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Slip Planes in BCC Tantalum: Towards Resolving the Discrepancy Between Modeling and Experiments

Christopher R. Weinberger

Jay Carroll, Lucas M. Hale, Hojun Lim, Garritt J. Tucker, Ping Lu , Jonathan A. Zimmerman, Khalid Hattar, Corbett C. Battaile, Brad L. Boyce, and Stephen M. Foiles

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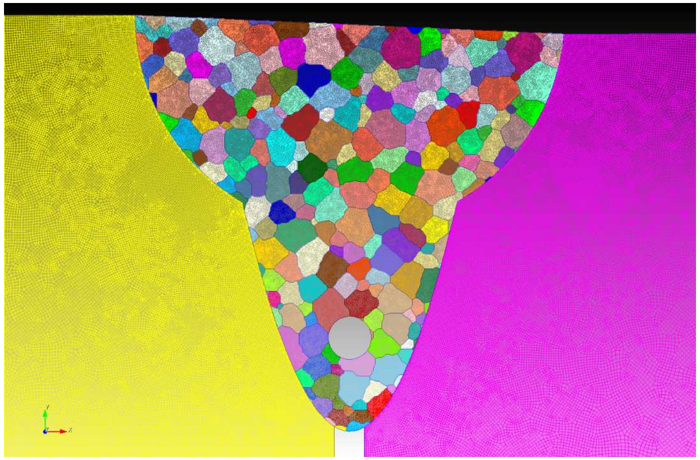
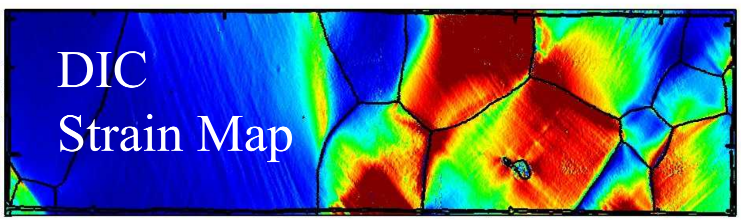
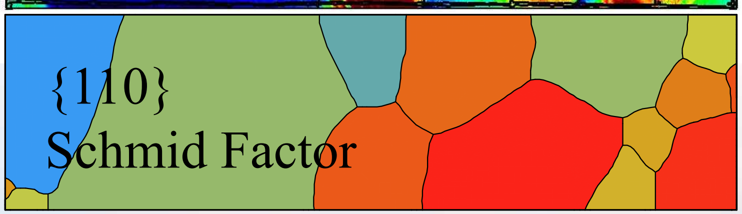
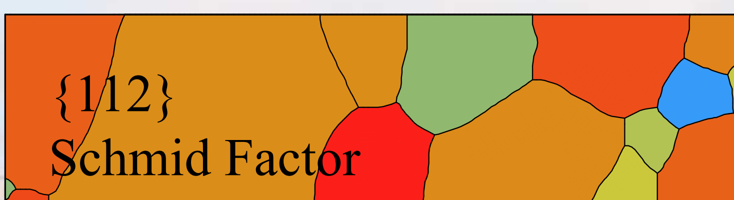
Why Study Slip Planes in BCC Metals?









- Inputs to large scale models

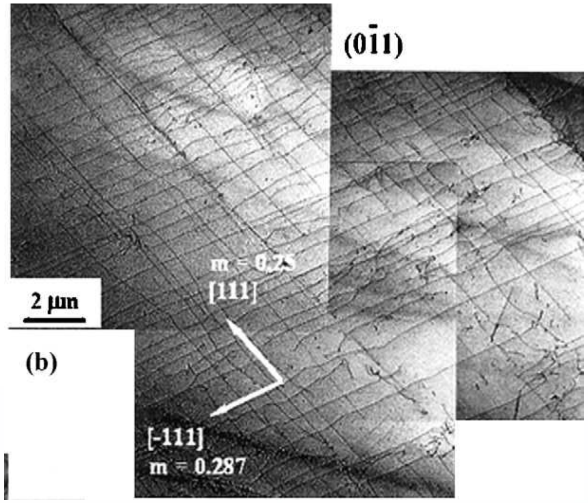
$$\mathbf{D} = \sum_{s} \dot{\gamma}^{(s)} \mathbf{M}^{(s)}$$

$\mathbf{M}^{(s)} \rightarrow$ Schmid Tensor

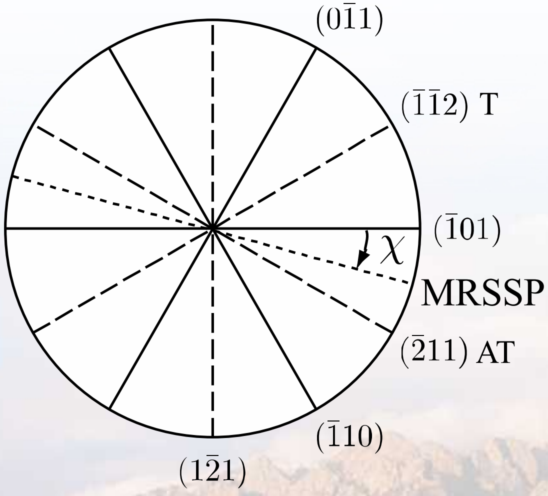
$\dot{\gamma}^{(s)} \rightarrow$ $$\frac{\dot{\gamma}}{\dot{\gamma}_o} = F\left(\frac{\mathbf{M}^{(\mathbf{s})} : \sigma}{\tau_*^{(s)}}\right)$$

- Understand large scale experiments

Ambiguity of Slip Planes in BCC Metals



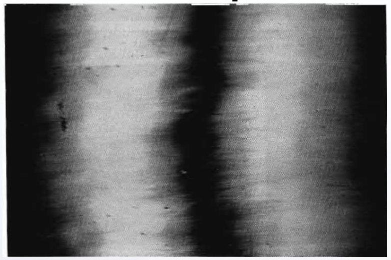
Hsiung MSEA (2010)



- Screw dislocations dominate at low temperatures.
- Slip planes in BCC metals are often ambiguous
  - Slip traces have been observed on:
    - {110}
    - {112}
    - {123}
- Prevalence of Cross-Slip?

Previous Observations of Slip in Tantalum

- Slip trace analysis in Ta:
  - Wavy Slip at 4.2 K and above
  - Slip lines identified are all {110}
  - Adding trace impurities indicates {110}
  - Slip tends towards the MRSSP as temperature increases

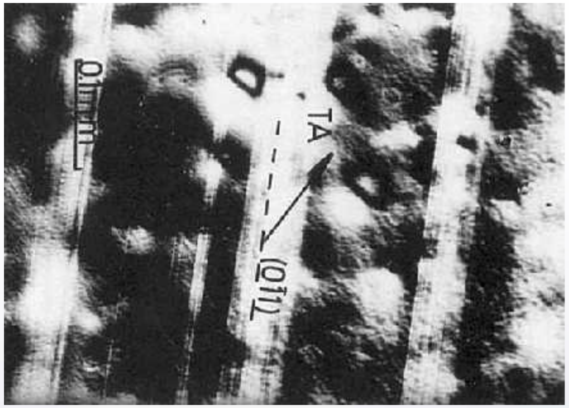


Diffuse slip in Ta at 4.2 K
Wasserbach, PSSA (1995)
Smialek and Mitchell, Phil Mag (1970)

- Indentation experiments suggest {110} at RT.

Biener et al. PRB (2007)

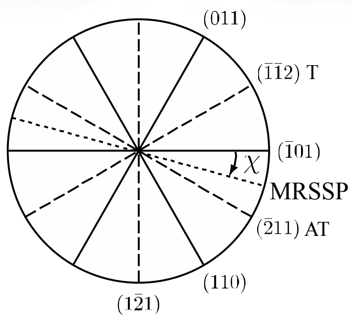
Smialek and Mitchell, JPSJ (1976)
Smialek and Mitchell, Phil Mag (1970)
Takuechi et al., Acta Metall (1979)
Takeuchi and Maeda, Acta Metall (1977)
Shields et al., MSE (1975)
Byron and Hull, JLCM (1967)
Hull et al., CJP (1967)
Wasserbach & Novak, MSE (1985)
Wasserbach, PSSA (1995)



Anomalous slip in Ta on {101} planes at 77K
Wasserbach, PSSA (1995)

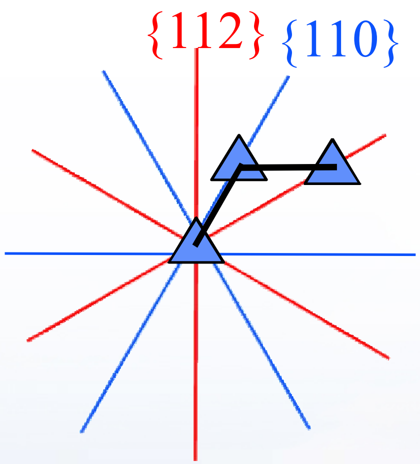
Review Paper: Weinberger, Boyce and Battaile, Int. Mater. Rev., In Press (2013)

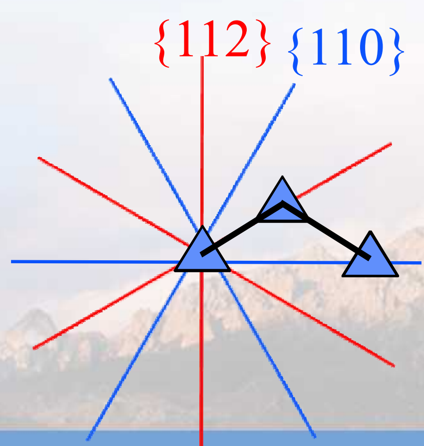
Composite Slip



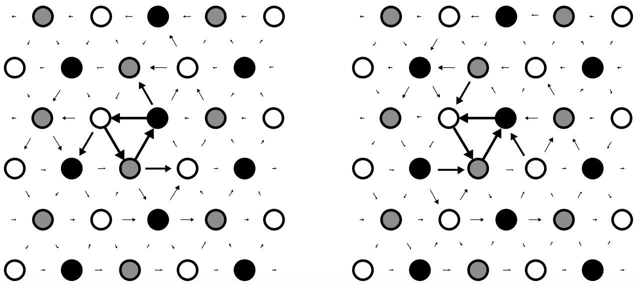
- Observations of {110} and {112} slip can be explained by competing slip planes.

- They can also be explained by cross slip
  - Screw dislocations are prevalent in BCC metals
  - {112} slip can be comprised of {110} slip steps
  - {110} slip can be comprised of {112} slip steps

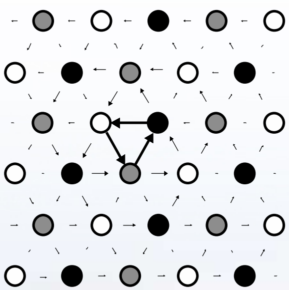




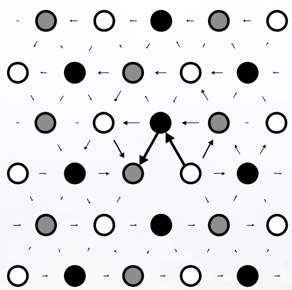
Metastable Core Structures: Predictions From Atomistics



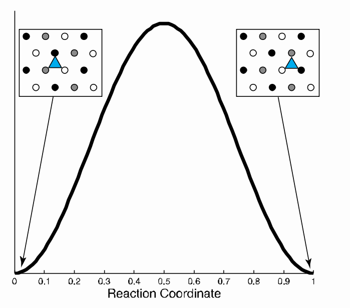
Polarized Cores

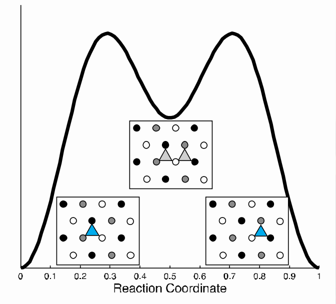


Compact Core



Split Core

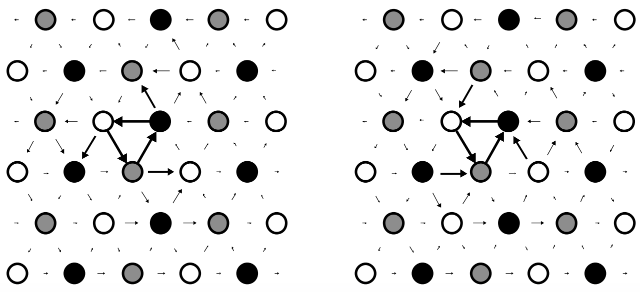




- Many atomistics simulations exhibit a polarized core
  - Obeys C3 symmetry
  - Has 2 degenerate structures: A & B
- Compact Core
  - Obeys D3 Symmetry
- Split core
  - Only satisfies the diad symetry
  - Triply degenerate
  - Sits on a {110} plane
  - Metastable state between compact cores

How does {112} slip work in Atomistics?

Polarized core



B A

Wen and Ngan, Acta Mater (2000)

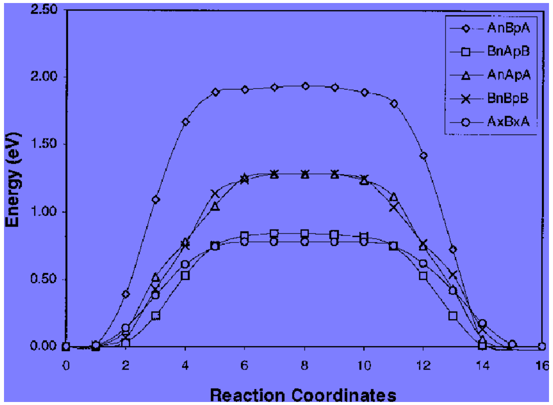
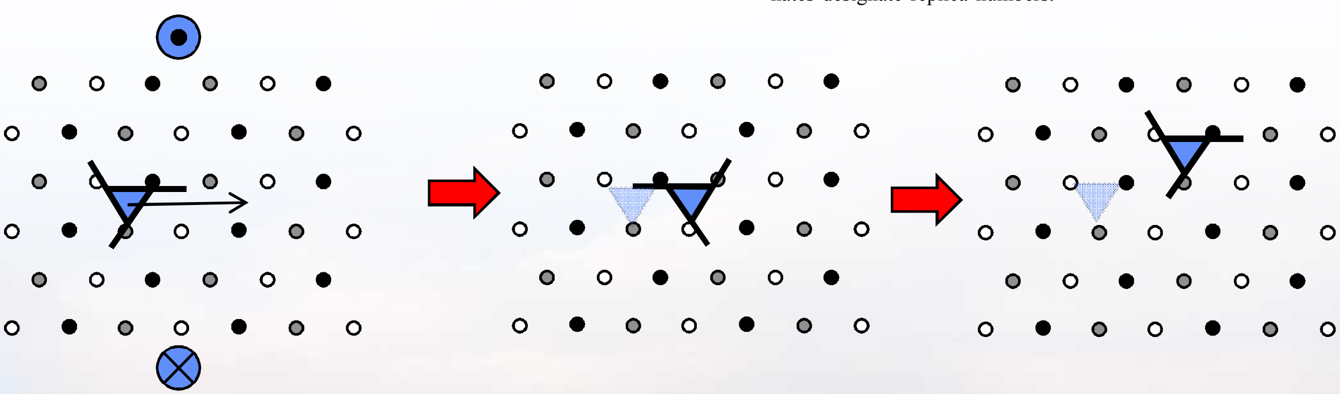


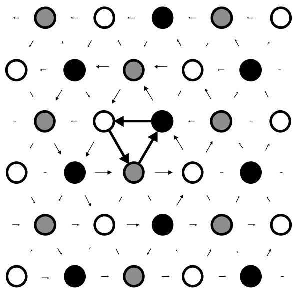
Fig. 4. Comparison of MEPs of kink-pairs. Reaction coordinates designate replica numbers.

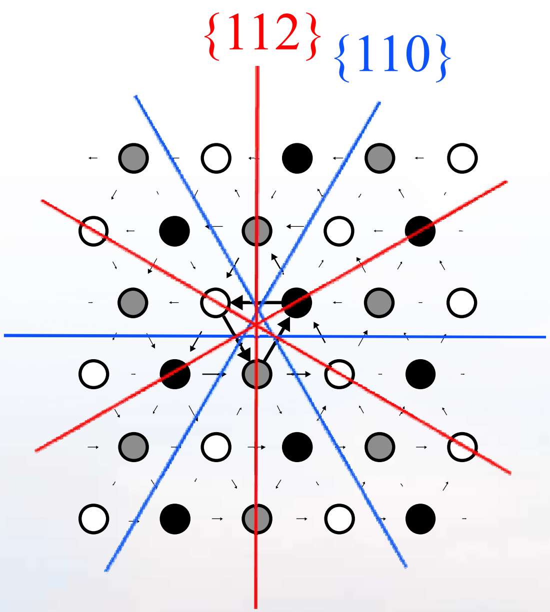
Lowest To Highest Energy:
A->B
A->A
B->B
B->A
For motion to the right
Flips for motion to the left



Polarized cores can result in a favored slip direction, which, in conjunction with polarity flips results in net {112} slip from {110} slip steps

Previous Atomistic Results: Ta





- Most models predict a compact core for Ta
- Interatomic potentials often show {112} slip
  - Comprised of {110} slip events

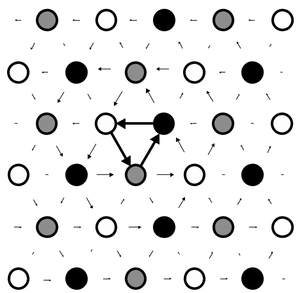
Ito and Vitek, Phil Mag 2001
Mishin and Lozovoi, Acta Mater 2006
Yang and Moriarty, Phil Mag 2001

- DFT shows similar results

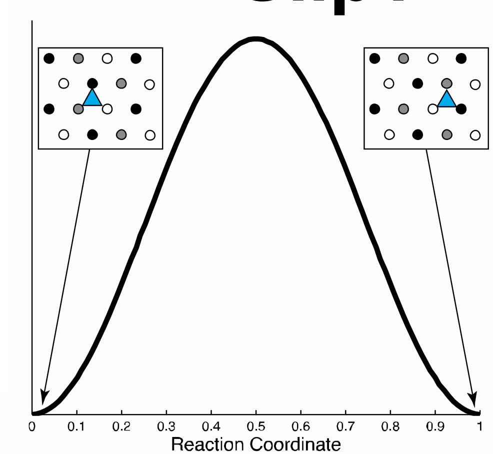
Woodward and Rao, PRL 2002
Segall et al., PRB 2003

How do we reconcile the experimental observations of {110} slip at low temperatures with atomistic simulations of {112} slip?

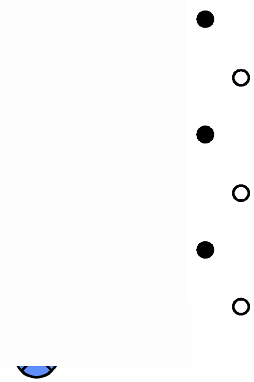
How Do Compact Cores Give Rise to {112} Slip?



Compact core
D3 symmetry



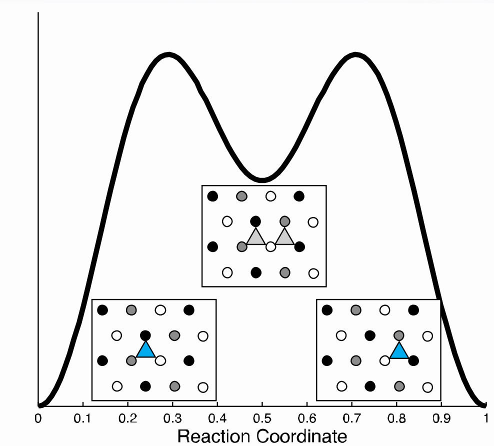
Peierls Potential



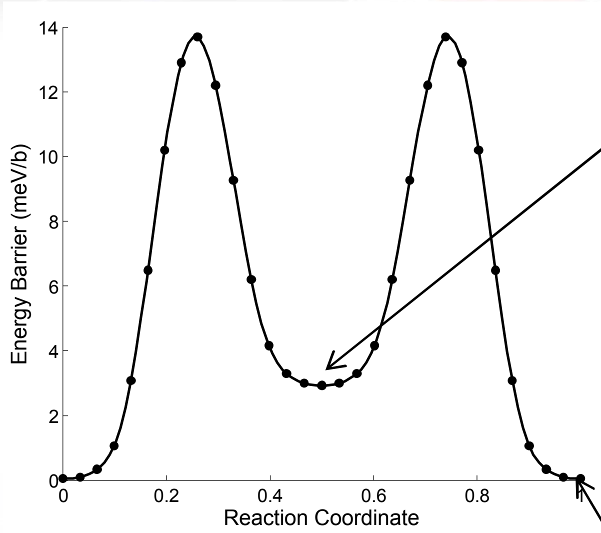
Why would a compact core, which has no structure preference for direction glide, give rise to {112} net slip from {110} slip steps?

Many Interatomic potentials that predict {112} slip with a compact core also predict a split core.

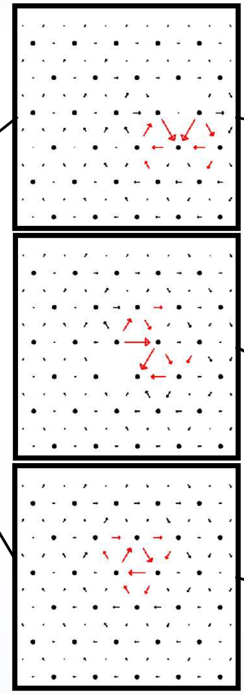
Does this influence the choice of slip planes?

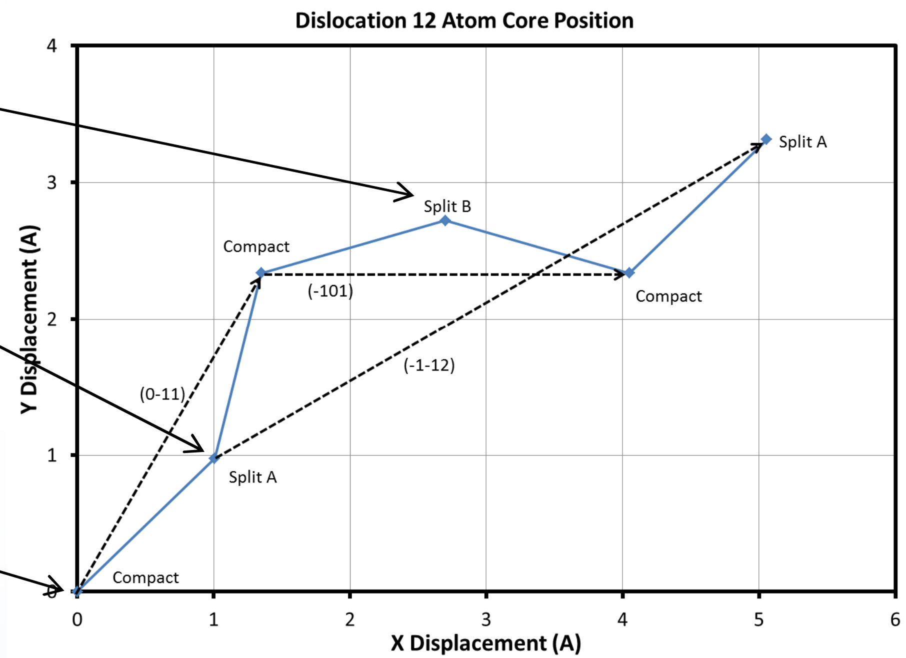


Atomistic Results for Ta Potentials



Computed Peierls Potential





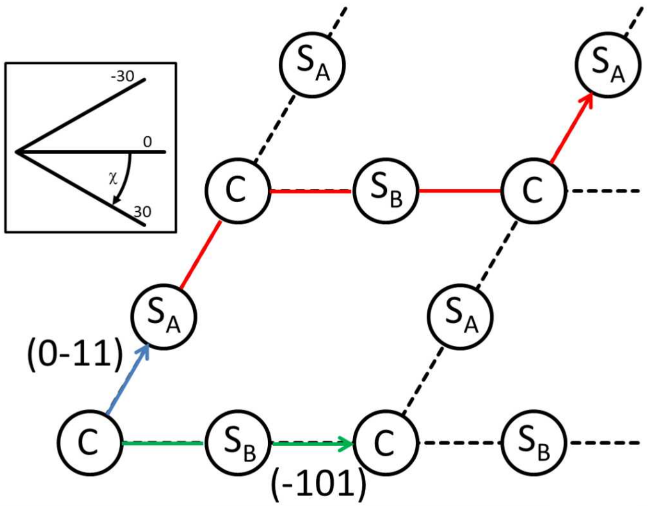
Slip path of a strain dislocation

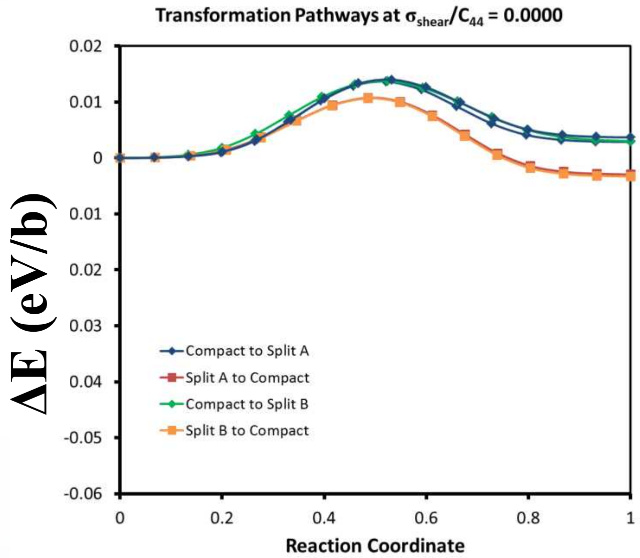
- Compared 5 interatomic models
  - All predict compact cores
  - All exhibit net {112} slip

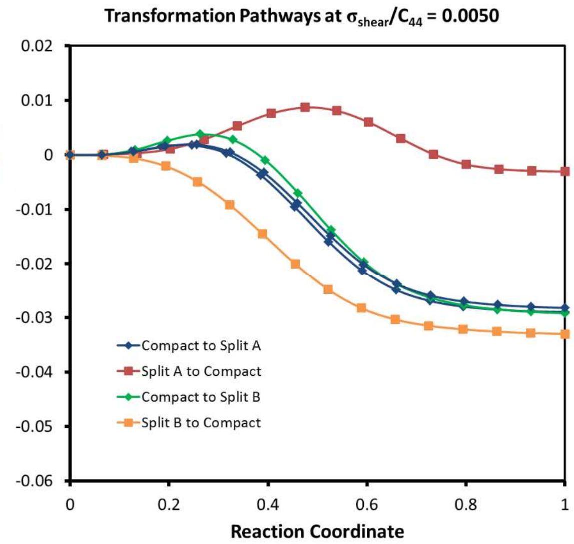
Angular Dependent Potential (Mishin)
Acakland Thetford Finnis-Sinclair
Zhou (EAM)
Guelil (EAM)
Li (force matched EAM)

- Core Transformations typically occur first
  - Compact->Split
- Slip then occurs from
  - Split -> Split

How Does the Compact Core Influence Slip?



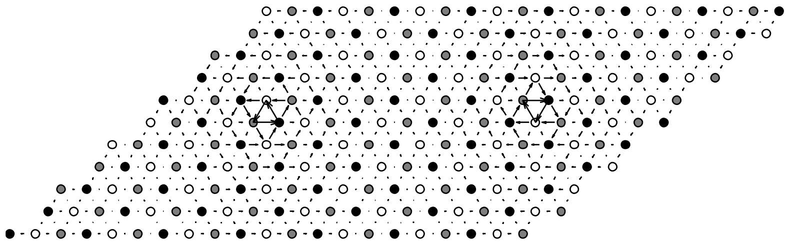


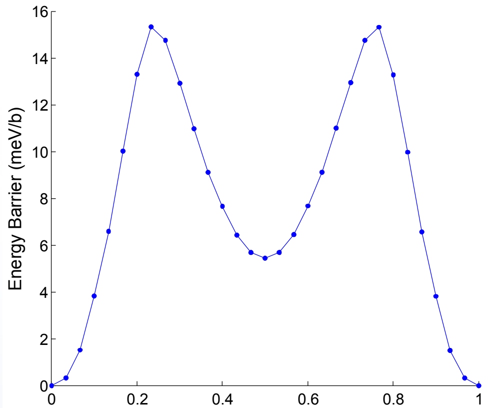


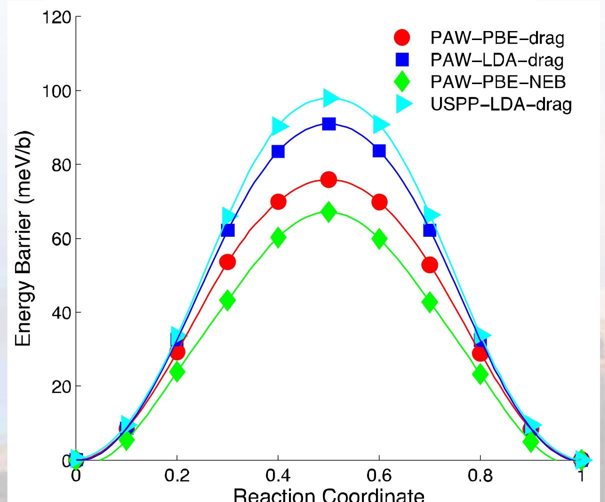
- Low temperature / High stresses:
  - The energy barrier from C->SA drops faster than C->SB even when the stress favors C->SB
  - High stresses required to move from SA destabilize other core structures -> slip occurs SA->SA
- At higher temperatures / low stresses -> energy barriers between C->SA and C->SB are similar which leads to cumulative {112} slip.

The stability of the Split core influences {112} slip.
Does the split core actually exist?

Density Functional Theory



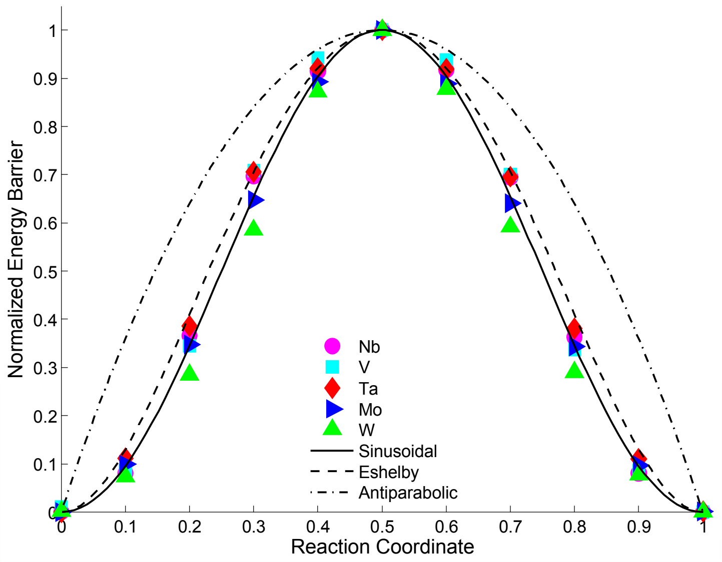


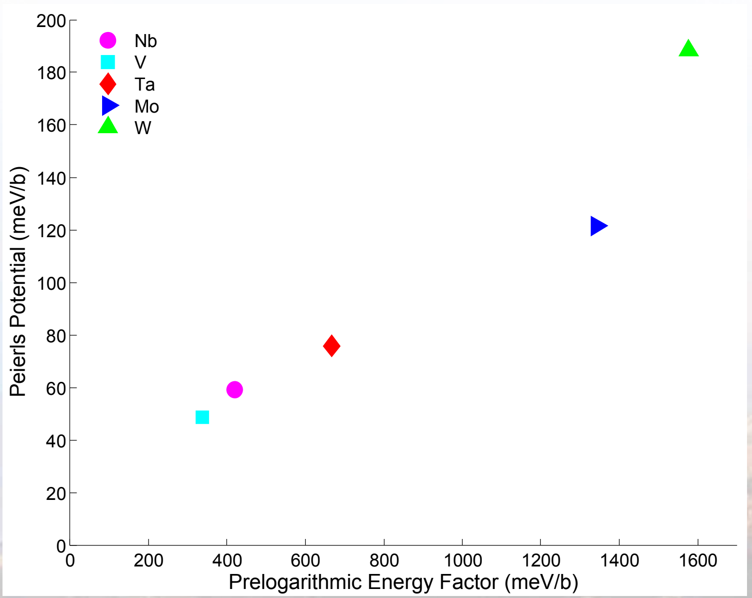


- Due to PBCs, we use a a dislocation dipole, 231 atoms.
- Empirical potentials exhibit the camel hump Peierls potential.
- DFT does not show a metastable state
  - Different XC: PBE (GGA) & LDA
  - Different PP: PAW & USPP

Weinberger, Tucker, Foiles, PRB (2013)

An Aside on Universality





- Consider 5 different BCC metals: Ta, V, Nb, Mo, W
- All Materials modeled show similar Peierls potentials
- Peierls potential height scales with the dislocation line energy.

Weinberger, Tucker, Foiles, PRB (2013)

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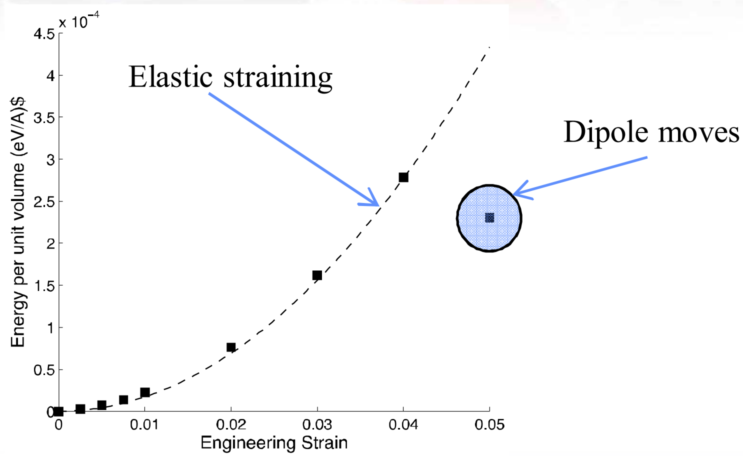
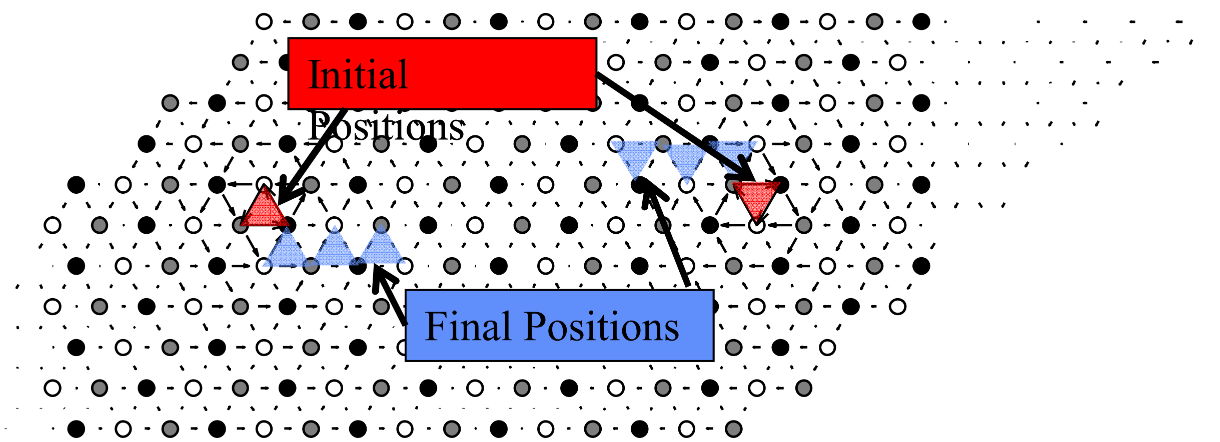
Slip planes Ta predicted by DFT

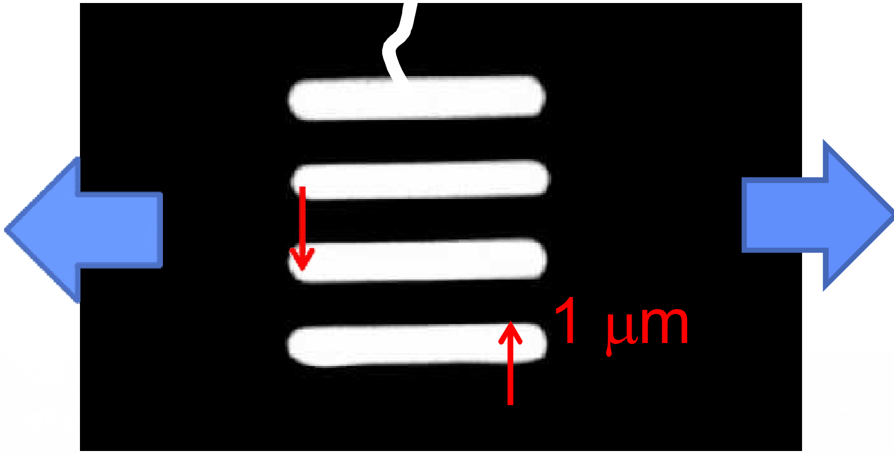


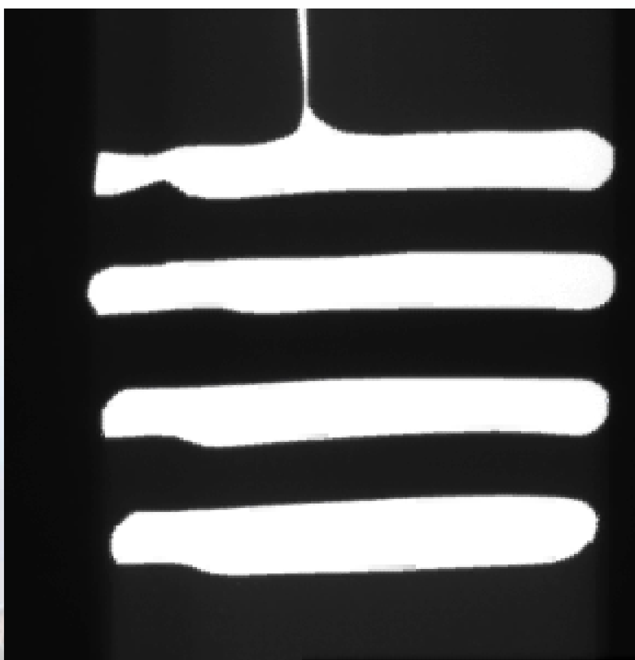
- Previous reports with DFT suggest {112} slip
  - Isolated dislocation: Woodward and Rao (2002)
  - Dipole: Segall et al.
- Conducted straining
  ons on dipoles using
  PBE
  LDA
  x slip, not {110} but
  2}



Dipoles may not be the best test case for {112} slip
Can {112} slip exist for compact cores w/o split cores?

FIB-milled Tensile Straining Bars

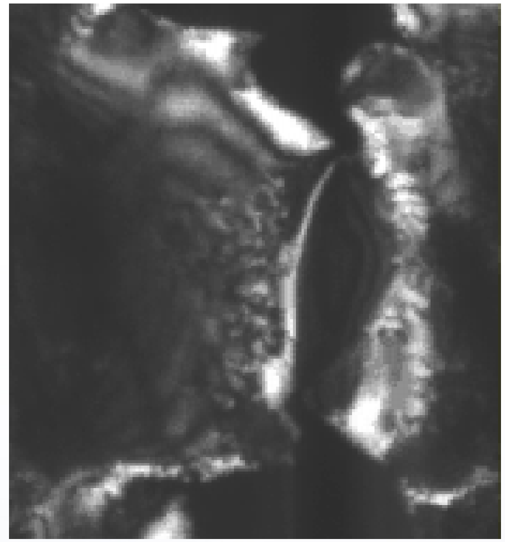


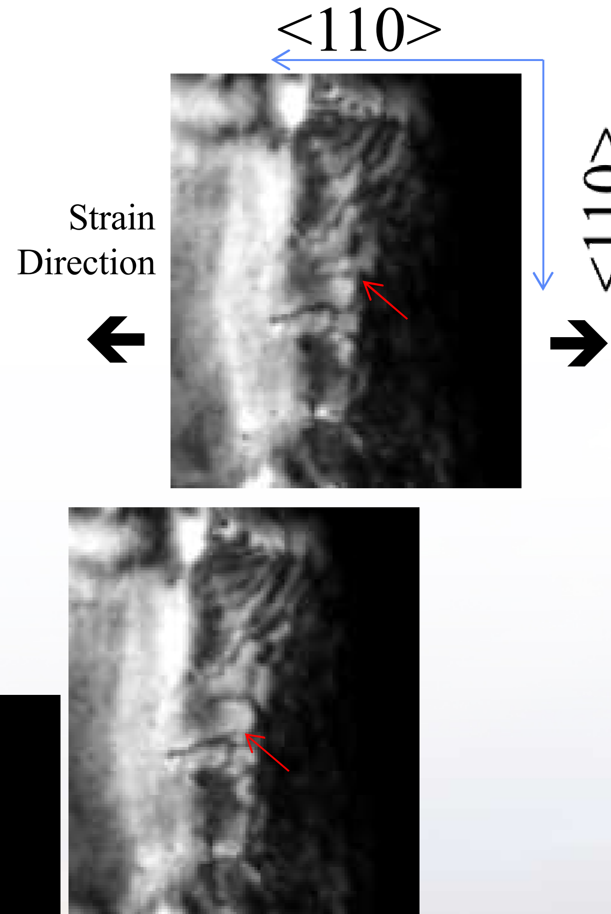


- Micron bars, created by ion milling and FIB, will be used for in-situ TEM straining – generation, propagation and interaction
  - Uniform gauge length
  - Large electron transparent region
  - To better control the fracture process
  - To study the dislocation dynamic beyond crack tip

Produces large uniform electron transparent tensile bars, but require extensive FIB-milling and annealing

Dislocation Dynamics in Micro-straining Bars

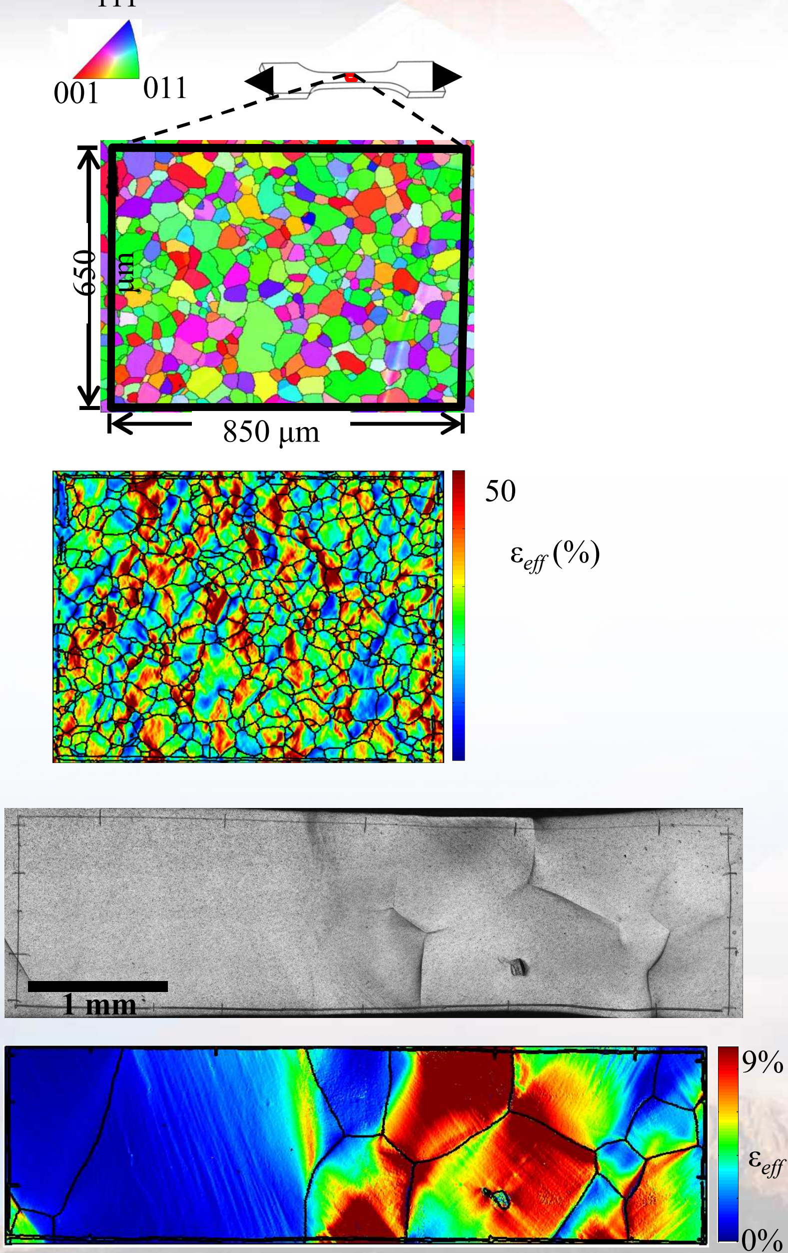




- Dislocation motion in a {110} plane
- Dislocations direction is <111>

Dislocation motion can be observed in the plastic zone ahead of the fracture tip, as full line dislocations

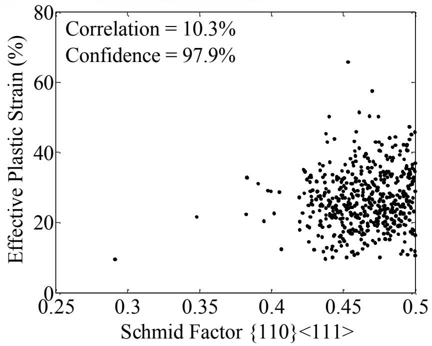
Deformation of Polycrystals and Oligorystals



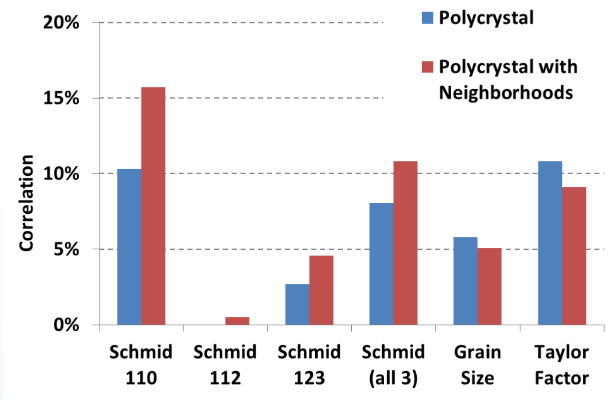
- Tensile tests on polycrystalline and oligocrystalline Ta.
- Surface Strains are measured using Digital Image Correlation
- Grain Orientations determined by EBSD
- This allows us to correlate Schmid Factors and Accumulated Plastic Strain.

Carroll, Clark, Buchheit, Boyce & Weinberger, submitted (2013)

Correlation of Accumulated Plastic Strain and Schmid Factors

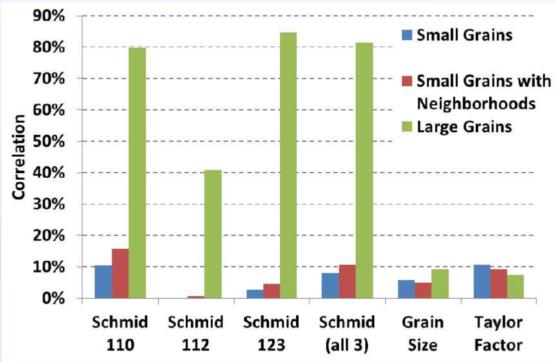


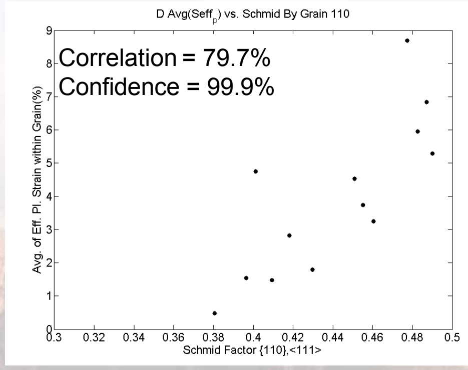
- Use a Spearmin Correlation to relate effective plastic strain to Schmid Factors.



- In poly crystals, {110} shows the strongest correlation

- Higher correlations by including "grain neighborhoods" (<20^{o} misorientations).



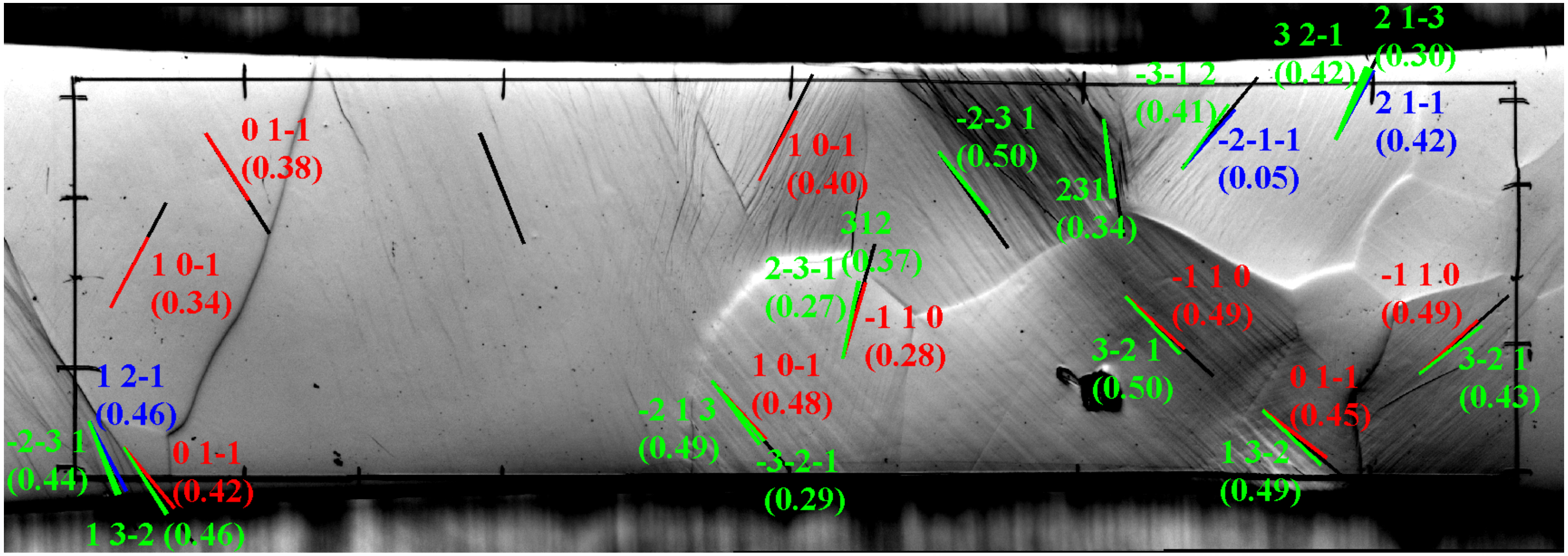


ls show stronger

s.

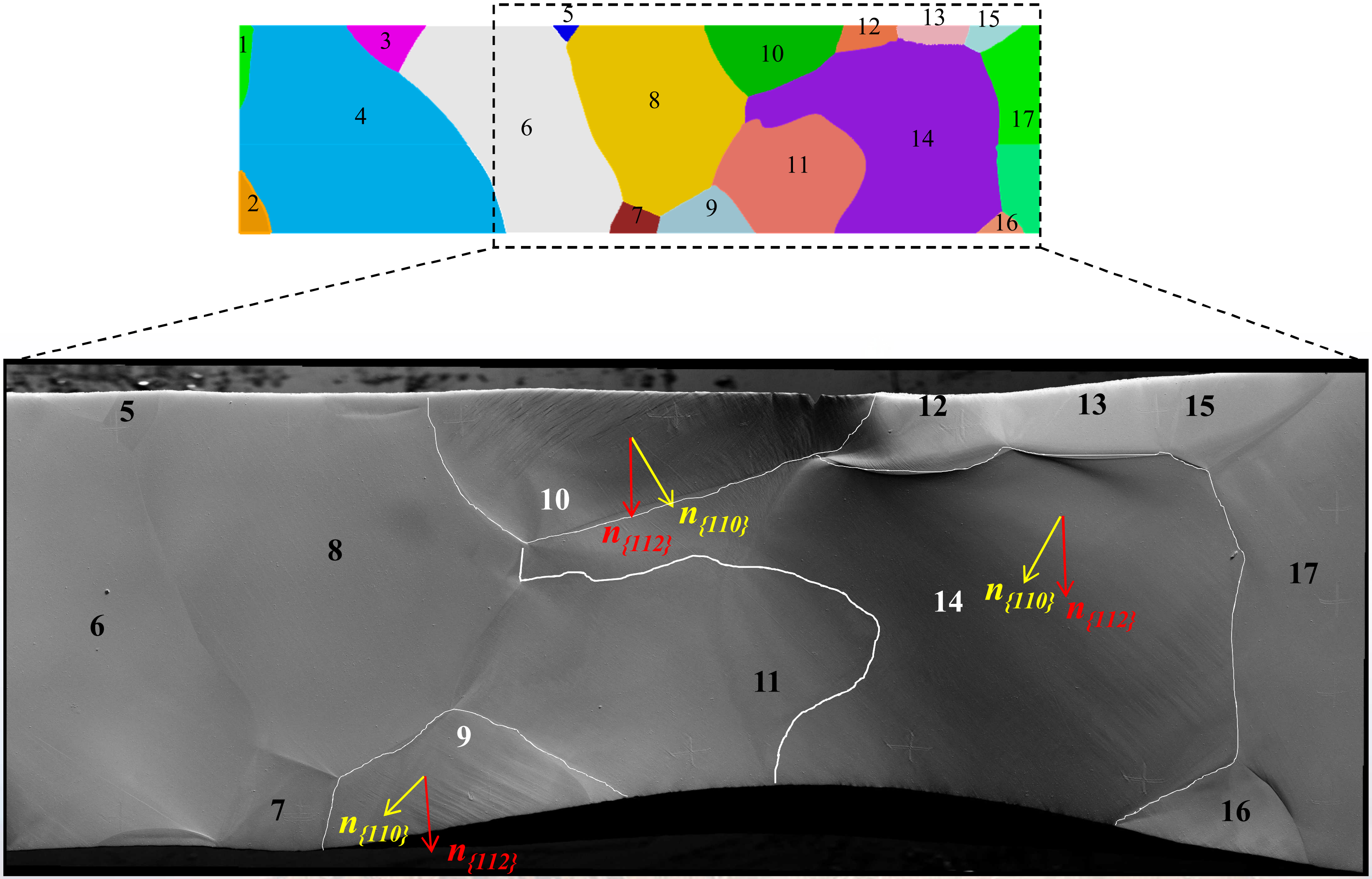
Carroll, Clark, Buchheit, Boyce & Weinberger, submitted (2013)

Slip Trace Analysis: Oligocrystal



- Slip trace analysis performed on the oligocrystal shows confusing picture of slip.
  - Only slip planes within 5 degrees are shown.
  - Most slip traces align with either {110} or {123}
  - Very few align with {112}
  - Agrees well with Schmid factor correlation

Slip trace analysis: Ta oligocrystal 2



n: slip plane normal of the most active slip plane calculated from the initial crystal orientation

Discussion

- Literature suggests {110} slip in Ta at low T tending to MRSSP slip at high T.
- Most simulations show {112} slip at 0K
  - ADP simulations show {112} slip at all temperatures
  - {112} slip caused by core structures and their stability
    - Core polarization
    - Split core and compact core stability
  - DFT simulations show {112} slip & {110}?
- {112} slip in simulations seems strongly dependent on core structures predicted.
- RT in-situ TEM straining experiments show {110} slip
- RT polycrystal and oligocrystal experiments support {110} slip.

This work supports {110} slip in Ta