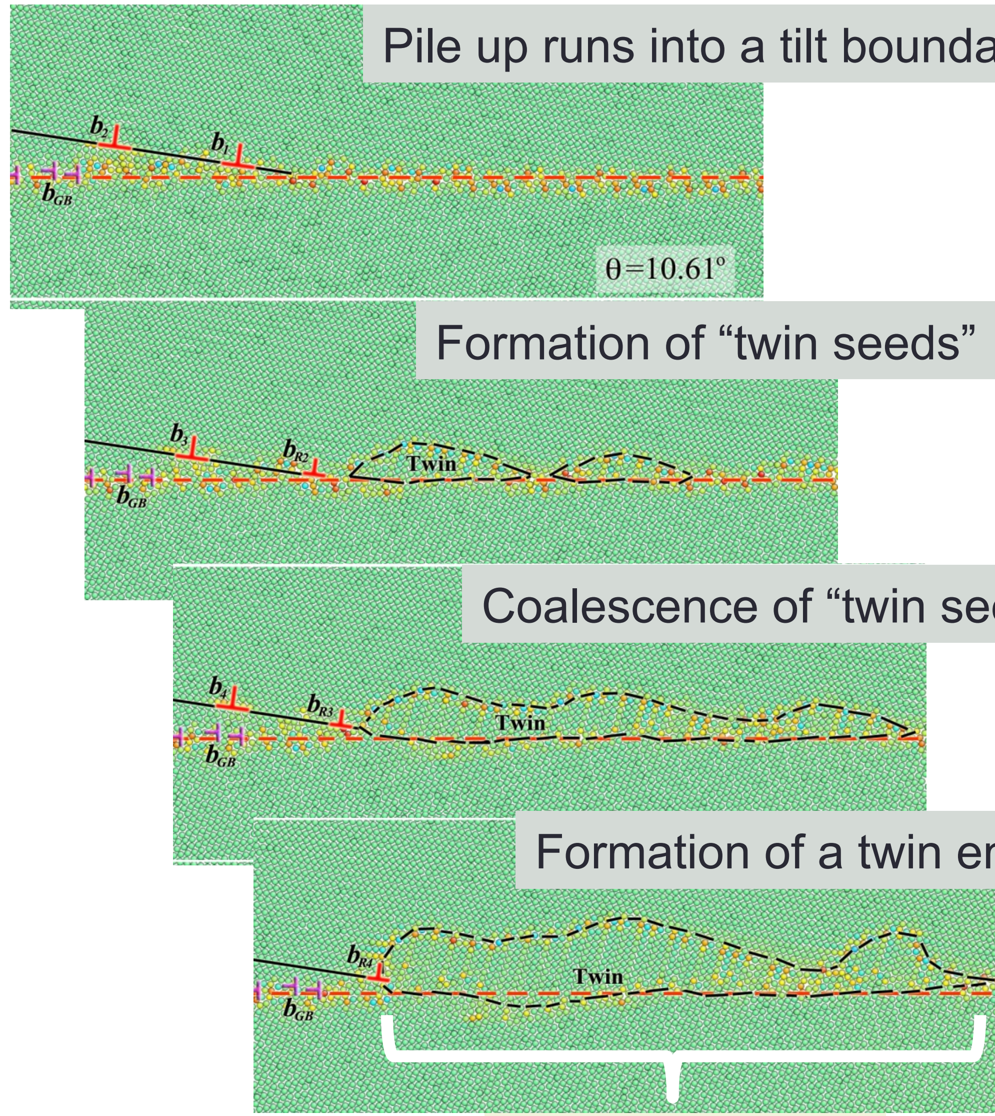


Wang, Beyerlein, MMTA 2012; Wang and Beyerlein 2012, MSMSE

MD simulation of twin nucleation



Wang, Beyerlein, MSMSE, 2012
Wang, Beyerlein, Tome, IJP, 2014



Pile up runs into a tilt boundary

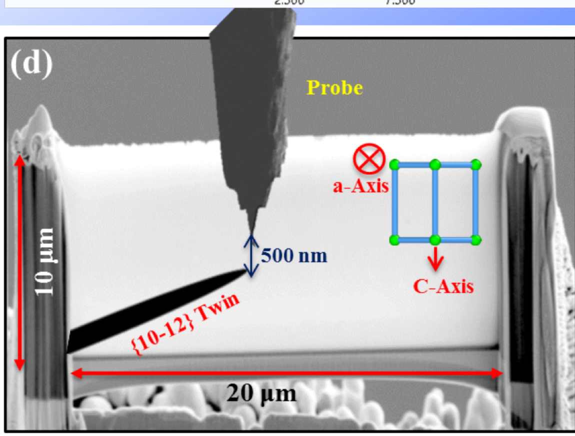
Formation of “twin seeds”

Coalescence of “twin seeds”

Formation of a twin embryo

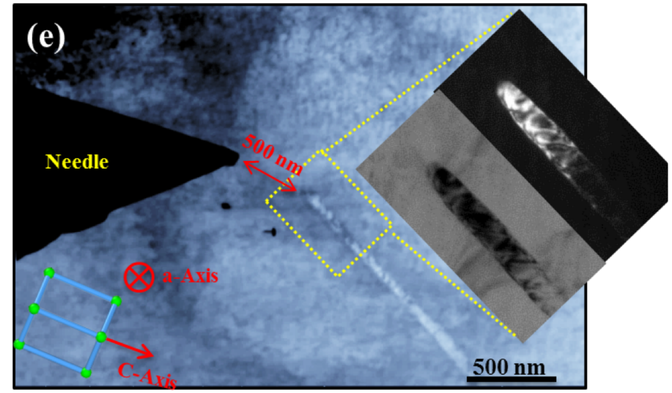
Characteristic size

Experimental observations

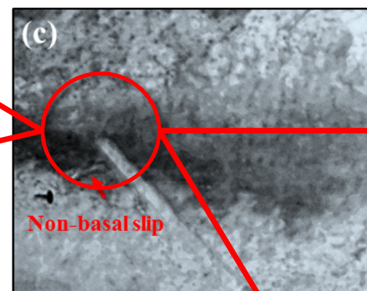


Local <a>-axis load applied to the SX Mg film

SX Mg thin film contains a pre-existing {10-12} twin

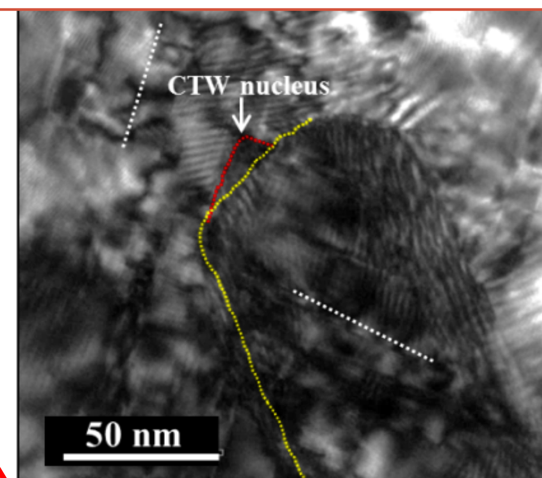


1) **The {10-12} twin tip advances**
2) **It moves forward but does not widen**

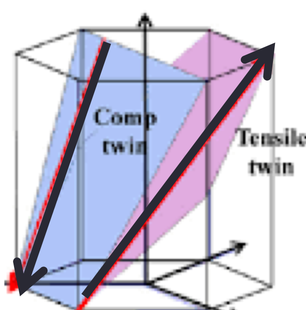


500 nm

2) a second {10-11} twin emanates from the growing {1012} boundary



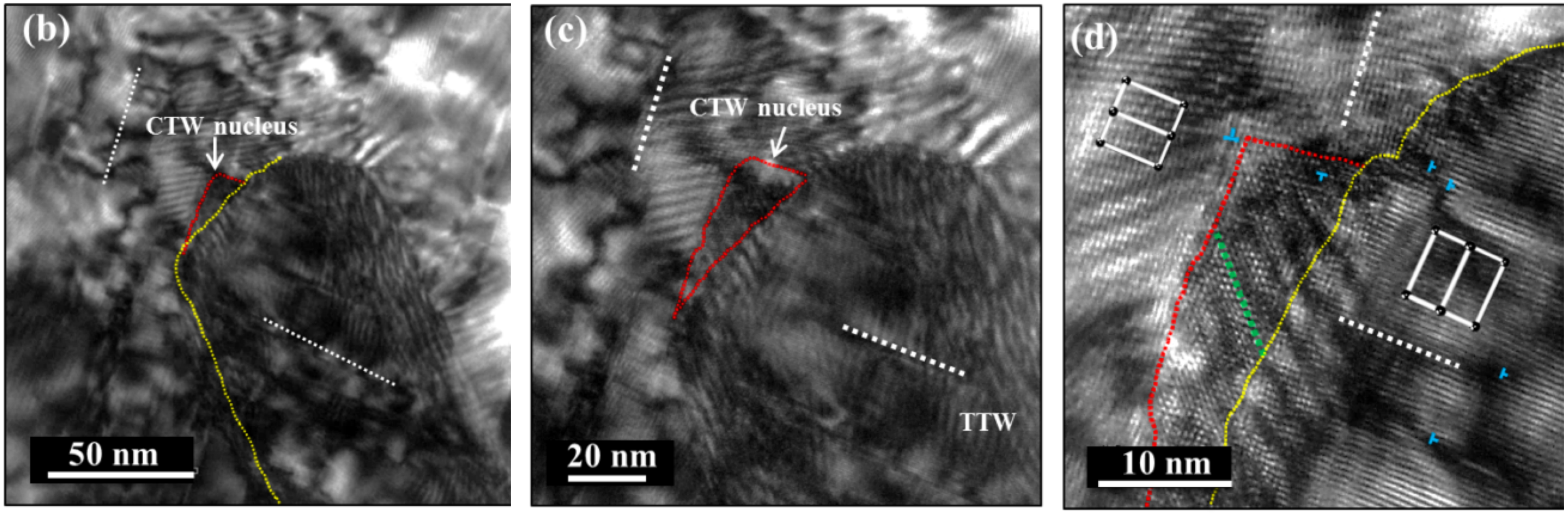
C-axis contraction (10-11) Twin



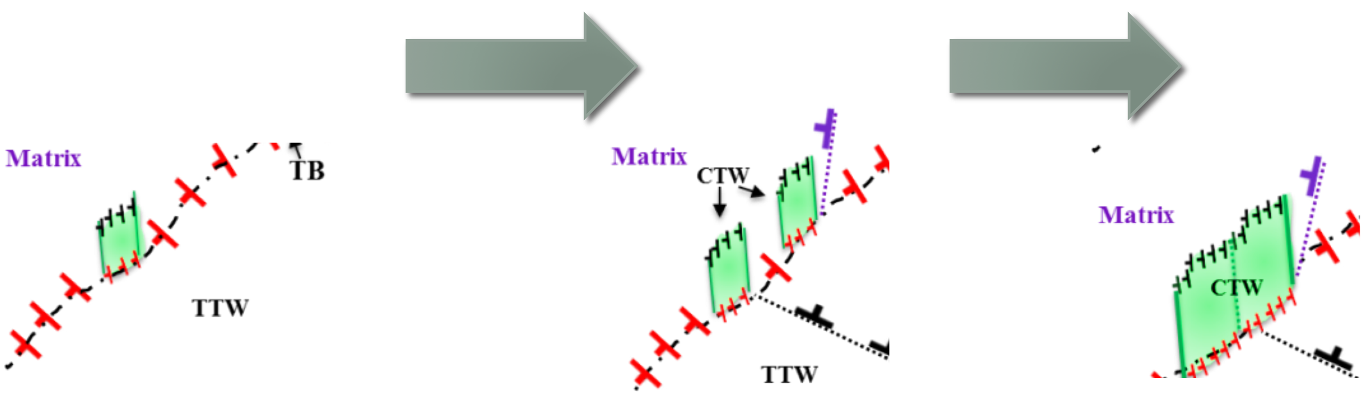
C-axis extension (10-12) Twin

L.Jiang et al. MSE-A, 2019

A contraction {10-11} twin embryo forms as load is applied



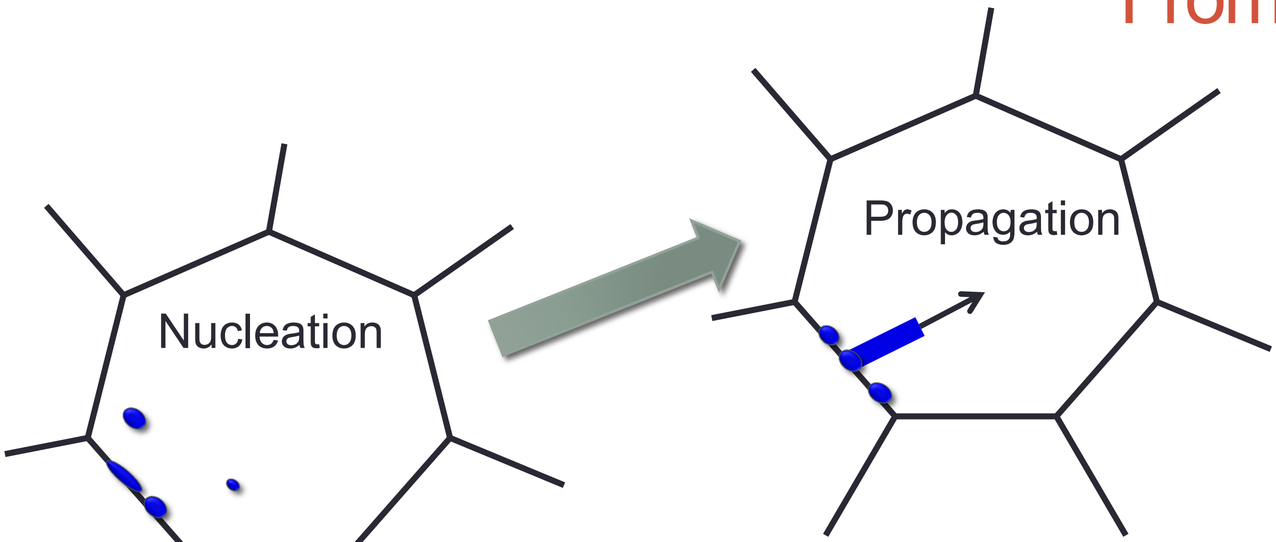
More <a> axis applied strain



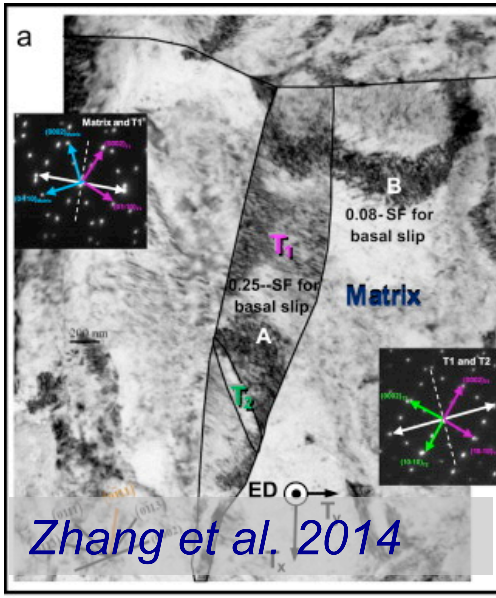
Compared with the local stress calculation, the CTW has the highest TRSS according to the calculation of the local stresses

PROPAGATION

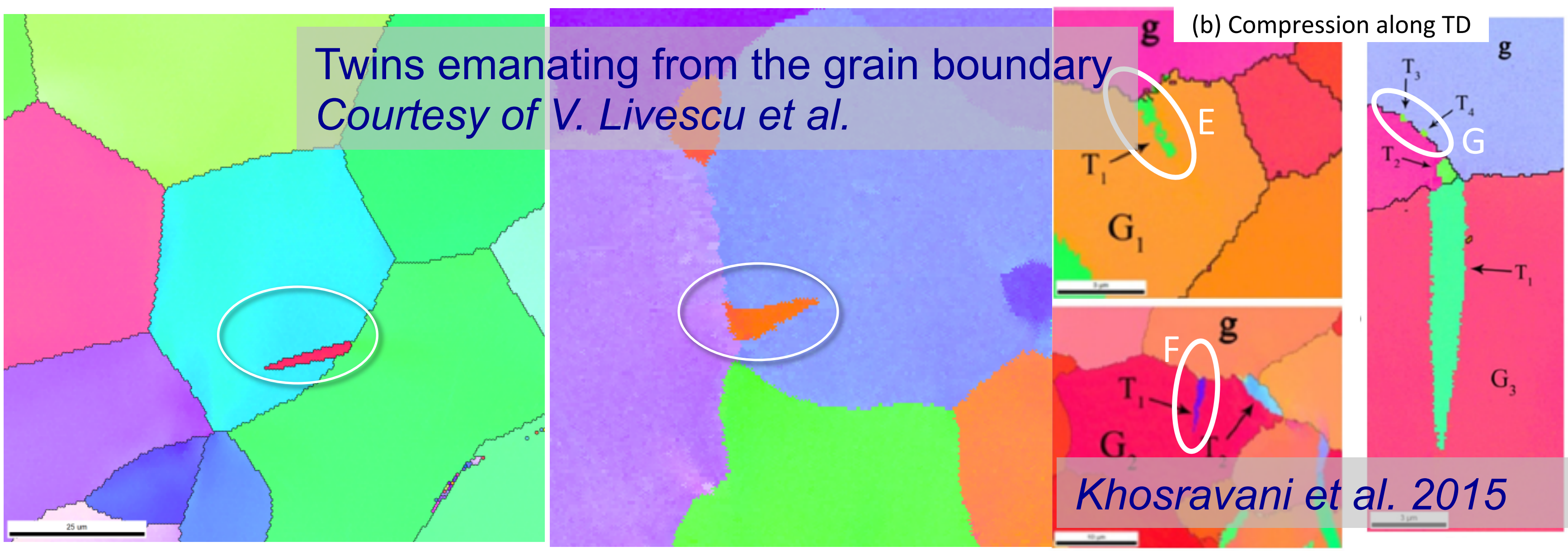
From embryo to lamella



They extend into wedge like shape



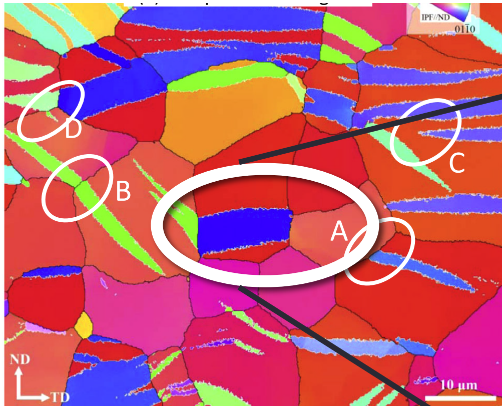
Zhang et al. 2014



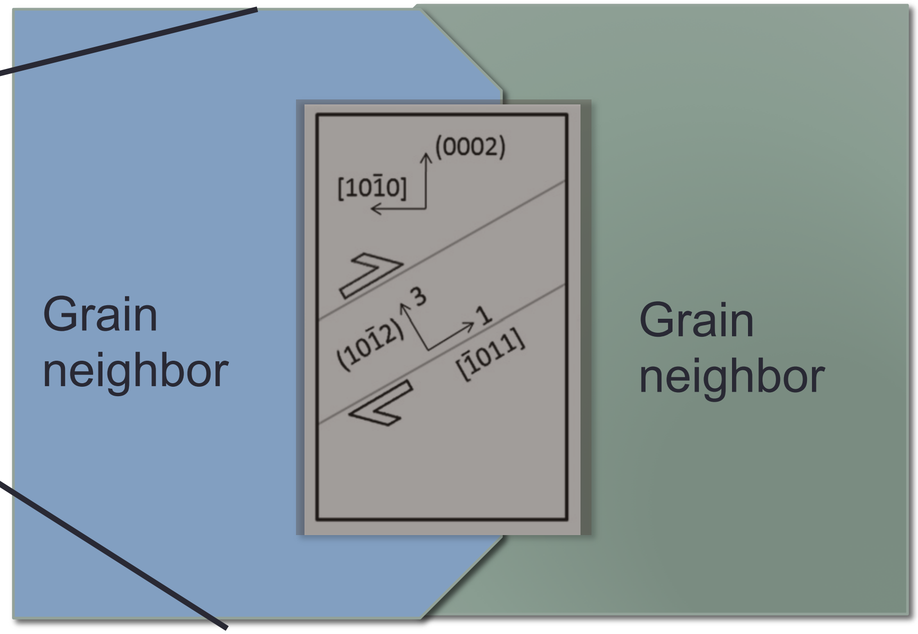
Twins emanating from the grain boundary
Courtesy of V. Livescu et al.

Khosravani et al. 2015

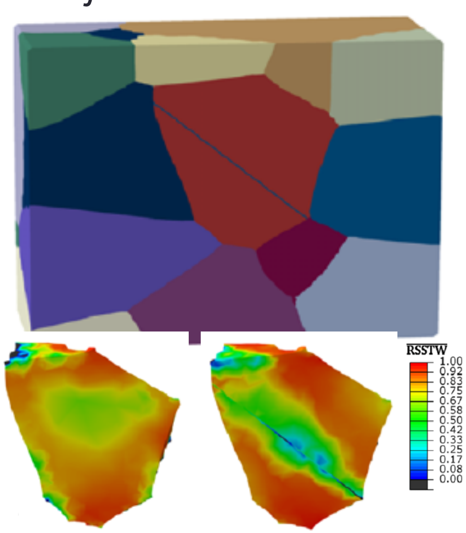
Including discrete twins in CP modeling



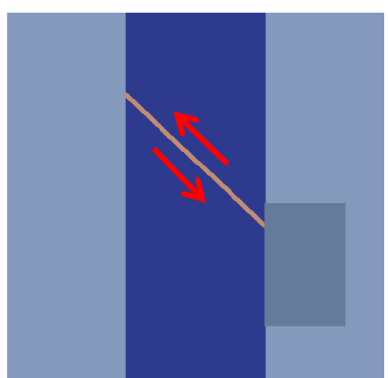
EBSD of deformed twin structure

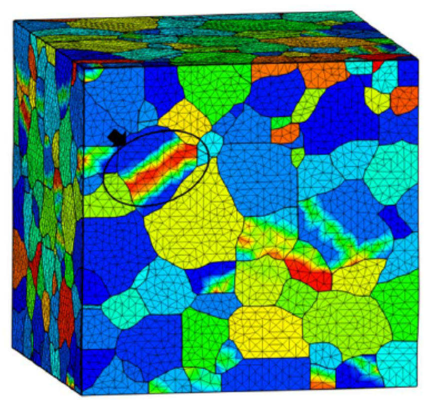


Ardeljan et al. CMAME 2016

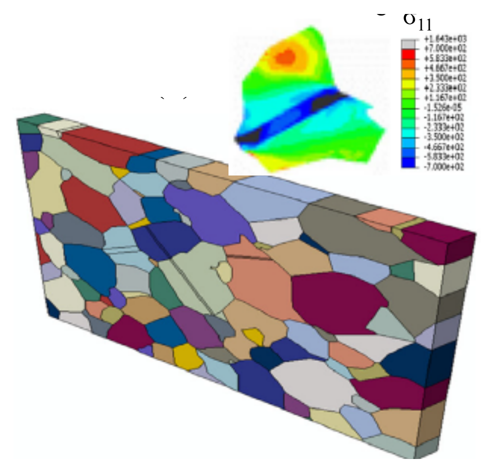


Arul Kumar et al. AM 2015; 2016





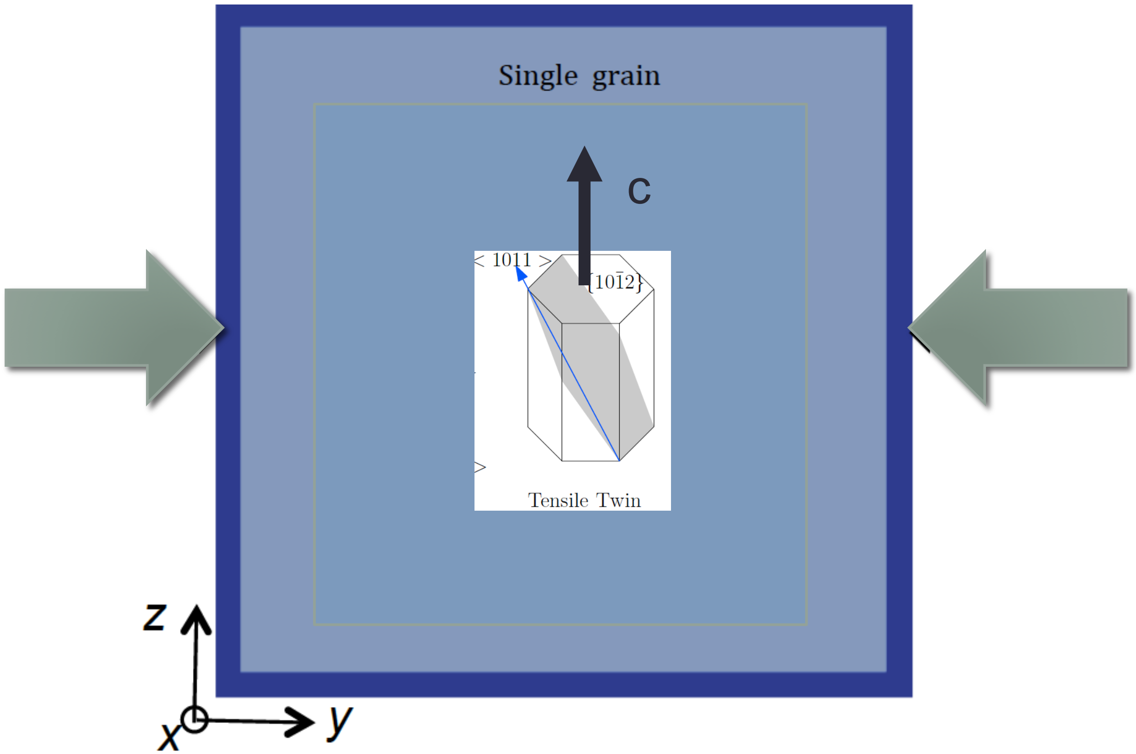
Cheng and Ghosh. 2017



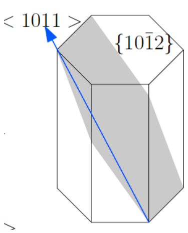
Abdolvand and Wilkinson 2016

Single crystal with an embedded twin

Individual grain with a twin inside a material



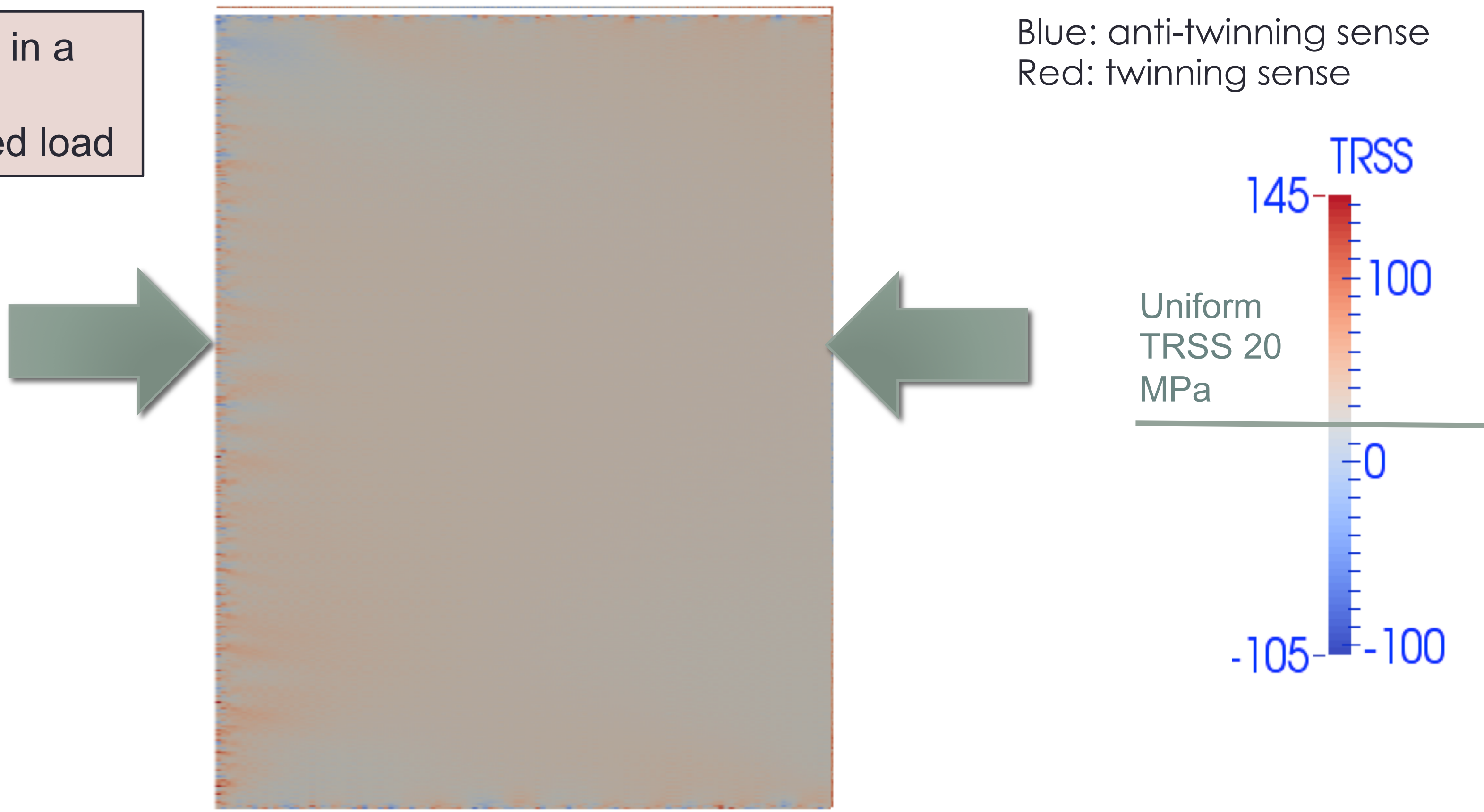
Twin resolved shear stress (TRSS)



{10-12} twin

TRSS field created by a {10-12} twin inside a crystal

Example grain in a polycrystal
Far field applied load

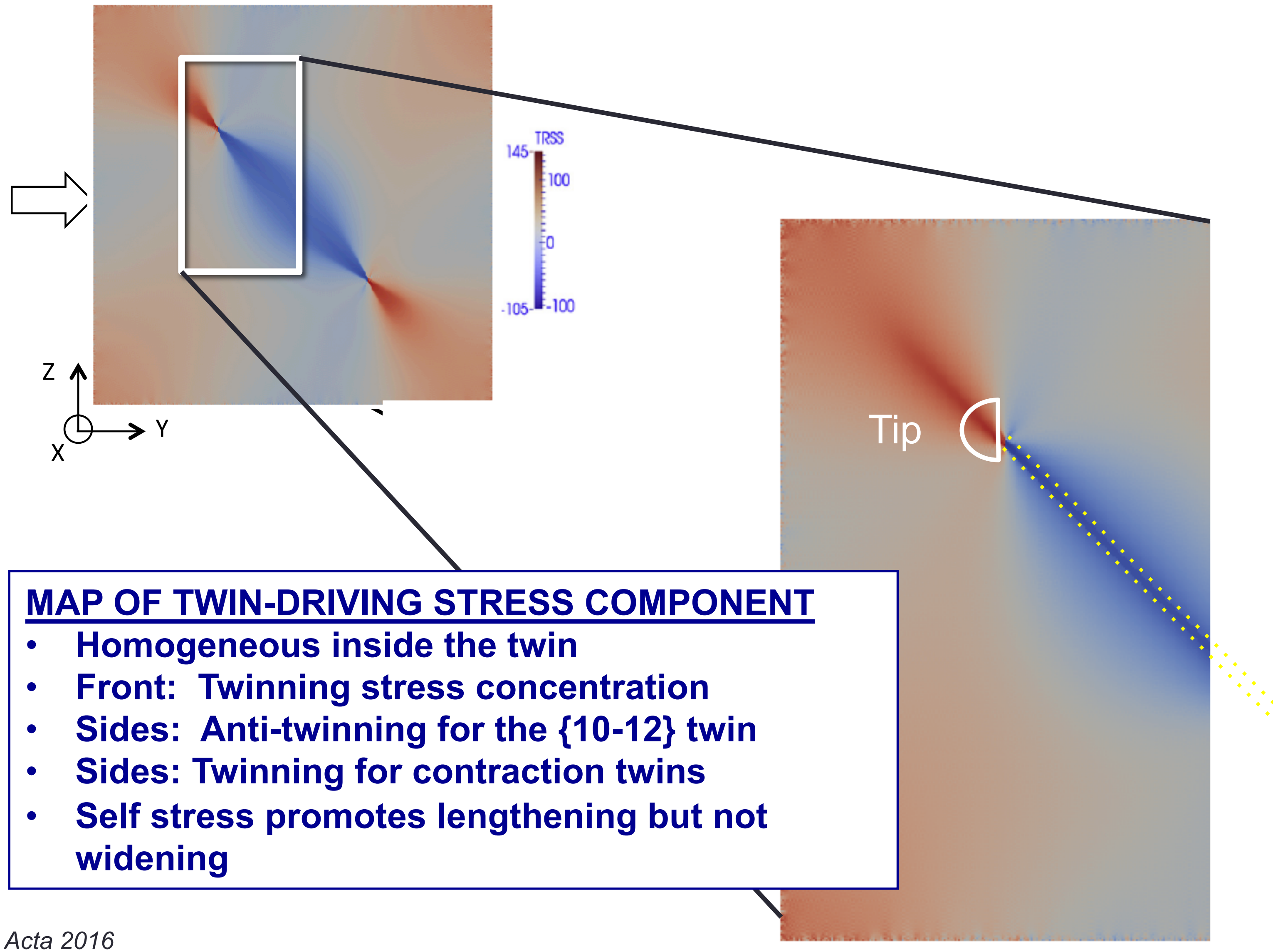


<u>MAP OF TWIN-DRIVING STRESS COMPONENT</u>

- **Front: Twinning stress concentration**
- **Sides: Anti-twinning for the {10-12} twin**
- **Self stress promotes lengthening but not widening**

"Self stress" of a twin

Consider "self" stress field:
single twin inside its parent single crystal



<u>MAP OF TWIN-DRIVING STRESS COMPONENT</u>

- **Homogeneous inside the twin**
- **Front: Twinning stress concentration**
- **Sides: Anti-twinning for the {10-12} twin**
- **Sides: Twinning for contraction twins**
- **Self stress promotes lengthening but not widening**

Arul Kumar et al. Acta 2016

References

- I. J. Beyerlein, X. Zhang, and A. Misra, "Growth twins and deformation twins in metals", *Annual Reviews in Materials Research* **44** (2014) 329-363.

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- D. Zhang, L. Jiang, B. Zheng, J. M. Schoenung, S. Mahajan, E. J. Lavernia, and I. J. Beyerlein, "Deformation Twinning (Update)", In: Reference Module in Encyclopedia of Materials: Materials Science and Materials Engineering, Elsevier B. V. (2016). 1-24

- C. N. Tomé, I. J. Beyerlein, R. J. McCabe, and J. Wang, "Multi-scale statistical study of twinning in HCP metals", In: *Engineering (ICME) for Metals: Reinvigorating Engineering Design with Science*, Wiley Press, 2018 (Horstemeyer, M.F., ed.).