

Basics of Dislocations in High Purity Niobium

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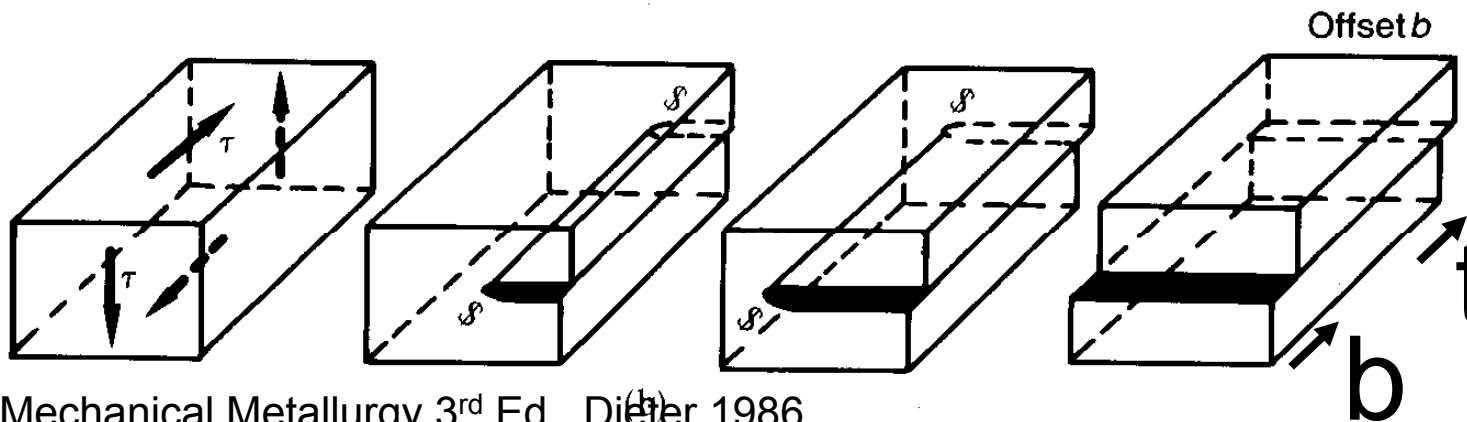
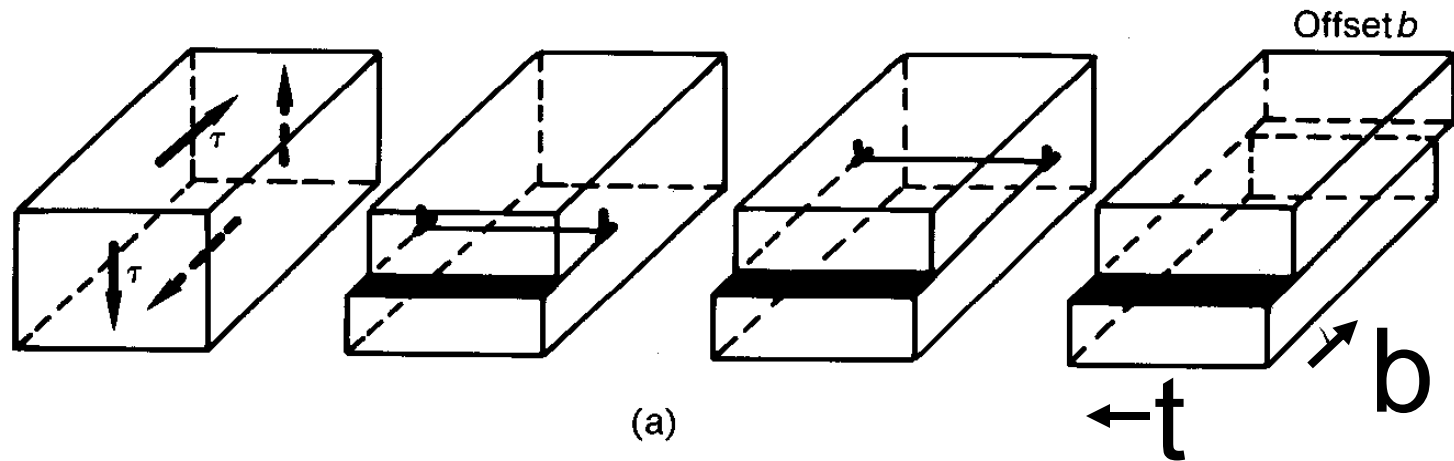
Support from Fermilab, DOE

Dislocation substructure, recrystallization, and texture are important for SRF community

- Polycrystalline Nb
 - Would like to determine textures best suited for given forming process (e.g. hydroforming)
 - Need accurate crystal plasticity model
- Large grain/Single crystal Nb
 - Tubes (welded or seamless) for hydroforming
 - Will deform differently in different crystal directions
 - Relating dislocation substructures to recrystallized grain orientations would aid design of desired textures
- Electric/Superconducting properties
 - Romanenko's thesis on high-field Q-slope correlates hot spots to higher local misorientation of lattice (higher dislocation density)
 - Phonon scattering due to dislocation lines parallel to phonon travel

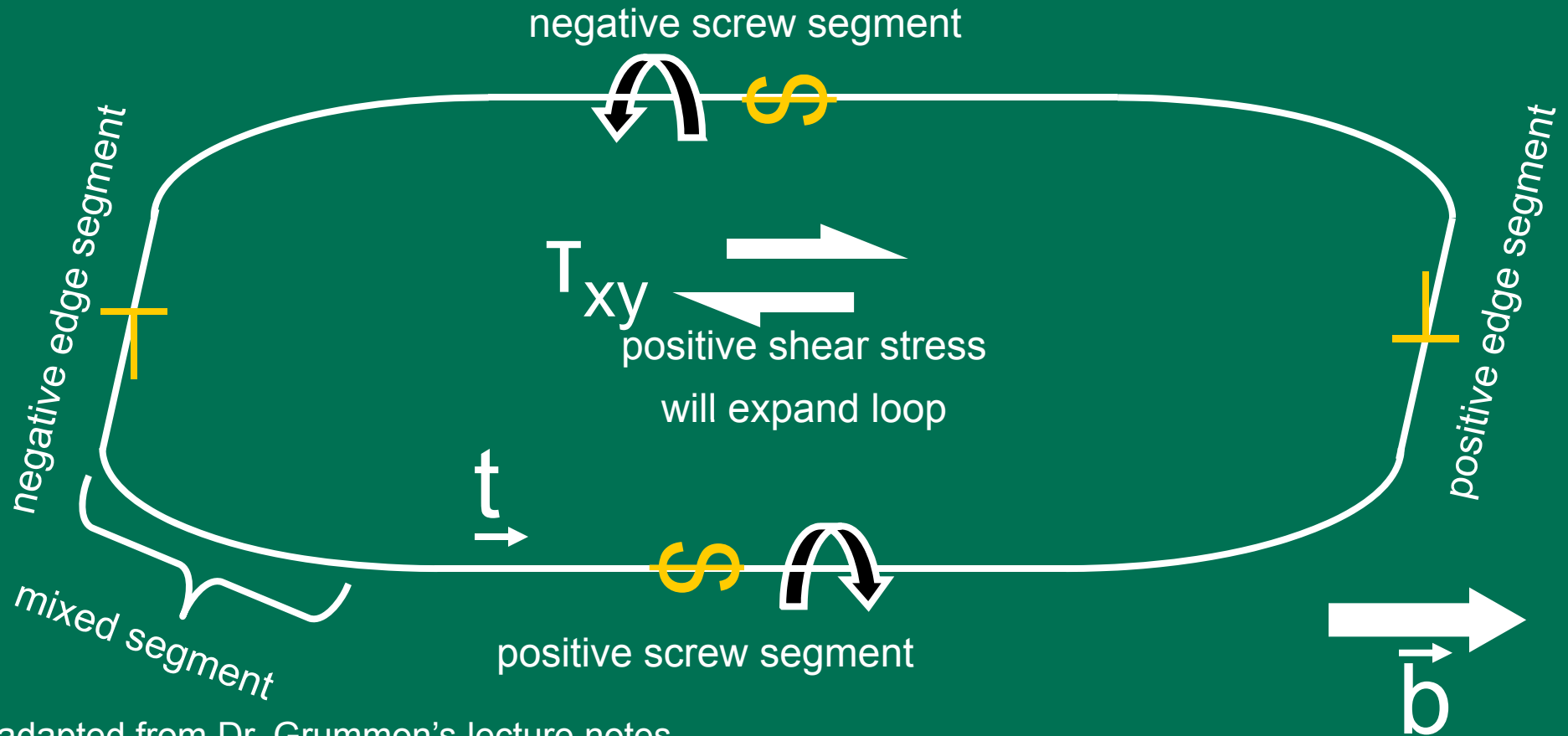
Difference between screw and edge dislocations

- Line defect in crystal lattice, burgers vector (b) and line direction (t)
- Edge has well defined slip plane ($b \times t = n$), Screw does not ($b \parallel t$)
- Sufficient shear stress resolved on slip plane and in burgers vector direction \rightarrow glide



Glide loops develop inside a crystal and expand into space, and terminate against a grain boundary

- Dislocation terminates on itself



adapted from Dr. Grummon's lecture notes

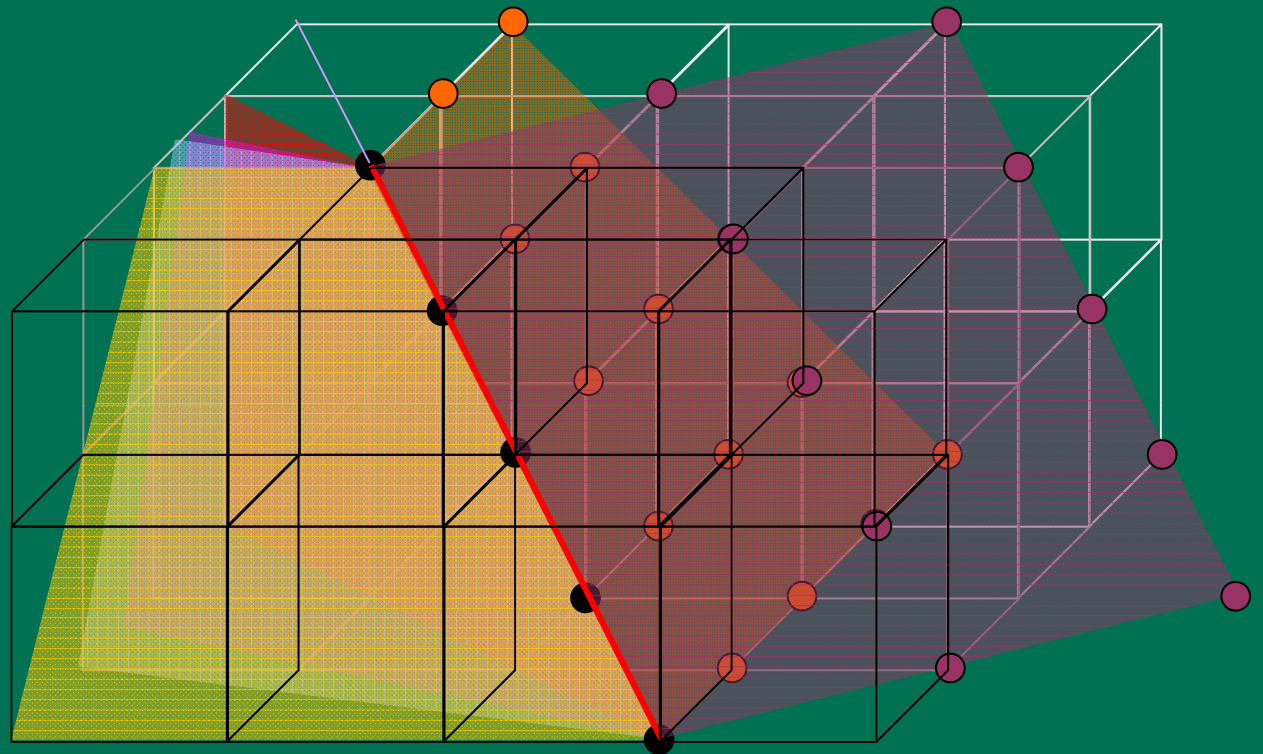
High purity BCC Slip Systems

Slip is expected to be easiest (lowest CRSS) on*

{110} planes,
which have highest
planar density,

and {112}

{123} at large strain



6 of the 48 available are illustrated and listed:

$$[-1 \ 1 \ 1] \ (1 \ 1 \ 0)$$

$$[-1 \ 1 \ 1] \ (1 \ 0 \ 1)$$

$$[-1 \ 1 \ 1] \ (0 \ -1 \ 1)$$

$$[-1 \ 1 \ 1] \ (1 \ -1 \ 2)$$

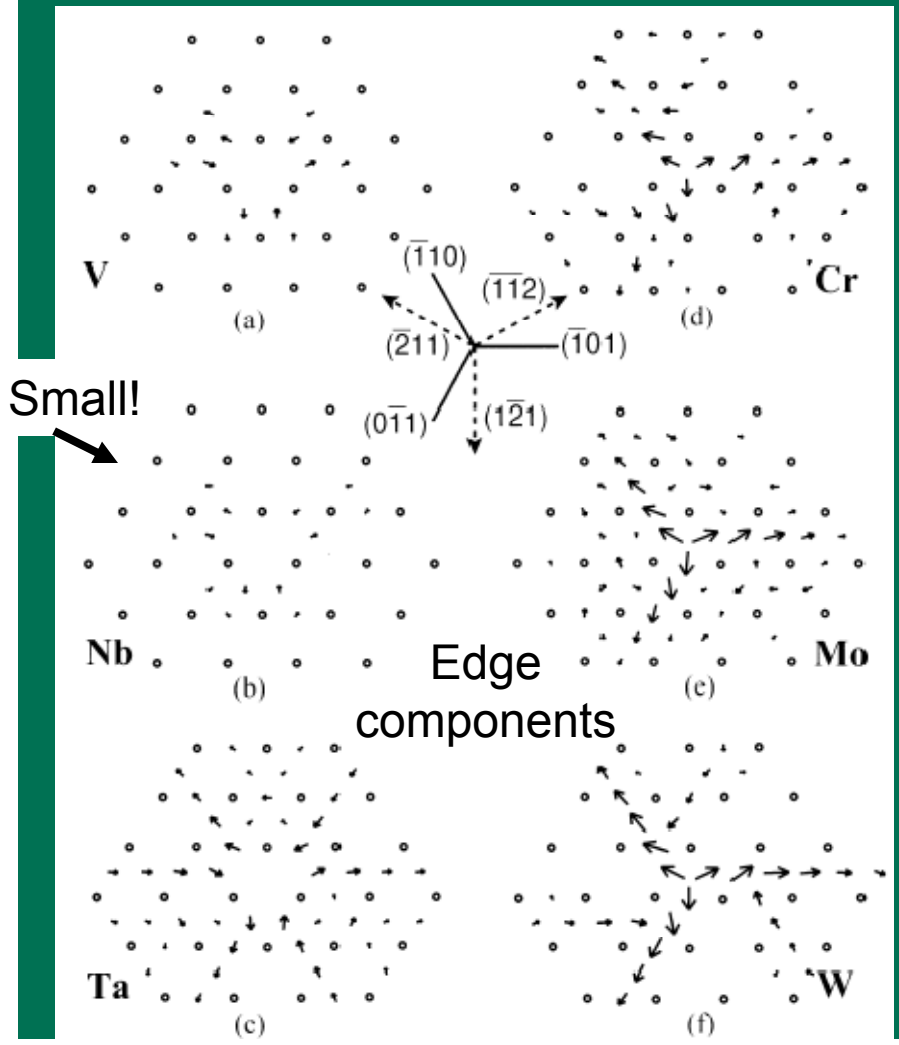
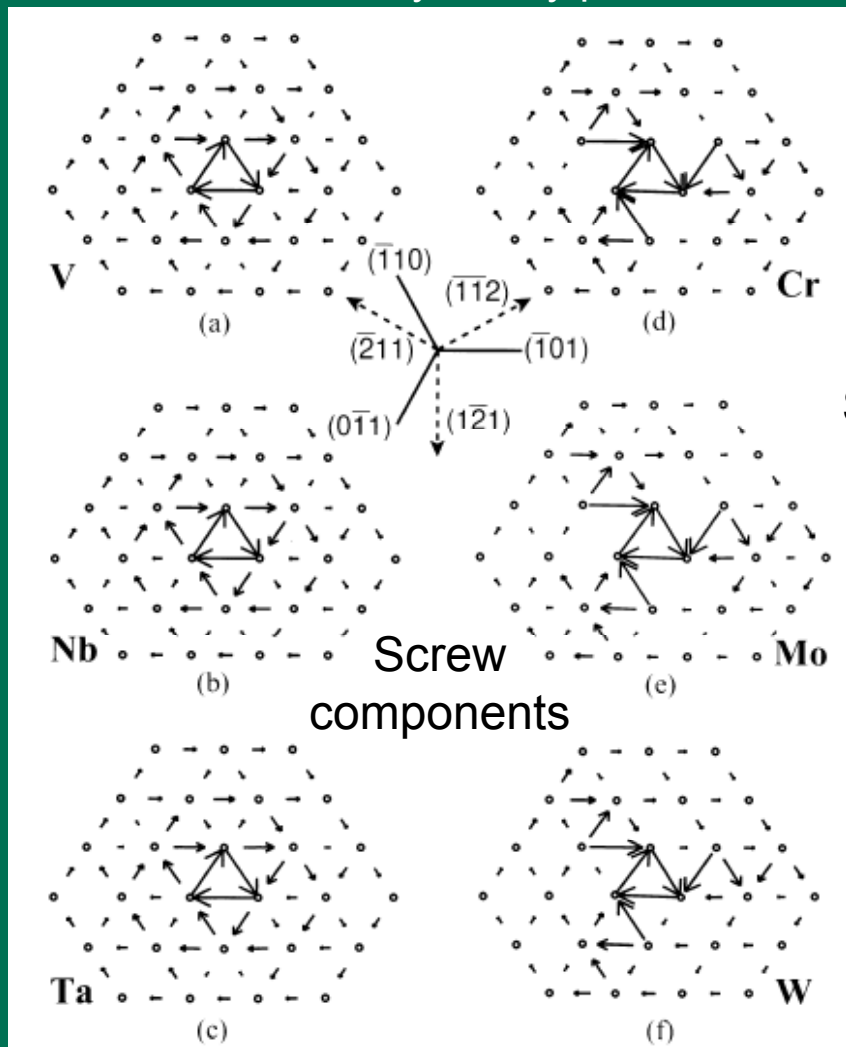
$$[-1 \ 1 \ 1] \ (-1 \ -2 \ 1)$$

$$[-1 \ 1 \ 1] \ (2 \ 1 \ 1)$$

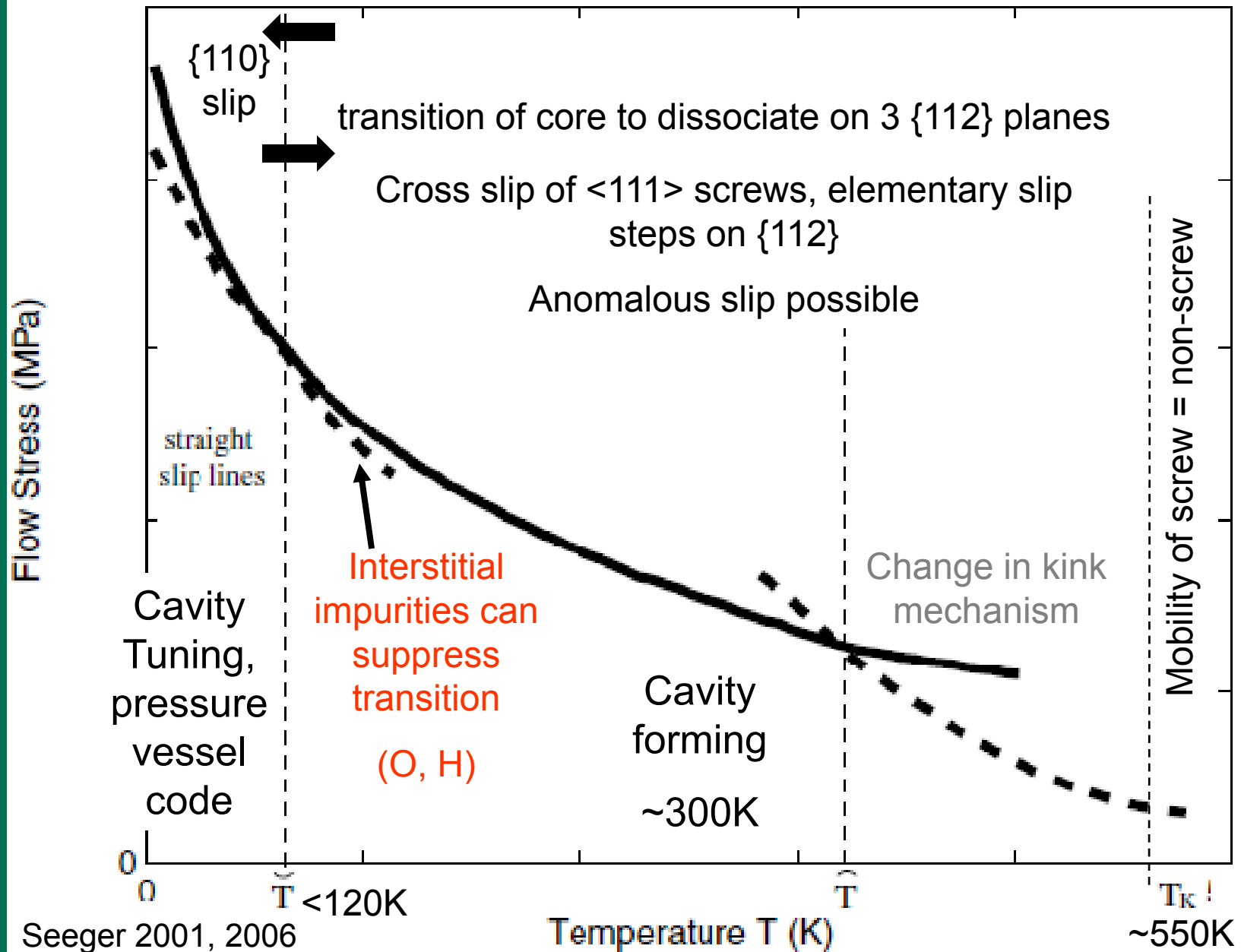
* Critical Resolved Shear Stress

Screw Dislocations in BCC

- Core dissociates in 3D on three symmetric $\{110\}$ planes $\llcorner \bar{T}$
- Non-glide shear stresses interact with edge components \rightarrow CRSS varies with orientation
- Edge components small in Nb, dependence of CRSS on crystal orientation is small
 - In FCC, core already mostly planar



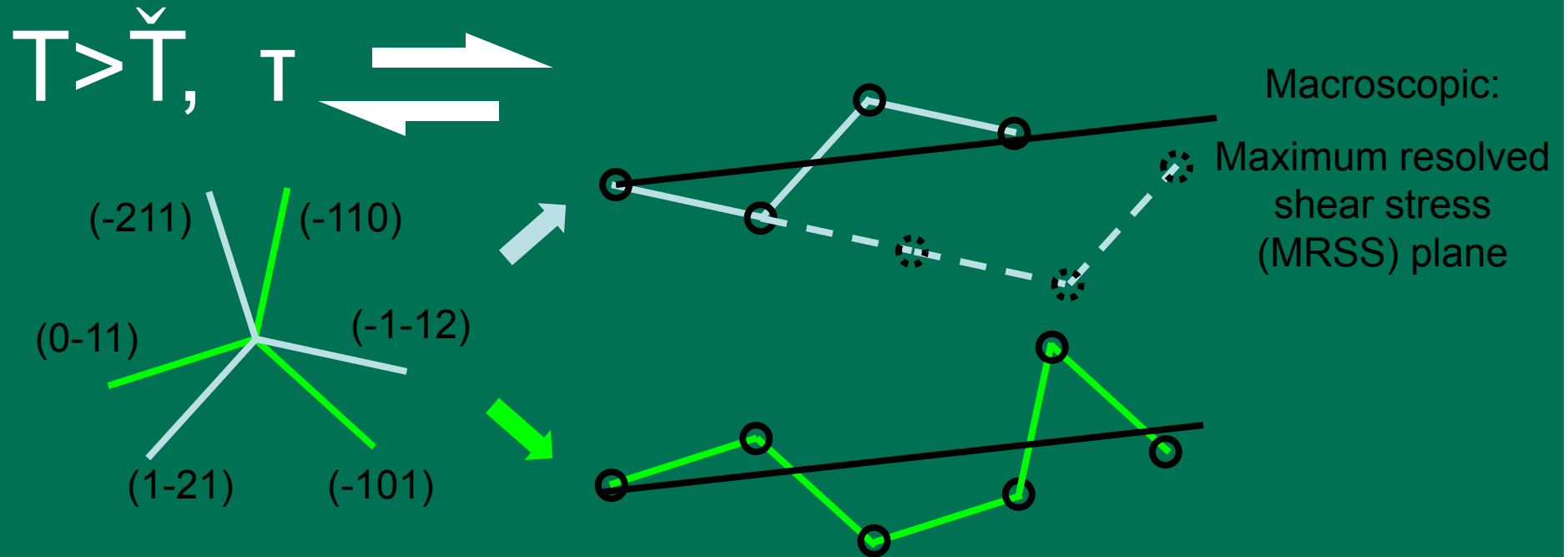
Favored slip planes change with T & purity



Possible issue of hydrogen contamination

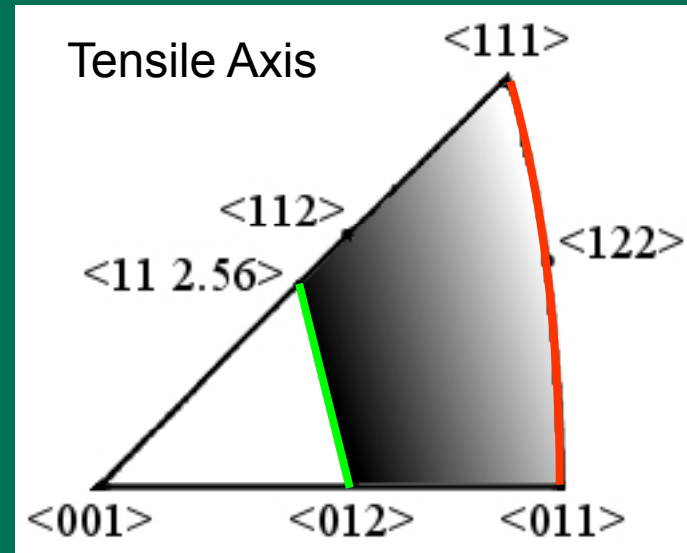
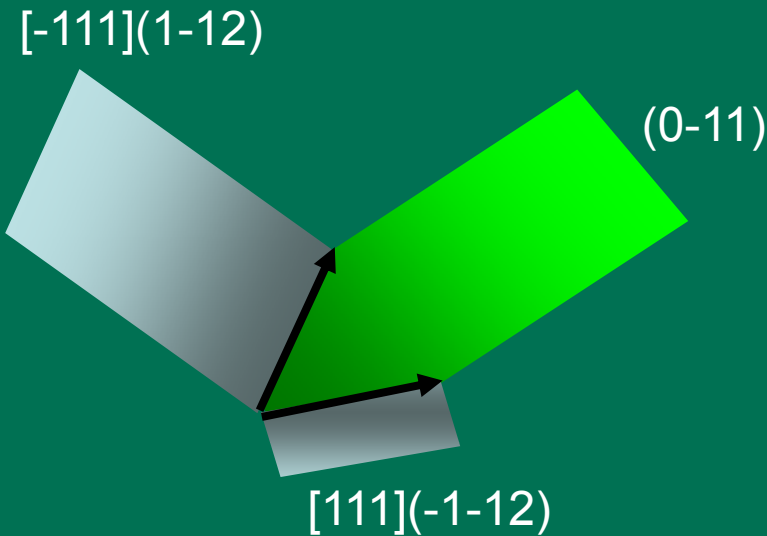
- Hydrogen penetration during
 - Deformation (thin oxide cracks)
 - Rough calculation: H may move 4mm in 5min at RT in Nb
 - How much of an effect?
 - Etching/Electropolishing
 - Not usually done before forming, sometimes remove Fe
- Stabilizes {110} dissociation
 - Promotes Slip on {110}
 - Dislocations, vacancies trap H
- Include in CPFEM modeling of forming process

Can we tell from slip traces?



- Complication: The distance between cross-slip events is unknown

Anomalous Slip



Most Likely

Much less likely

- Highest shear stress on two intersecting, equally active $\{112\}$ planes
- Cross-slip to mutual $\{110\}$ plane
 - of \sim half the resolved shear stress on $\{112\}$
- Maintains lower free energy

To avoid:

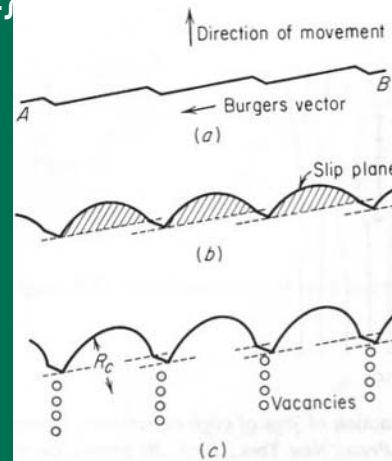
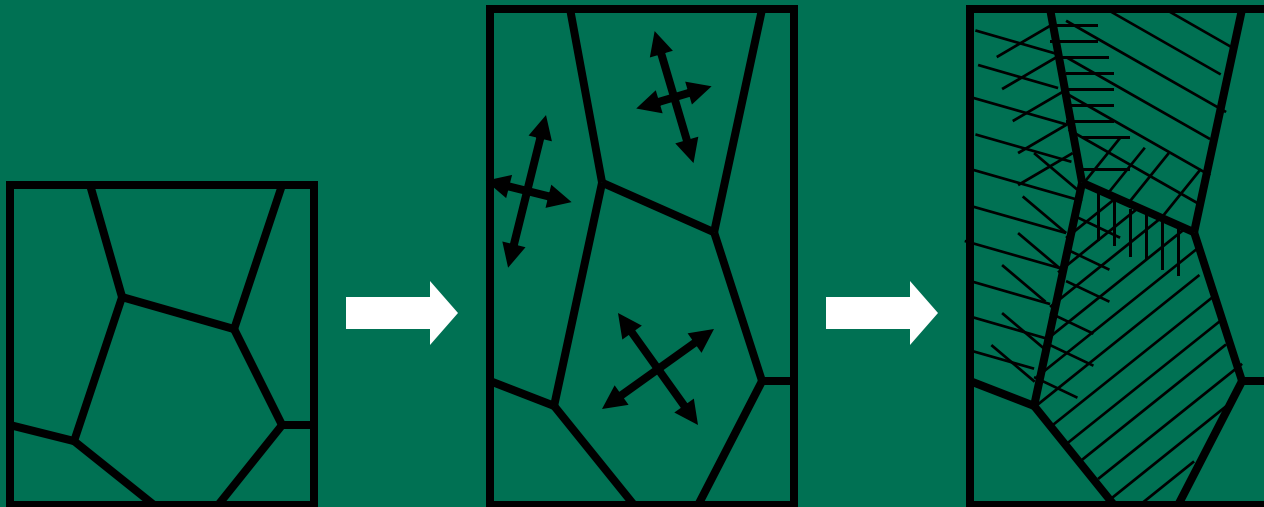


Figure 5-24 Movement of jogged screw dislocation. (a) Straight dislocation under zero stress; (b) dislocation bowed out in slip plane between the jogs due to applied shear stress; (c) movement of dislocation leaving trails of vacancies behind the jogs. (From D. Hull, "Introduction to Dislocations," p. 136, Pergamon Press, New York, 1965. By permission of the publishers.)

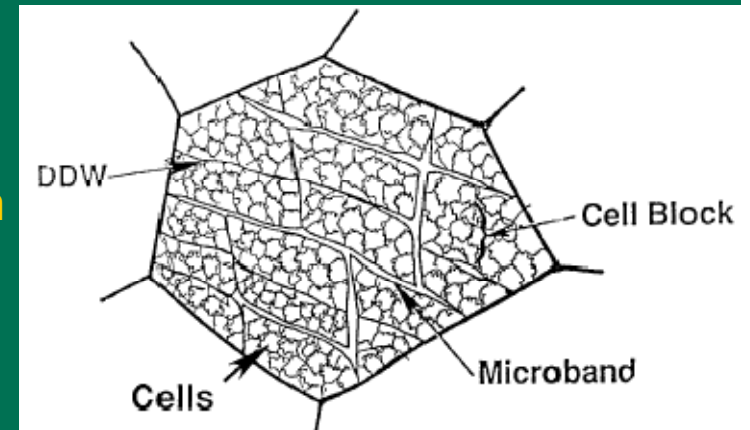
5 independent slip systems needed for arbitrary shape change (Von Mises)

- Taylor model often used for polycrystals
 - Strain of each grain same as that of aggregate
 - Different stress states in each grain
 - maintains grain boundary cohesion
 - Refined methods for selecting the 5 systems

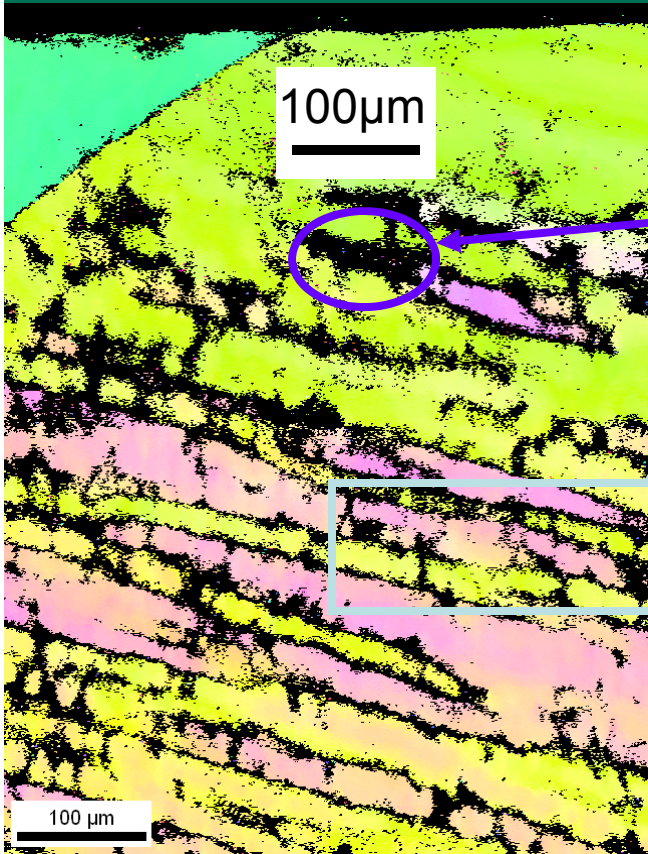


Dislocation structures

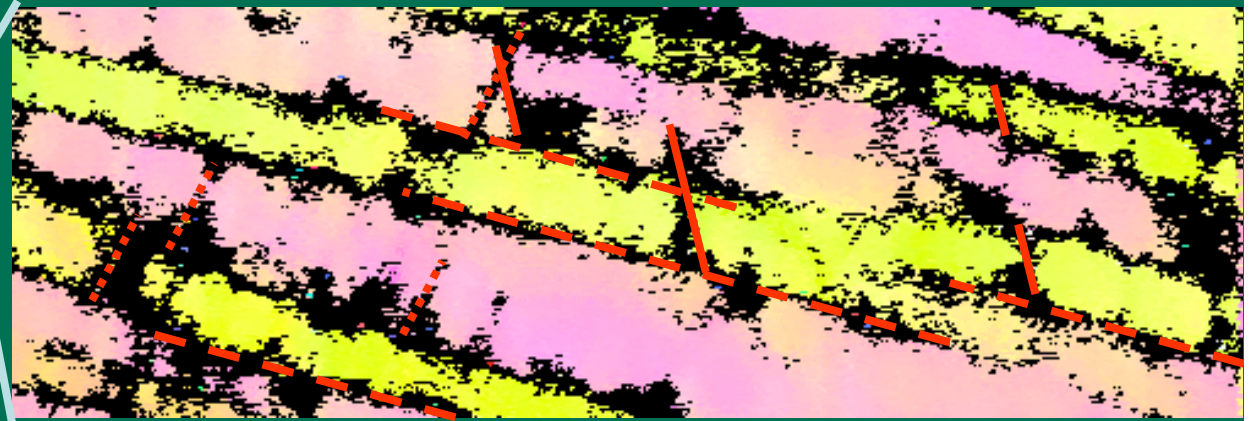
- Grains divide into
 - Cell Blocks (CBs) bounded by long flat boundaries
 - Microbands (MBs)- double walled, small strains
 - Dense Dislocation Walls (DDWs)- single walled, small strains
 - Lamellar boundaries (LBs)- appear at large strains, form very flat CBs, replace MBs and DDWs
 - All the above are considered geometrically necessary boundaries (GNBs)
 - Separate regions that deformed differently
 - Arranged in parallel families
 - Special macroscopic orientation relative deformation axis
 - Increasing strain- increase in misorientation angle and decrease in spacing, much more rapidly than IDBs
 - Cells within CBs (SSDs)
 - Equiaxed, bounded by incidental boundaries (IDBs)
 - Low misorientation angles



Shear bands at grain boundaries



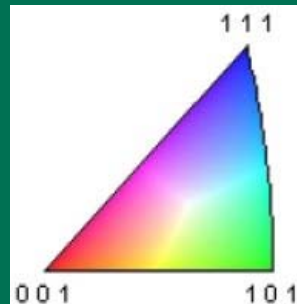
Dislocation substructures much larger than the coherence length are commonly observed



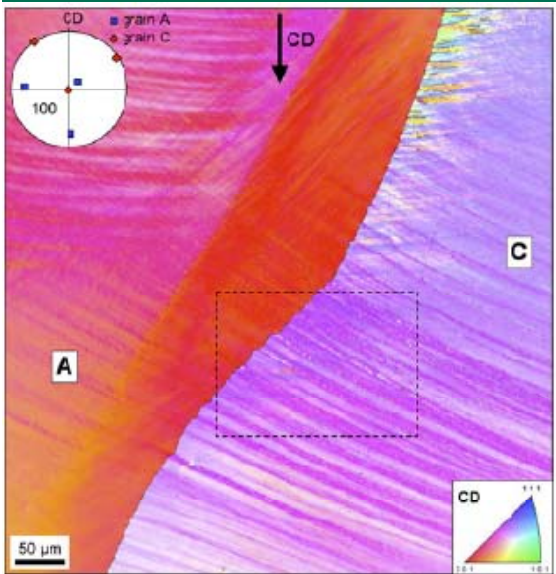
Evidence for multiple slip planes

Crystal directions \parallel
rolling direction

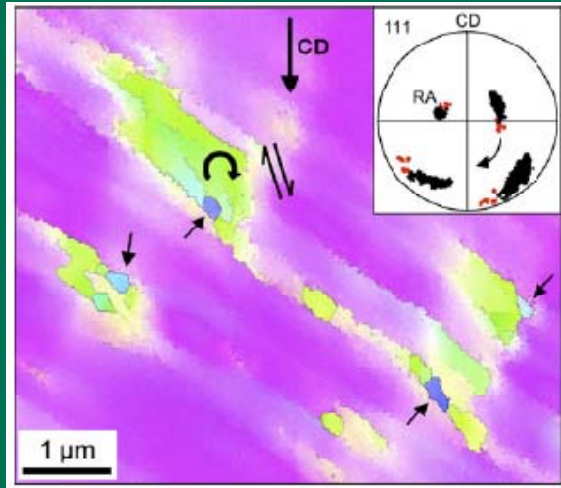
Bicrystal rolled 40%



Example of possible embryos/nuclei in Fe- 3wt% Si



Microshear bands at grain boundary. EBSD step size 1.4 μm.



Lattice rotations about $\sim\{111\}$ of possible embryos, black lines $>15^\circ$ misorientation

Intersecting slip systems lead to local rotation about a $\{111\}$ axis and make possible embryos within microshear bands



Summary

- Complex dislocation behavior most important for initial production of polycrystalline Nb sheet
 - Screw dislocation behavior controls plastic deformation behavior in sxl/large grain Nb
 - Awareness so can control deformation texture and therefore Rx texture
 - Need to incorporate screw behavior into crystal plasticity model
 - Others have done this, evaluate best method to use
- Complex BCC slip less of an issue in polycrystal
 - Closer to random texture more isotropic
 - Strong textures may be more affected
- Provocative questions
 - After Rx, why not leave the sheet alone?
 - After 800C Bake, why more EP?
 - Can we put furnace in Clean room?