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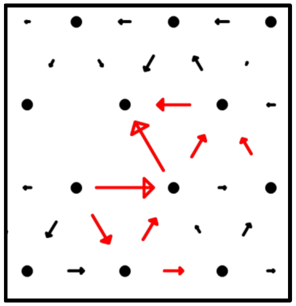
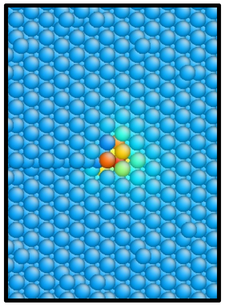
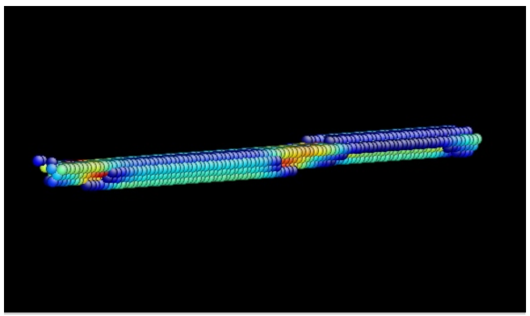
Simulations of bcc tantalum screw dislocations: understanding why classical inter-atomic potentials predict {112} slip







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NNSA National Nuclear Security Administration

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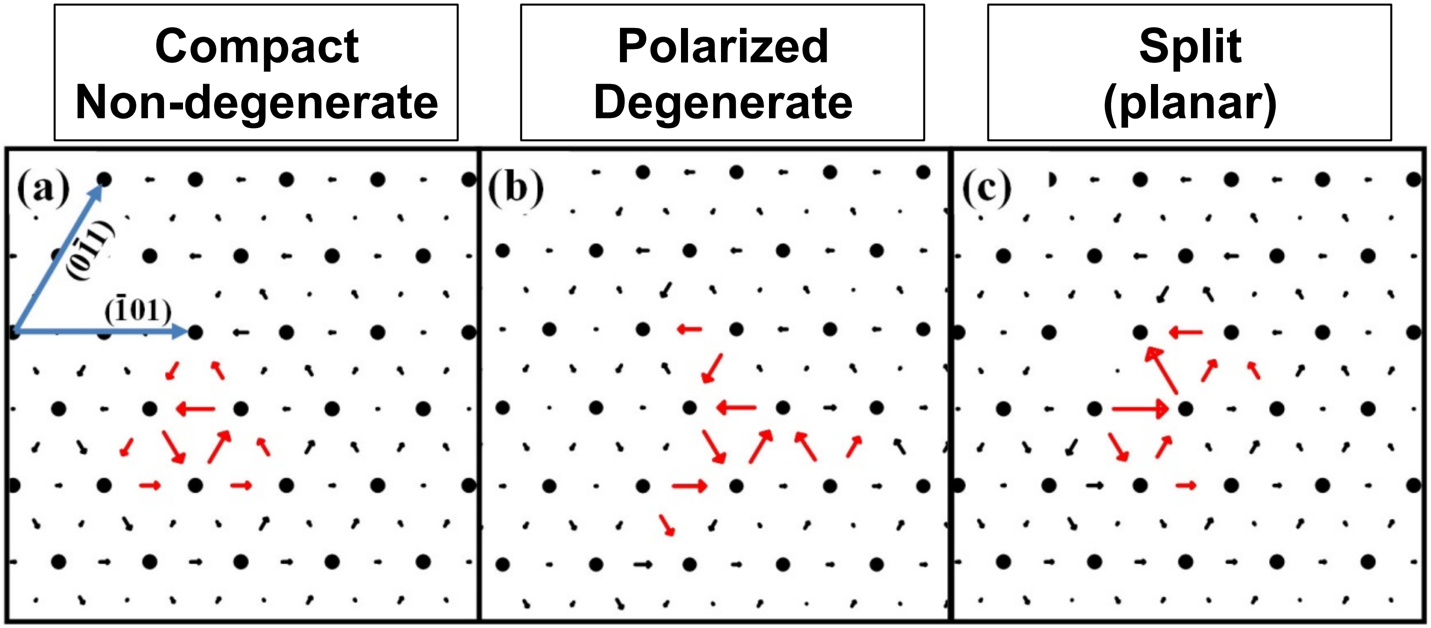
Motivation: Understand Dislocation Behavior in Tantalum

- We seek to develop a plasticity model for bcc metals based on accurate dislocation behavior
  - <111> screw dislocations dominate due to large Peierls Stresses
  - Slip is strongly temperature and orientation dependent
  - Multiple slip planes: {110}, {112}, {123}, wavy

- High lattice resistance is due the non-planar nature of the screw dislocation core in bcc metals (Hirsch, 1960; Caillard and Martin, 1975).
- The configuration of a dislocation core has not been confirmed experimentally, but has been identified using atomistic modeling and simulation.

Dislocation Core Structure and Slip Behavior



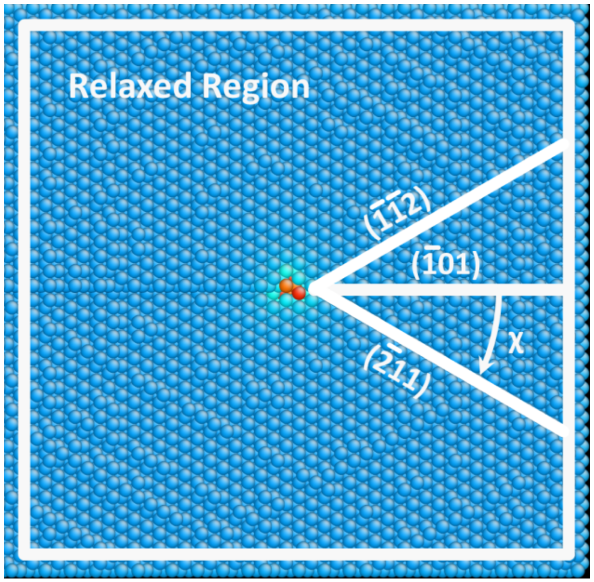
- Compact core results in {110} slip (Duesbery et al, 1973).
- Polarized core results in {112} slip via motion on alternating {110} planes (Duesbery et al, 1973).
- Also observed in simulation is a planar or split core – core appears “split” between two non-planar core locations, spread on a single {110} plane. Split core is metastable in classical potential atomistics (e.g. Gordon et al, 2010); unstable in many DFT calculations (Ventelon et al, 2007; Weinberger et al, 2013).

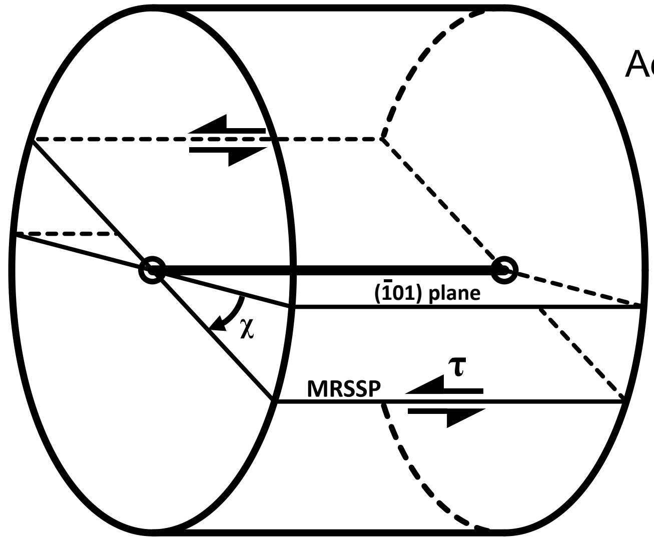
Slip behavior differs with dislocation core structure

- Polarization of the dislocation core does not cover all atomistic observations of {112} slip. Nearly all simulation with classical potentials (e.g. Duesbery and Vitek, 1998; Anglade et al, 2005) and some *ab initio* calculations (Woodward and Rao, 2002; Segall et al, 2003) report {112} slip occurring from a compact core.
- Experiments indicate that fundamental slip in Ta is on {110} planes (Takeuchi and Maeda, 1977; Tang et al, 1998).
- **We seek to establish the underlying cause for empirical potentials exhibiting {112} slip in atomistic simulation.**
- **We perform atomic simulations of single dislocation slip in Ta**
  - **Observe how dislocation reacts to stress and temperature**
  - **Measure critical resolved shear stress (CRSS) to activate motion**
  - **Determine necessary information in developing a larger scale model**

Thin Simulation Design

- Single dislocation in 200 X 200 X 22.9 Å system
- Periodic in z-direction, outside x- and y-boundaries fixed
- Strain applied according to anisotropic elasticity solution
- Middle of system relaxed with a force minimization algorithm
- Five classical potentials investigated: FS[1], EAM[2-4], ADP[5]
- Increase load and characterize and measure any changes



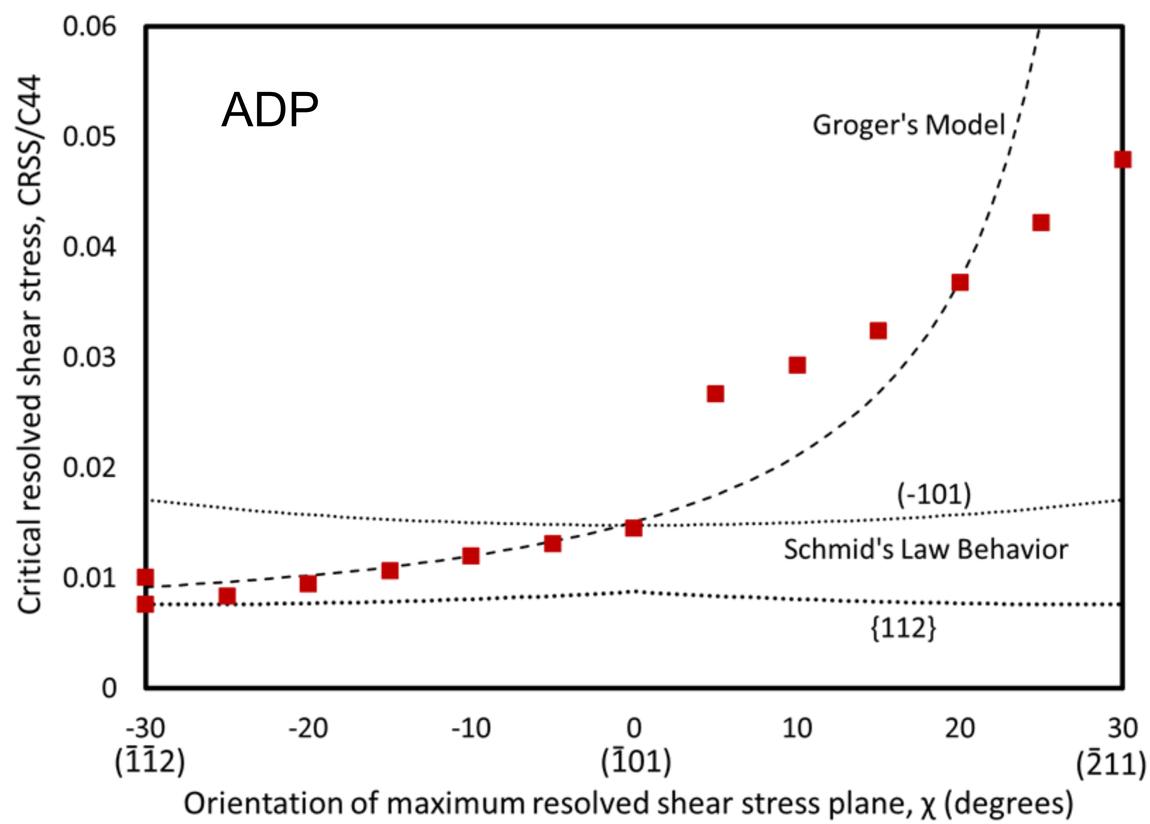


Adapted from [6]

[1] G. J. Ackland and R. Thetford, Phil Mag A **56,** 15 (1987).
[2] A. M. Guellil and J. B. Adams, J Mater Res **7,** 639 (1992).
[3] Y. H. Li, et al., Phys Rev B **67** (2003).
[4] X. W. Zhou, et al., Phys Rev B **69** (2004).
[5] Y. Mishin and A. Y. Lozovoi, Acta Mater **54,** 5013 (2006).
[6] M. R. Fellinger, et al., Phys Rev B **81** (2010).

Critical Resolved Shear Stress

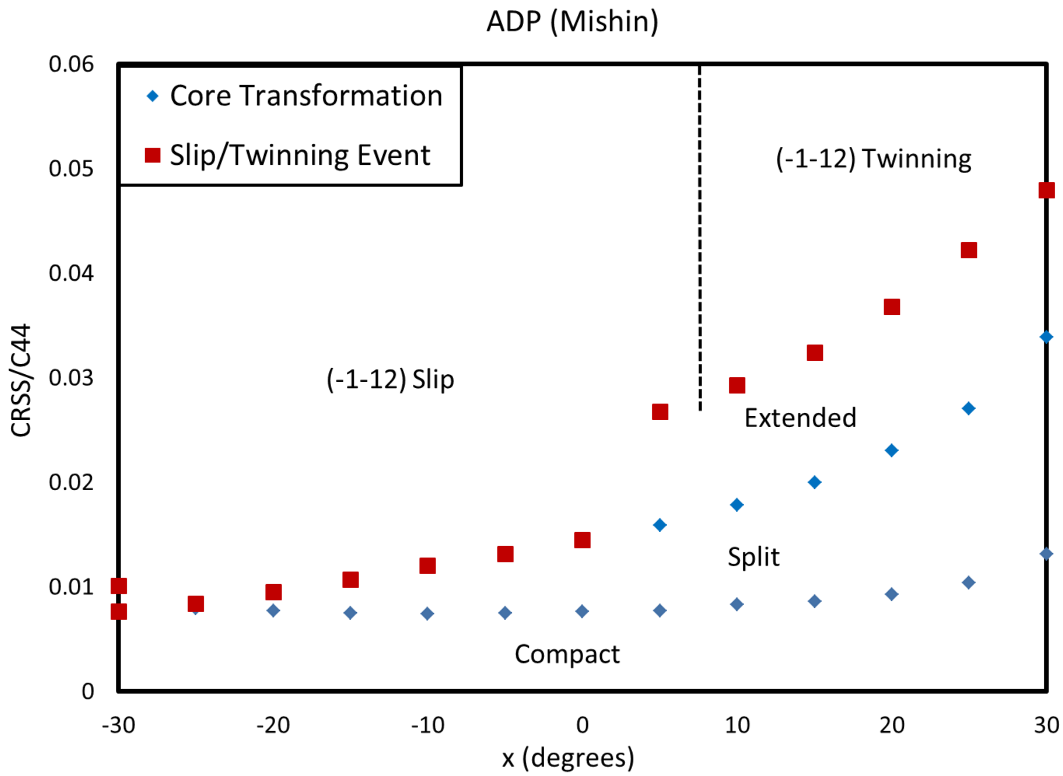
- Stress to activate unrestricted dislocation motion
- Like to understand/fit correct behavior
  - Deviation from Schmid's law
    - Twinning/anti-twinning {112} asymmetry
    - Groger's model
  - (-1-12) slip instead of expected (-101) slip
  - Discontinuities in CRSS vs. orientation

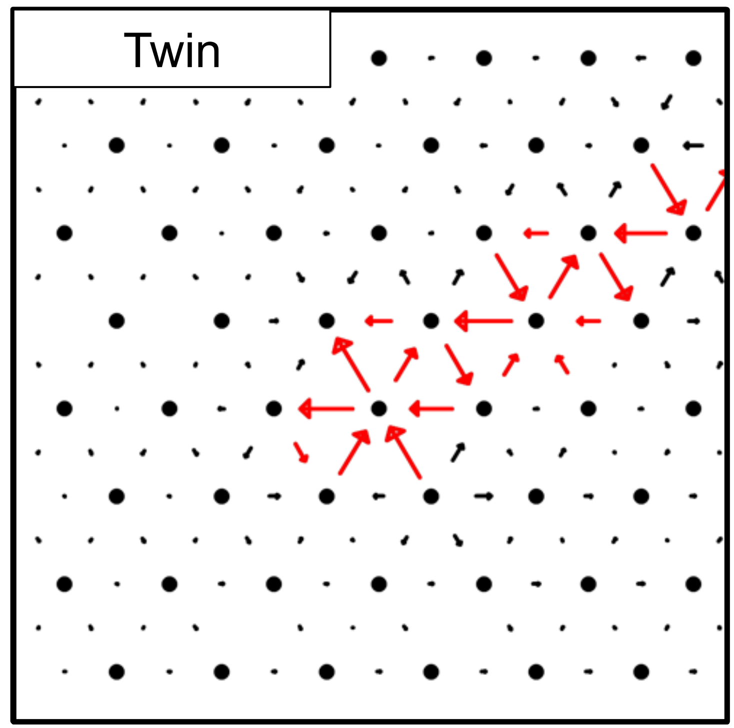


[1] R. Groger, V. Racherla, J. L. Bassani, and V. Vitek, Acta Materialia **56,** 5412 (2008).

Dislocation Core Transformations

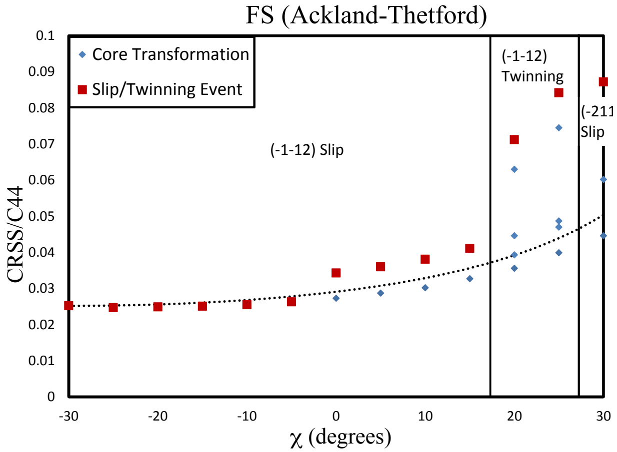
- CRSS discontinuities related to changing core structures (positions) and other critical events
- CRSS values obtained for ADP are close to *ab-initio* results by Woodward and Rao

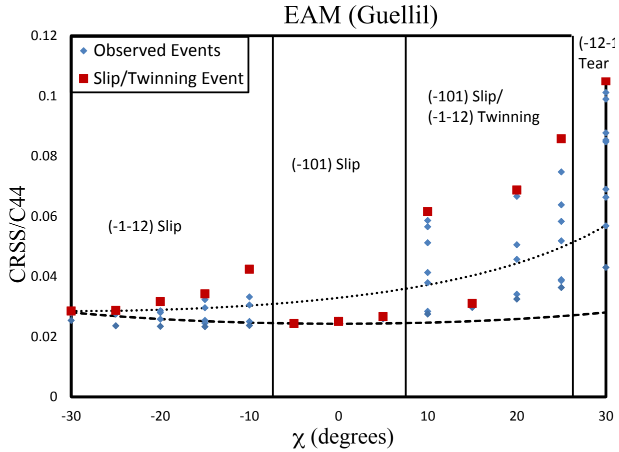


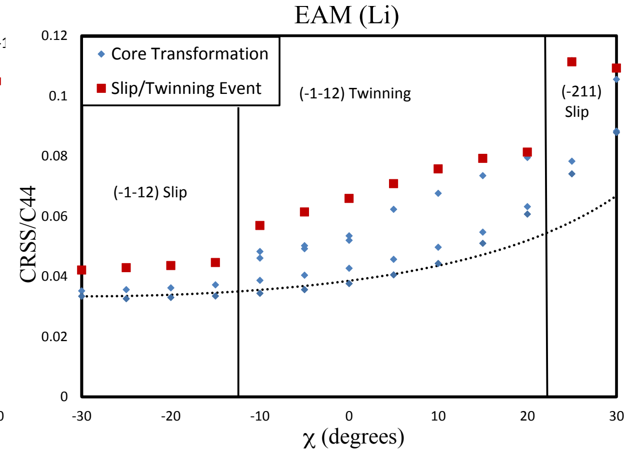


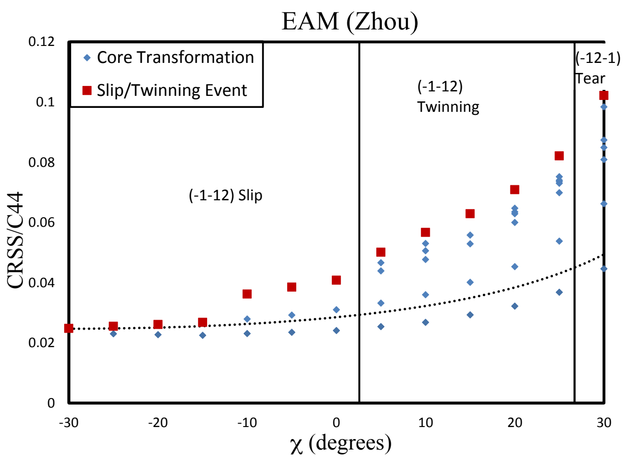
[1] C. Woodward and S.I. Rao, Phys Rev Lett **88,** 216402 (2002).

All Potentials Tested Show {112} Slip





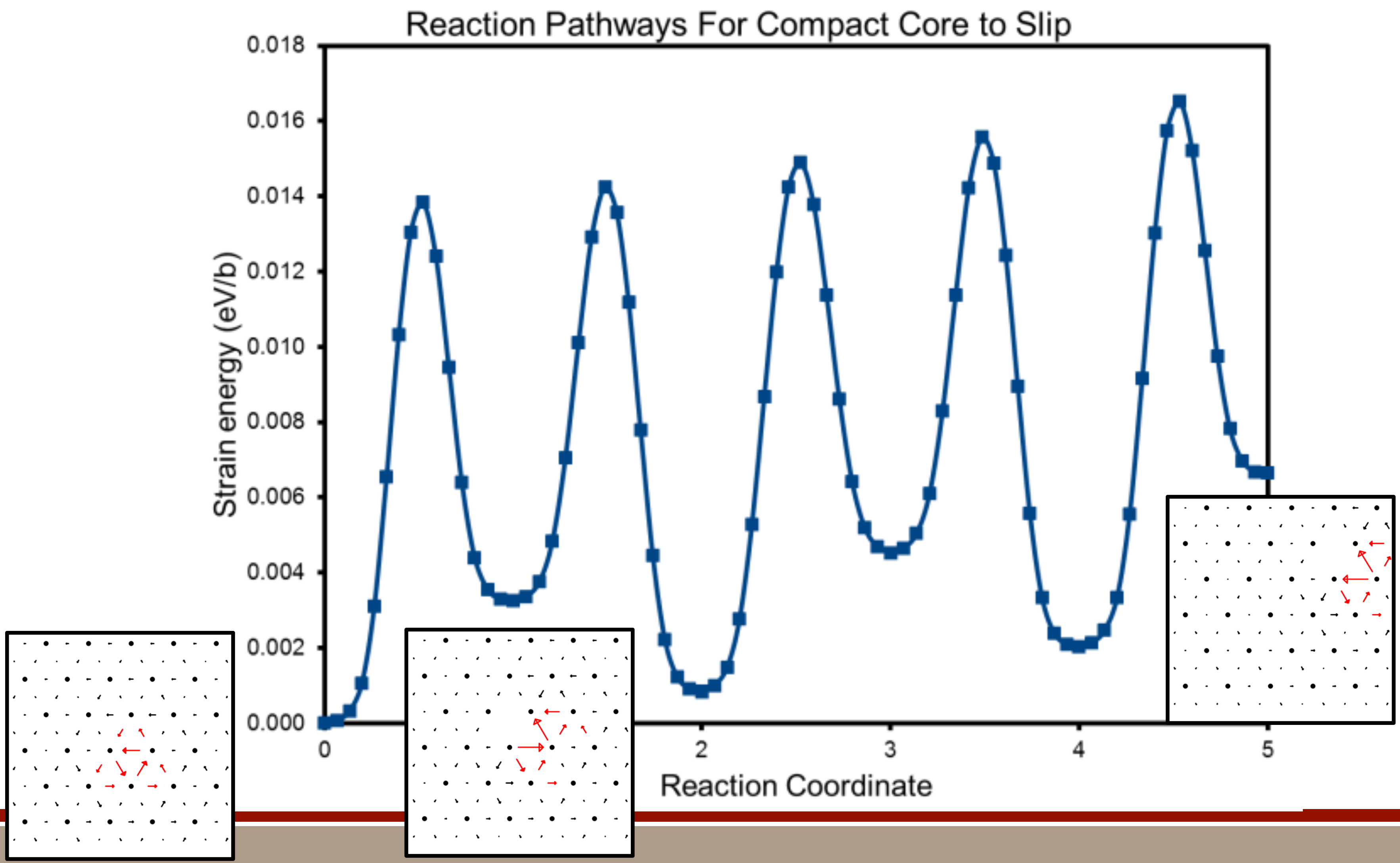




- Potentials available at project start were EAM-type variants
- New potentials have since been created that have yet to be evaluated:
  - MGPT by Moriarty et al. (2012)
  - MEAM by Fellinger and Wiklins (2013)
  - SNAP by Thompson et al. (under development)
  - BOP - ?

(-1-12) Zero Stress Slip Pathway

Nudged Elastic Band calculations of the reaction pathway and barriers



(-1-12) Zero Stress Slip Pathway

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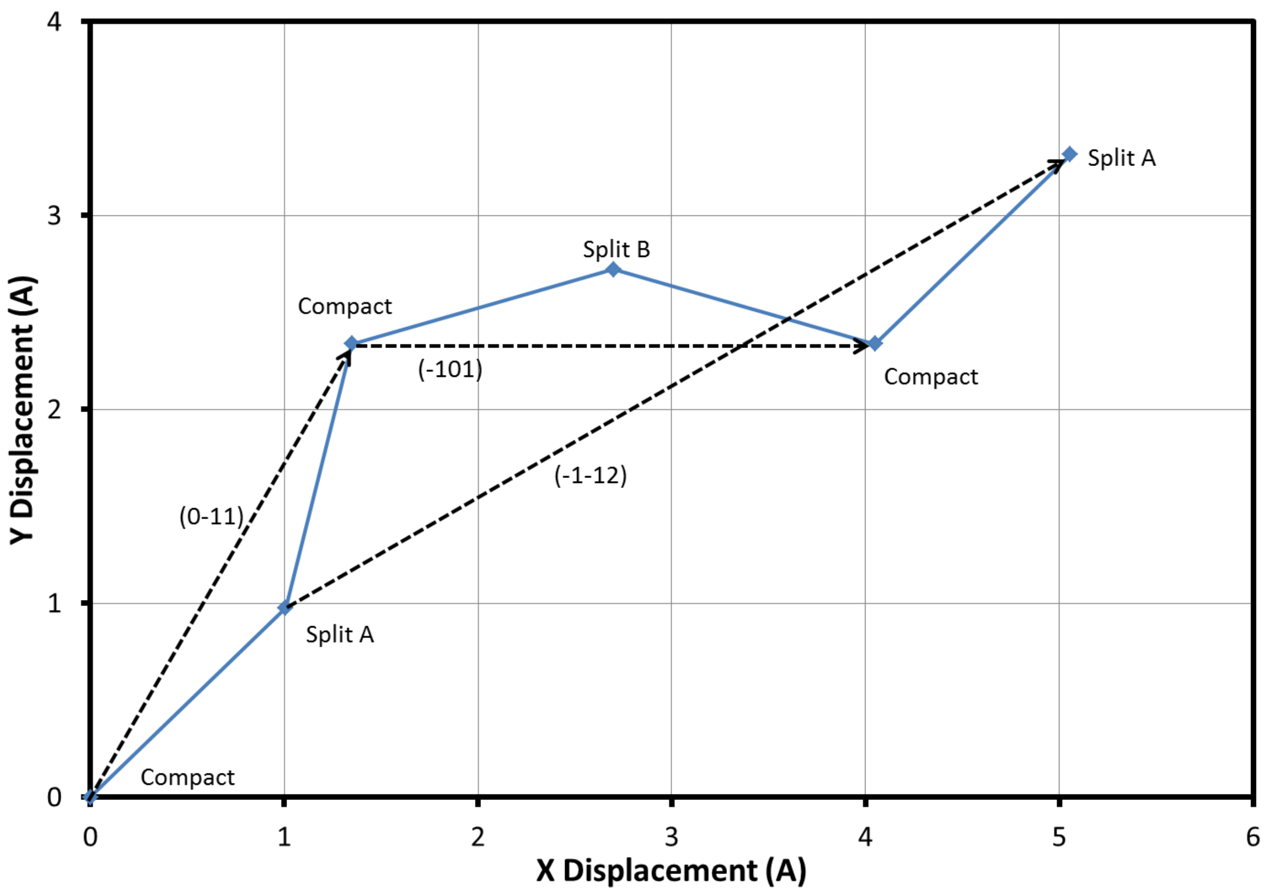
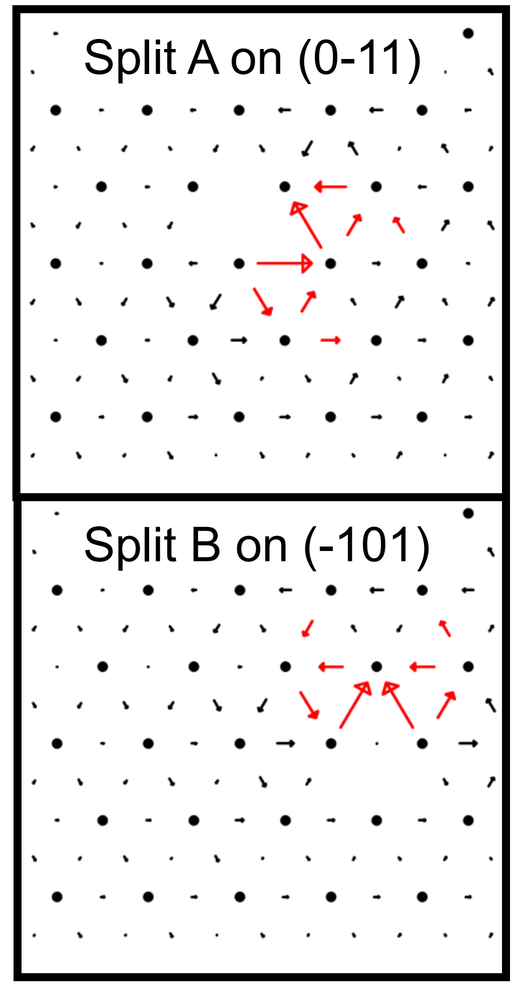
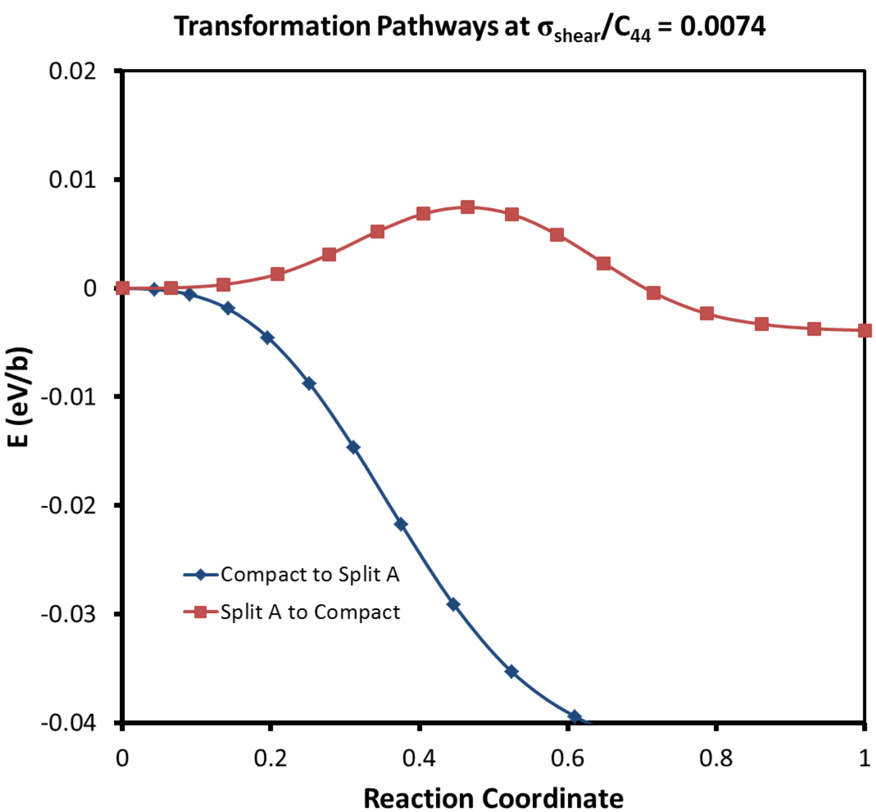
{110} glide steps on two different planes resulting in total {112} slip

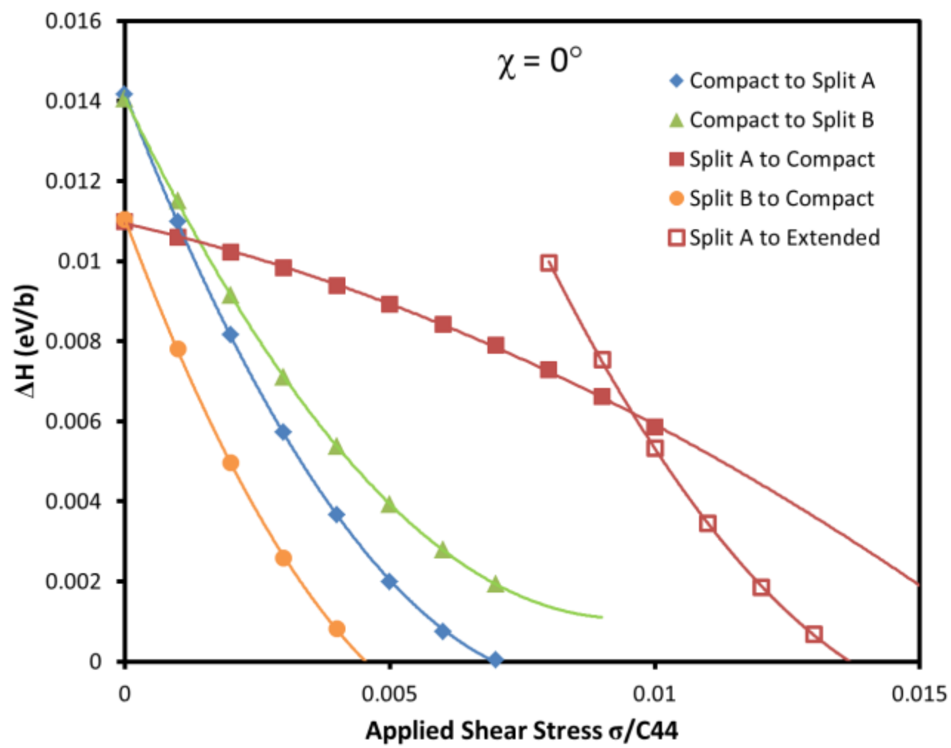




Stress Dependent Barriers

- Four unique barriers along slip pathway
- Activation enthalpy, ΔH, given by maximum energy along pathway
- Max resolved shear stress along (-101) – Split B favored by driving force
- Critical stress for Compact to Split A less than Compact to Split B!





Activation Enthalpies

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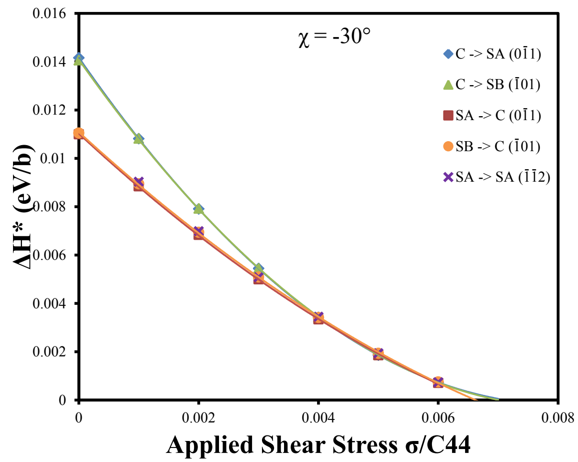

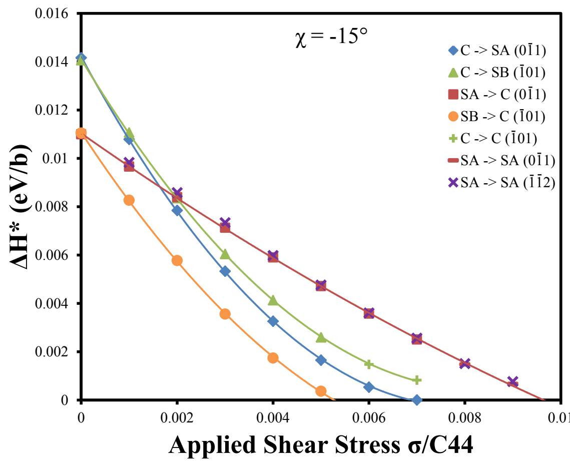

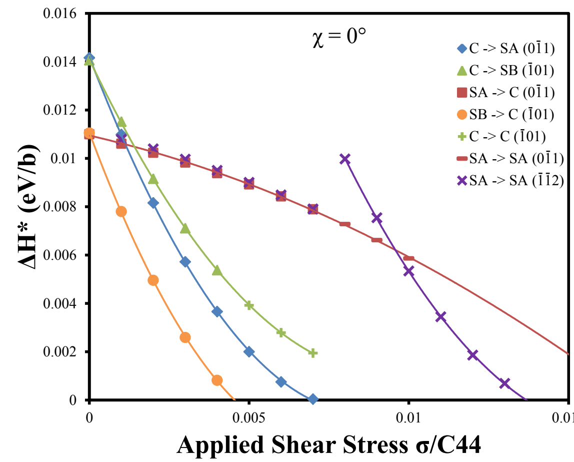

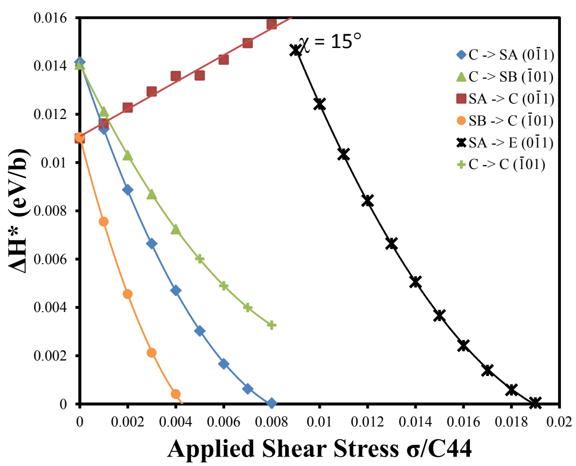

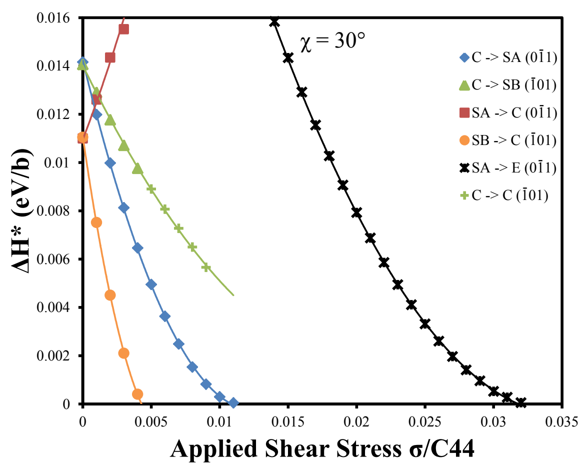

- Activation enthalpy for Compact to Split A less than Compact to Split B at all stresses and for all orientations

(-101) vs (-1-12) Slip Processes

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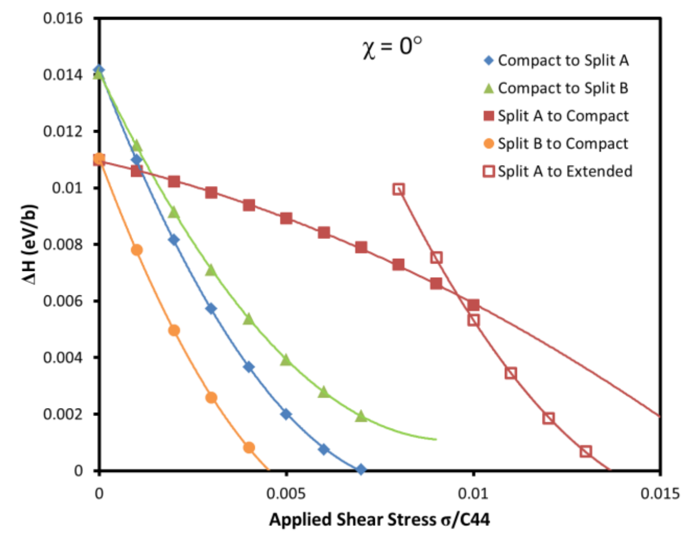
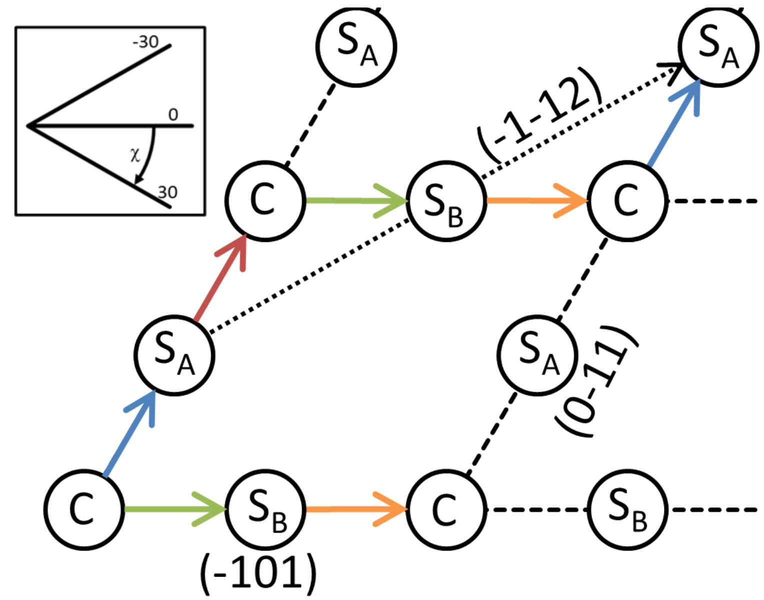
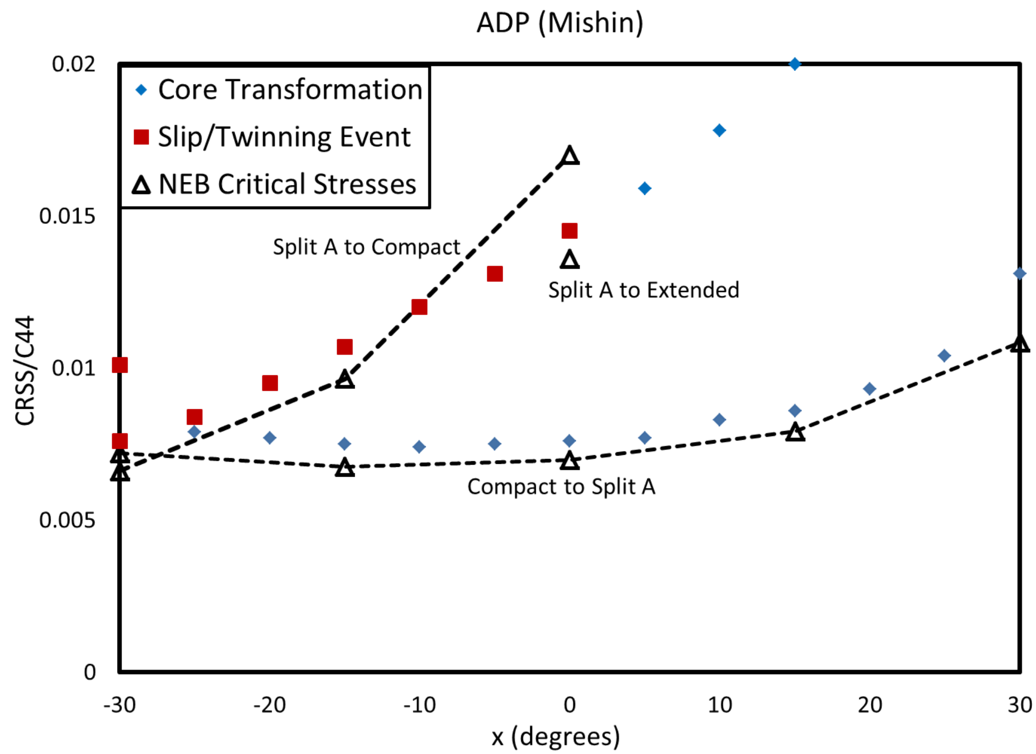
- Dislocation starts as a compact core at a C position
- First motion depends on if critical stress for $C \rightarrow S_A$ or $C \rightarrow S_B$ is lower:
- If $C \rightarrow S_B$ is lower
  - (-101) slip will occur when $C \rightarrow S_B$ and $S_B \rightarrow C$ are activated
- If $C \rightarrow S_A$ is lower
  - Dislocation will transform by shifting to S_A along the (0-11) plane
  - After transforming, only $S_A \rightarrow C$ possible along slip pathway
  - (-1-12) slip occurs if $S_A \rightarrow C$ is activated or bypassed





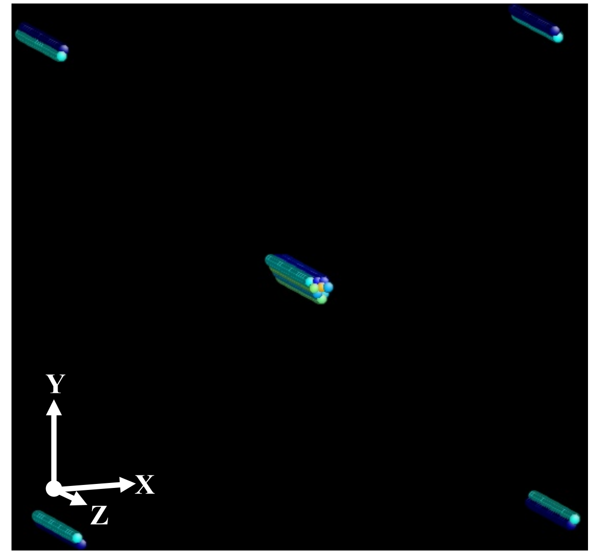
Barrier Dependent CRSS

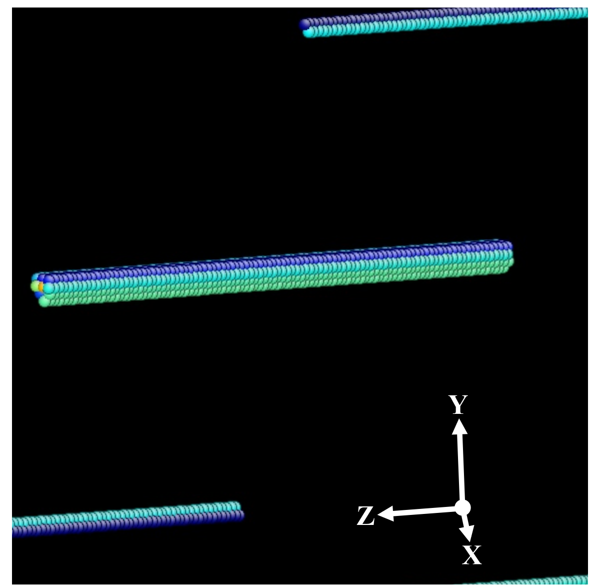
- Transformation and slip predicted by barrier critical stresses
- Barrier associated with CRSS changes with orientation
- Different critical barrier for (-101) and (-1-12) slip
- Model for slip at 0 K cannot assume only one critical barrier



Larger Simulations

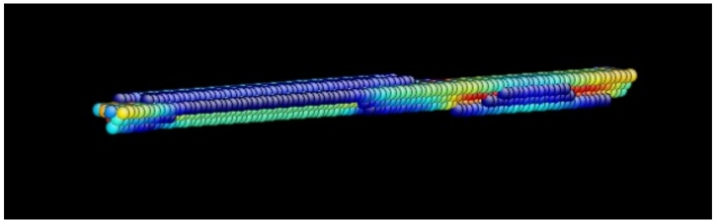
- Systems of roughly 208 X 208 X 286 Å created containing a single screw dislocation
- Surfaces in x- and y-directions free, z-direction periodic
- Shear stress added to system by adding a force in the z-direction to atoms in regions near the y surfaces
- System is updated dynamically with NVT integration
- Force increased incrementally until dislocation moves

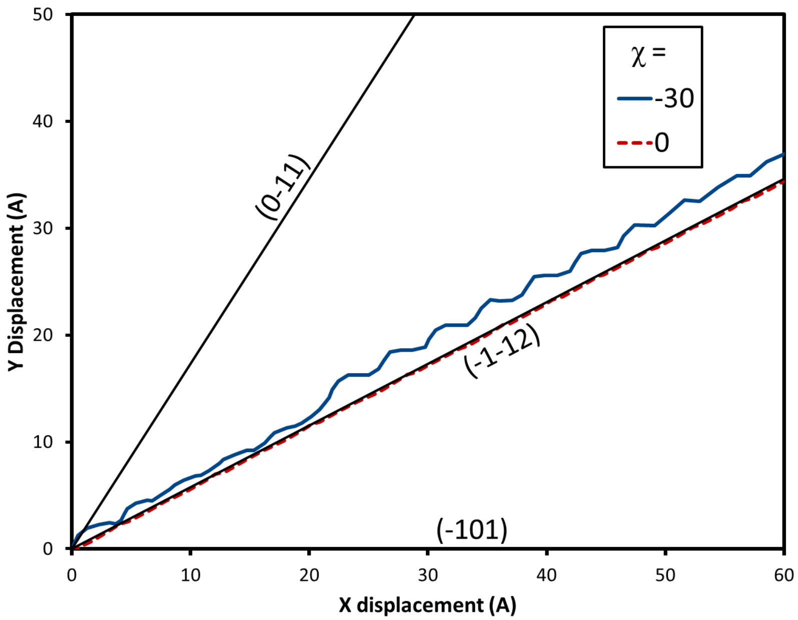


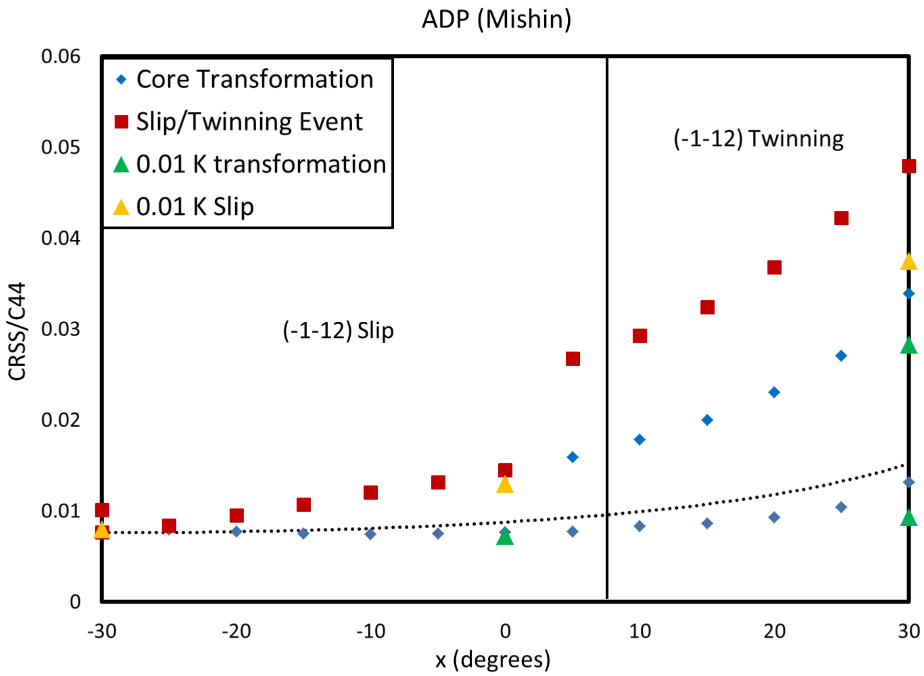


High Stress, 0.01 K Simulations

- Split core transformation observed
- Observed events match with thin simulations
- Alternating {110} motion for χ = -30°
  - Zero stress pathway S_A-C-S_B-C-S_A
- Motion exactly follows (-1-12) for χ = 0°
  - Extended core pathway and short kink
- Twinning observed for χ = 30°

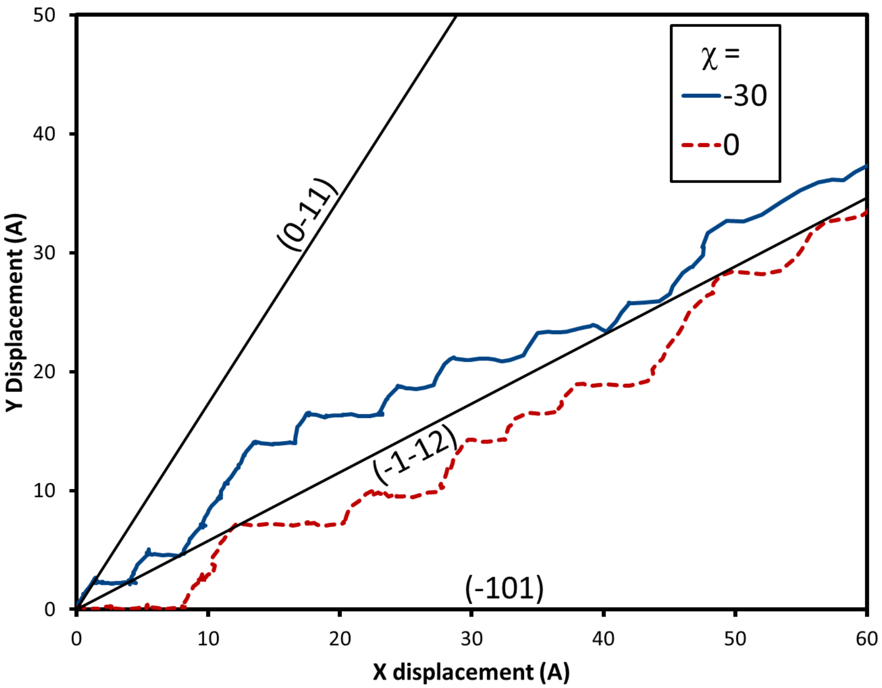


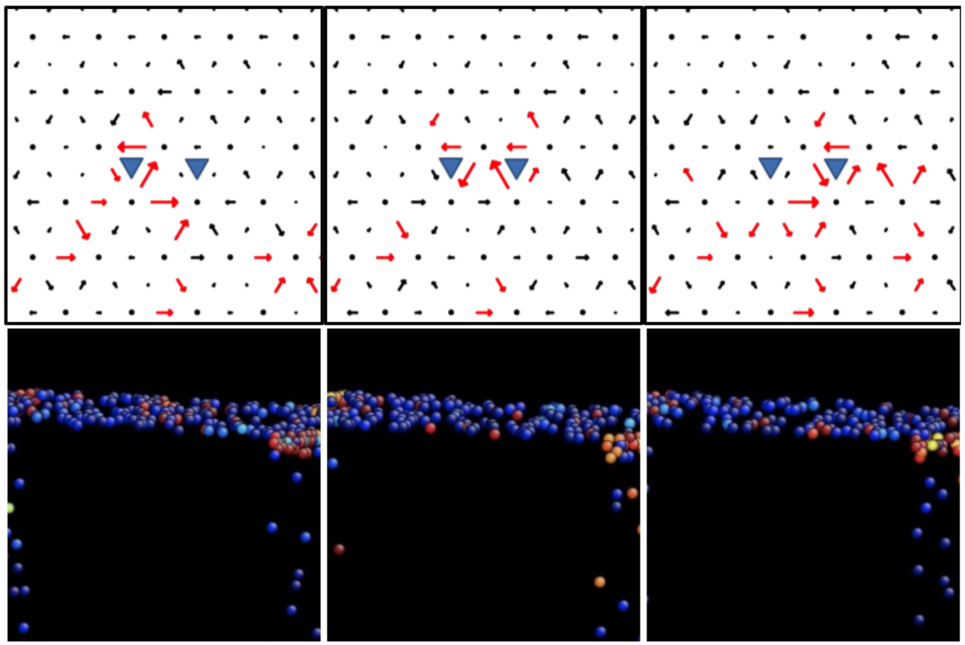




Low Stress, 300 K Simulations

- Split core is metastable state
- Nearly equal number of (0-11) and (-101) glide steps resulting in a cumulative (-1-12) slip
- No slip observed for χ = 30°up to 1 GPa shear stress





Conclusions

- Complex CRSS behavior due to multiple stress dependent barriers along slip pathway.
- {112} slip is the result of {110} motion on 2 different planes through multiple compact and split core positions.
- Activation enthalpy for moving compact to split along the (0-11) plane is smaller than a similar motion along the (-101) plane even though the resolved shear stress is greater along the (-101) plane. This counter-intuitive behavior is due to the stability of the split core structure.
- At finite temperatures, kink motion follows the same low-energy paths between split core configurations.
- Similar calculations have been done for bcc Iron using a potential for which the split core structure is unstable. {110} slip is observed, and the fitting of a single crystal yield law is in progress.