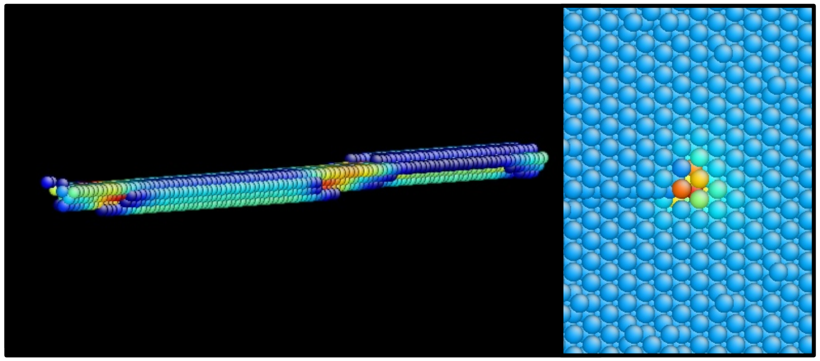
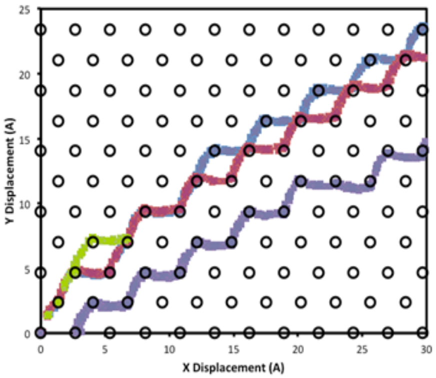
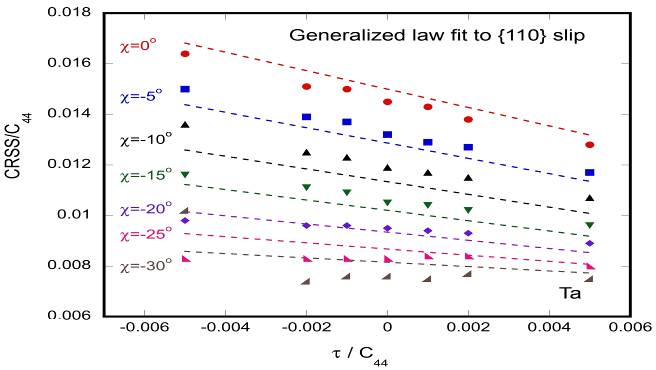
SAND2012-9262P

Exceptional service in the national interest

Sandia
National
Laboratories







PPM: Nanoscale Origins of Plasticity in Ta

Jon Zimmerman, Chris Weinberger, Lucas Hale, Hojun Lim, Garritt Tucker
Laura Smith, Diana Farkas (Virginia Tech)
Ping Lu, Khalid Hattar, John Sullivan

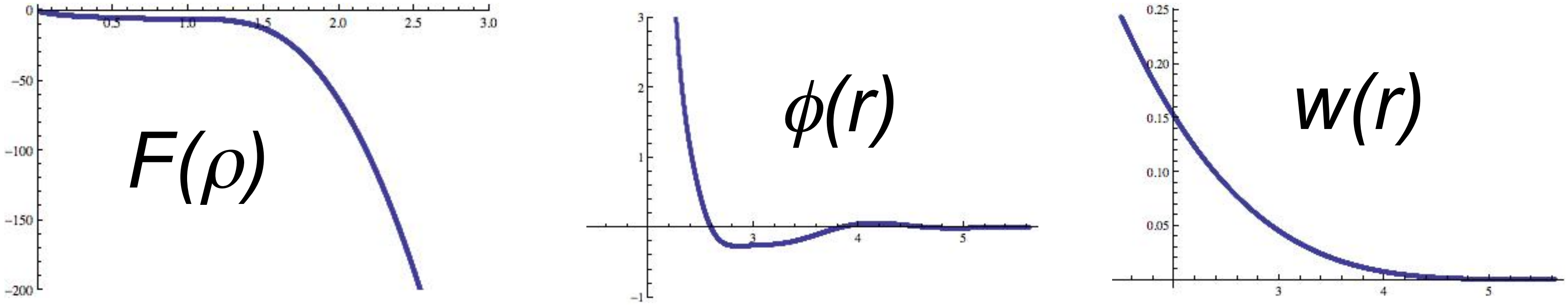
Motivation

- Gain a fundamental understanding on the atomic-level mechanisms and dominant defects relevant to incipient plastic deformation and ductile fracture of Ta.
- Early experiments in PPM did not conclusively show the traditional picture of void nucleation, growth and coalescence that characterizes FCC metals, but did show a lot of dislocation activity.
- Approach:
    - Identify "best" inter-atomic potentials for modeling dislocations in Ta
    - Perform atomic-level simulations of screw dislocation behavior to determine slip paths and systems
    - Use simulation results to quantify stress-dependent slip (Peirels) barrier and parameterize a single crystal yield law for use in mesoscale simulations
    - Perform simulations of nanocrystalline Ta to identify non-prescribed defects and deformation mechanisms and correlate with loading rate

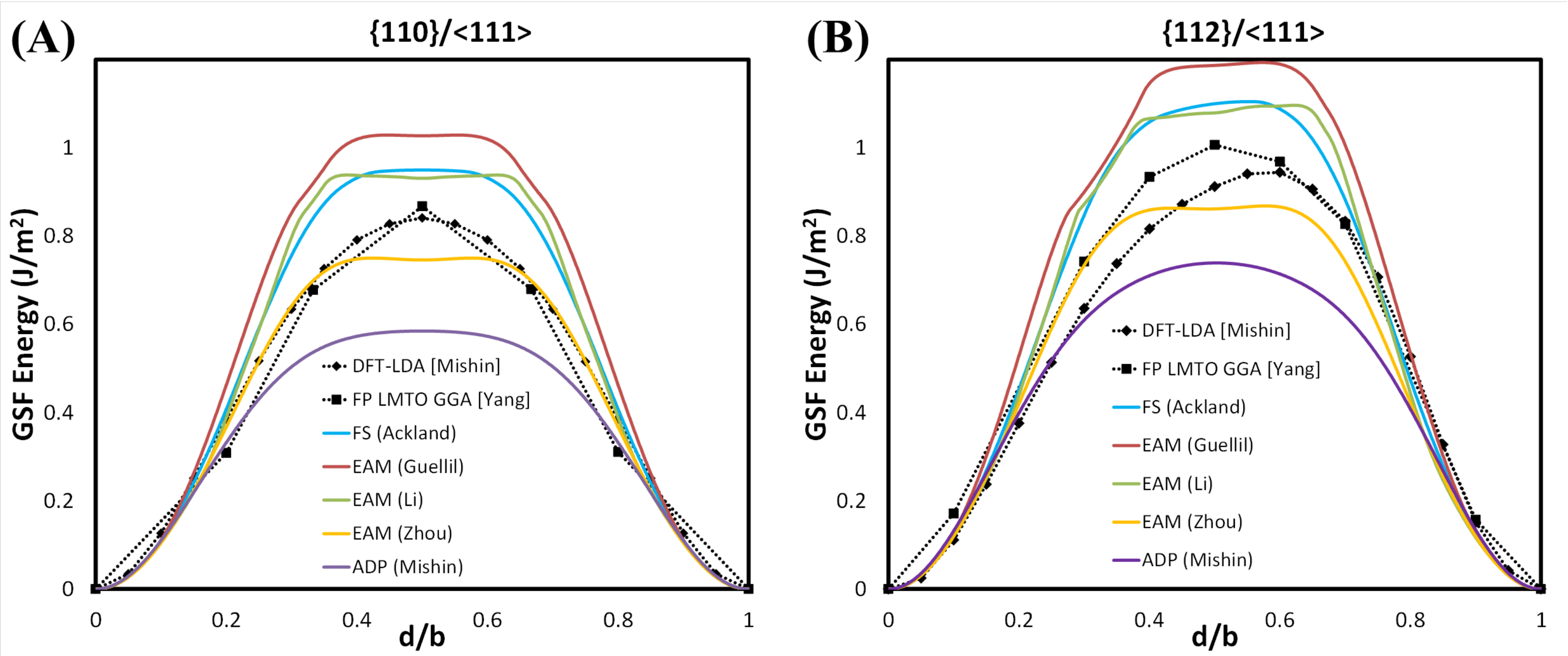
Interatomic Potentials for Ta

- Identified several inter-atomic potentials for Ta and evaluated them regarding relevant mechanical properties (e.g. elastic constants, stacking fault curve).
- Most promising:
  - Angular Dependent Potential (ADP) by Mishin and Lozovoi
  - Quantum-EAM (qEAM) by Strachan et al.
  - Force-matched EAM potential by Li et al.
  - Model Generalized Pseudopotential Theory (MGPT) by Moriarty et al.
- Performed Mathematica-based verification of new ADP-Ta tables provided by Yuri Mishin.
- ADP implemented into LAMMPS and verified using calculations of surface energies, vacancy formation energy, and cohesive energies for FCC, HCP and DC phases.

Interatomic Potentials for Ta



Above: Embedding function, pair potential, and quadrapole function of the ADP
Below: Generalized Stacking Fault curves for various Ta interatomic potentials



Dislocation Behavior in Ta

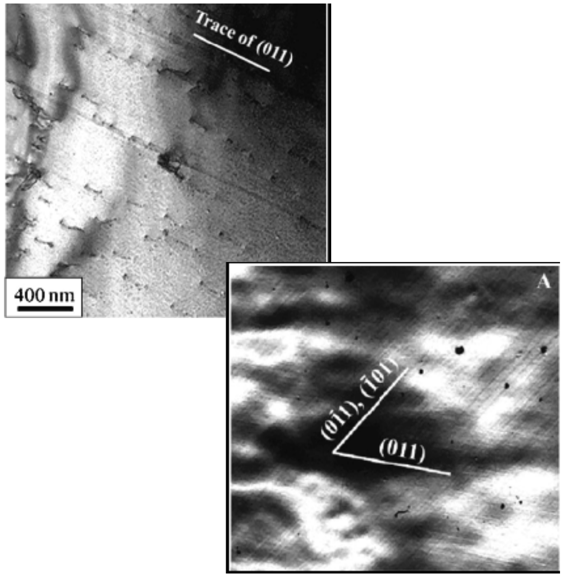
- Plasticity in bcc metals primarily governed by screw dislocations
  - High lattice resistance
  - Stress dependent Peierls Stress
  - Multiple different slip planes: {110}, {112}, {123}, wavy

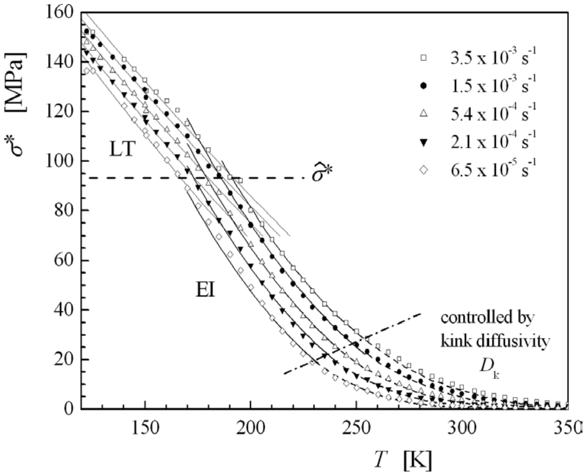
- Use atomic simulations to measure the critical resolved shear stress (CRSS) to observe motion of a single dislocation
  - Thin 0 K systems to investigate core structure and slip pathway
  - Large dynamic systems to study kinking and temperature effects

BCC Slip Plane Review Paper

(Weinberger, Boyce and Battaile)

- Two important questions
  - What are the macroscopic slip planes (crystal rotations)
  - What are the fundamental slip planes (planes kinks nucleate on)
- Currently covers the BCC transition metals
  - Iron, Molybdenum, Tungsten, Tantalum, Vanadium, Niobium
- Three sections:
  - Direct experimental observations: Slip trace analysis (optical, TEM, SEM), Laue X-ray, indentation, etch pit…
  - Inference from flow stress measurements: Use kink-pair theory to determine kink formation energy -> obtain slip planes
  - Atomistic simulations





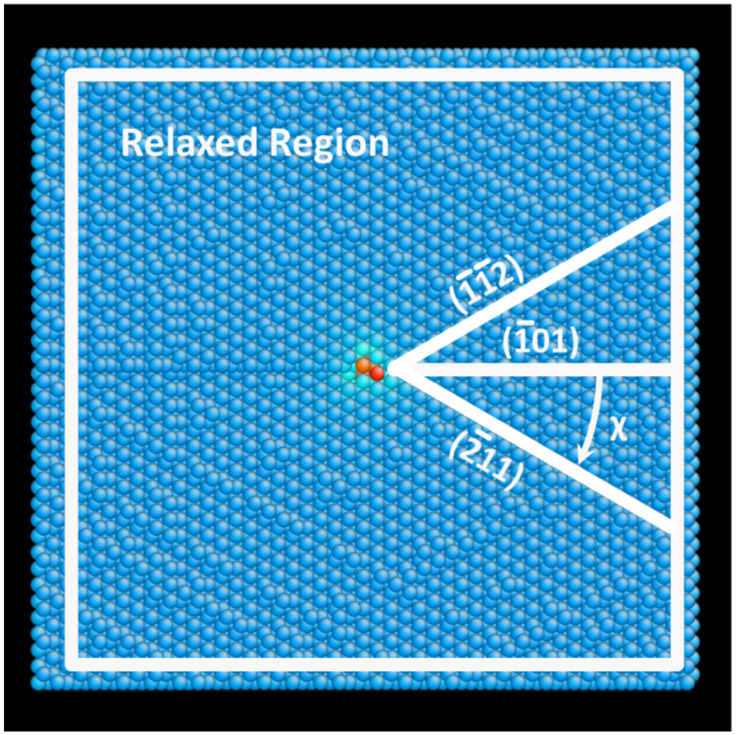
BCC Slip Plane Review Paper

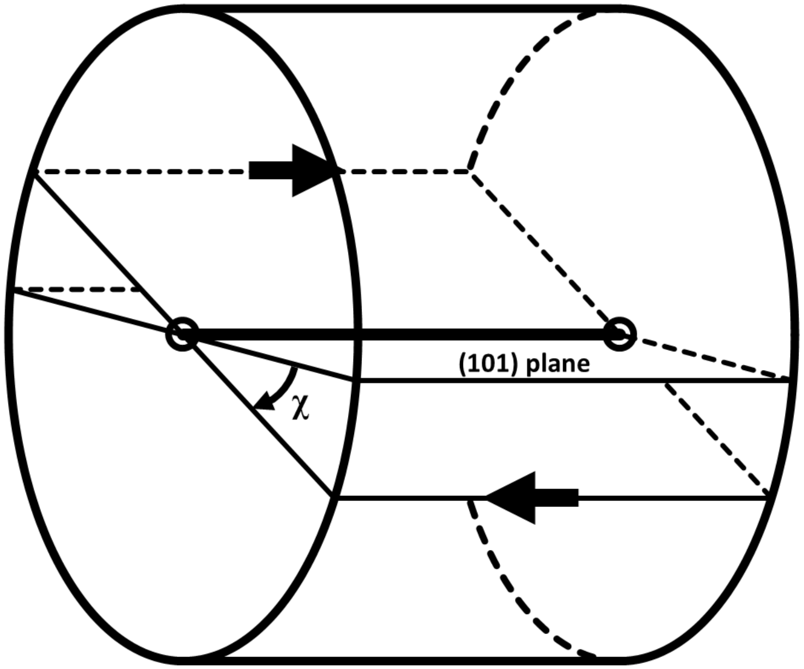
- Direct Experimental Observations:
  - At 4.2 K, slip clearly occurs on {110} planes, some {112} slip observed.
  - At higher temperatures, slip appears on planes near MRSS planes
  - Suggests slip occurs fundamentally on {110} planes with net slip on MRSS planes.
  - Mechanical Twinning sometimes occurs 77K and below.
- Flow Stress Measurements:
  - The work of Seeger has shown that kinks nucleate on {112} planes.
- Atomistics:
  - All interatomic models to date show that kinks form on {110} planes in all BCC transition metals (including Tantalum)
  - Most interatomic models for Ta at 0K show net slip on {112} planes

The literature is inconclusive with regards to both the macroscopic and fundamental slip planes.

Thin Simulation Design

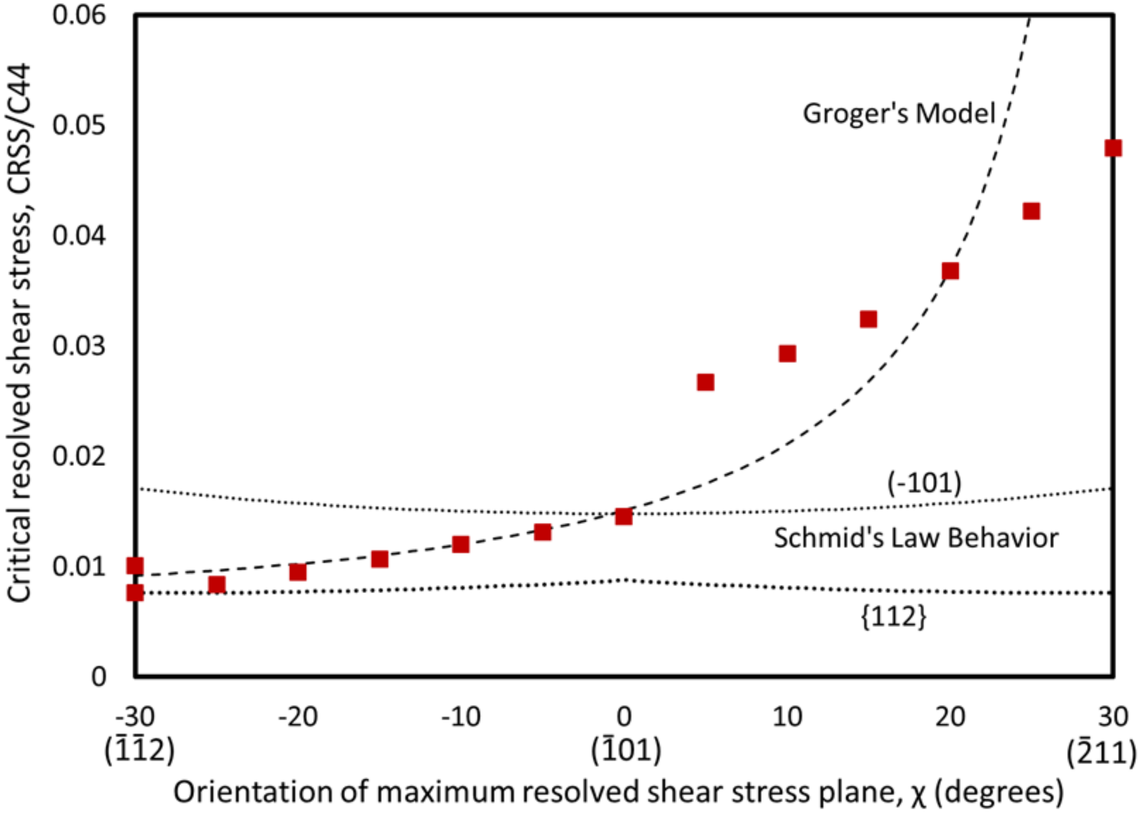
- Single dislocation in 200 Å X 200 Å X 22.9 Å system
- Strain applied according to anisotropic elasticity solution
- Middle of system relaxed with a force minimization





Critical Resolved Shear Stress Plot

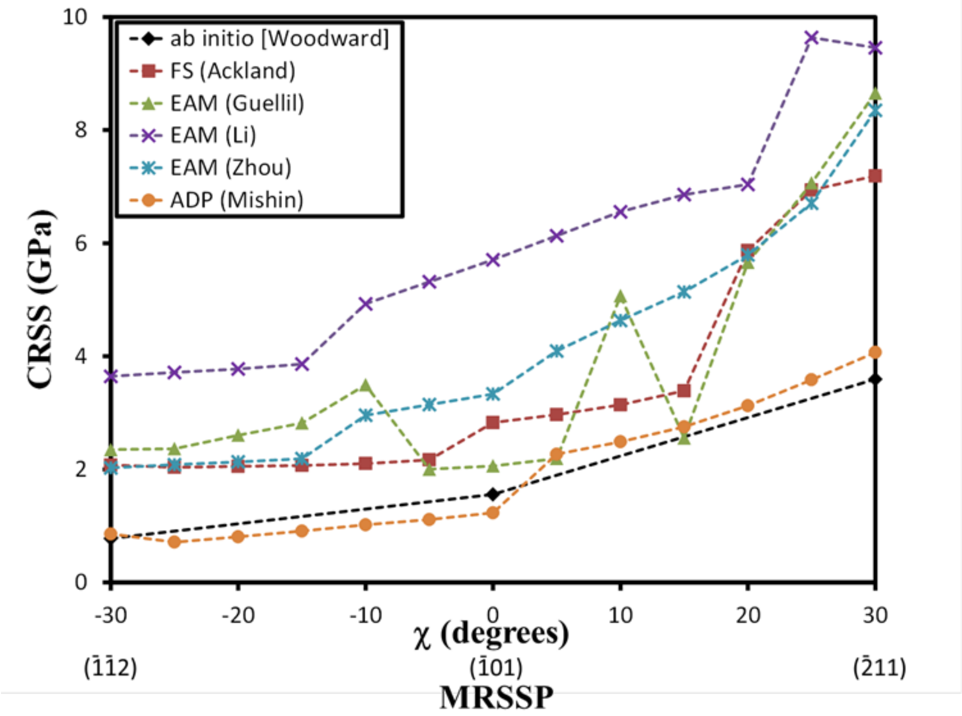
- Need to understand/fit correct behavior
  - Deviation from Schmid’s law →Groger’s model
  - Twinning/anti-twinning {112} asymmetry
  - (-1-12) slip instead of expected (-101) slip
  - Discontinuities in CRSS values with changing stress



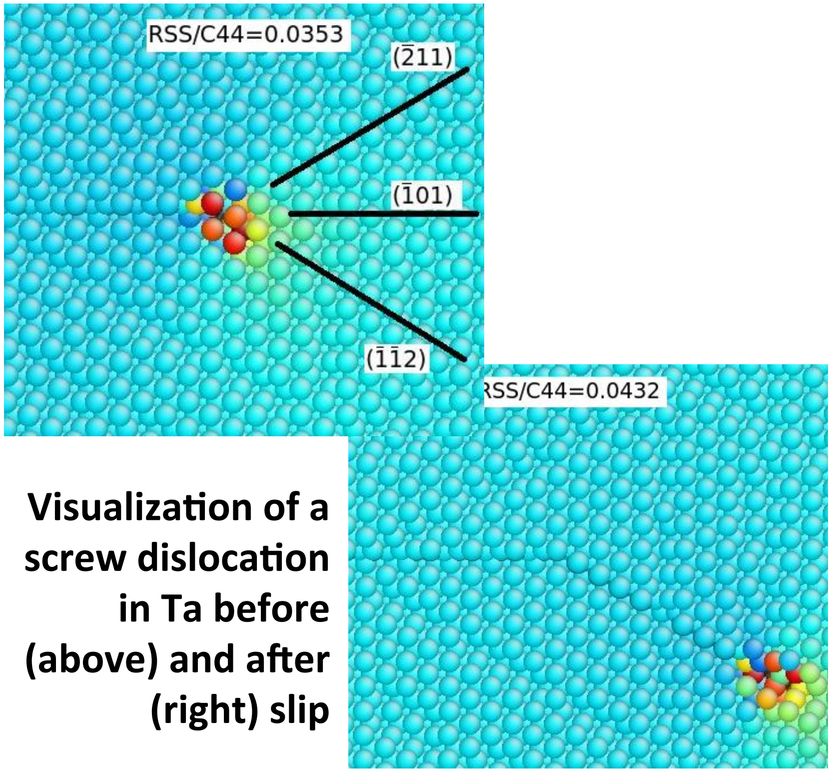
[1] R. Groger, V. Racherla, J. L. Bassani, and V. Vitek, Acta Materialia **56,** 5412 (2008).

Variation of CRSS among Potentials

- All potentials show {112} slip, only Guellil shows {110} as well
- ADP results in behavior closest to ab-initio predictions of CRSS



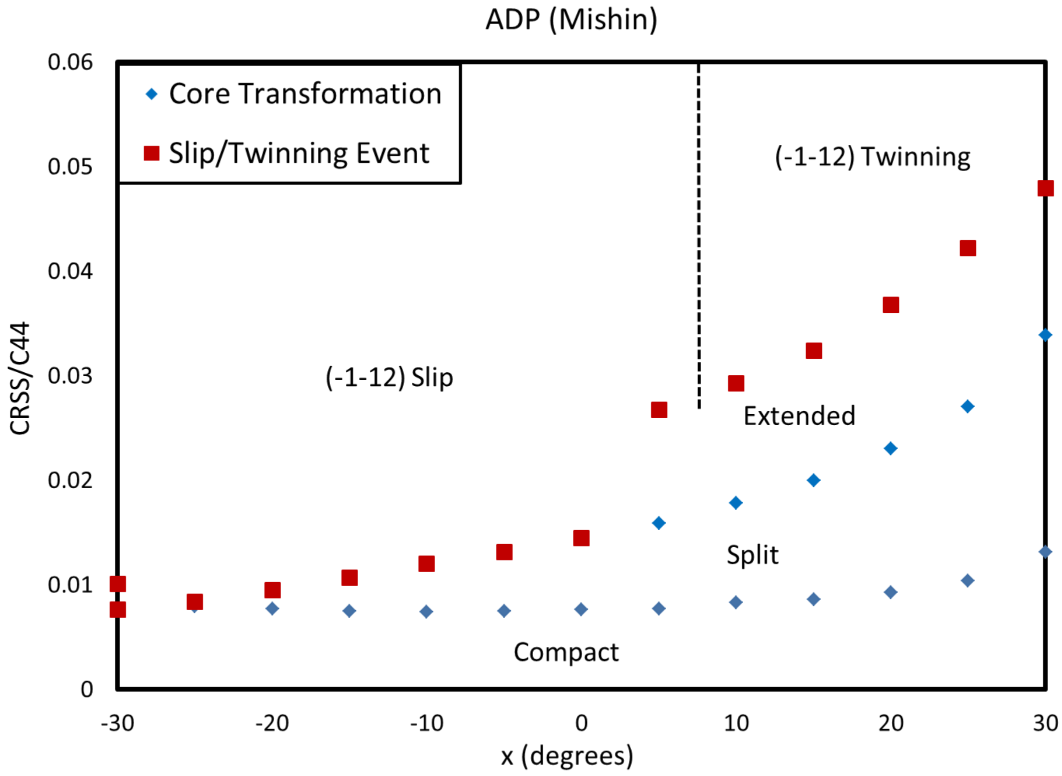
CRSS values (as a function of orientation with respect to the (-101) plane) comparing Ta potentials with ab-initio calculation

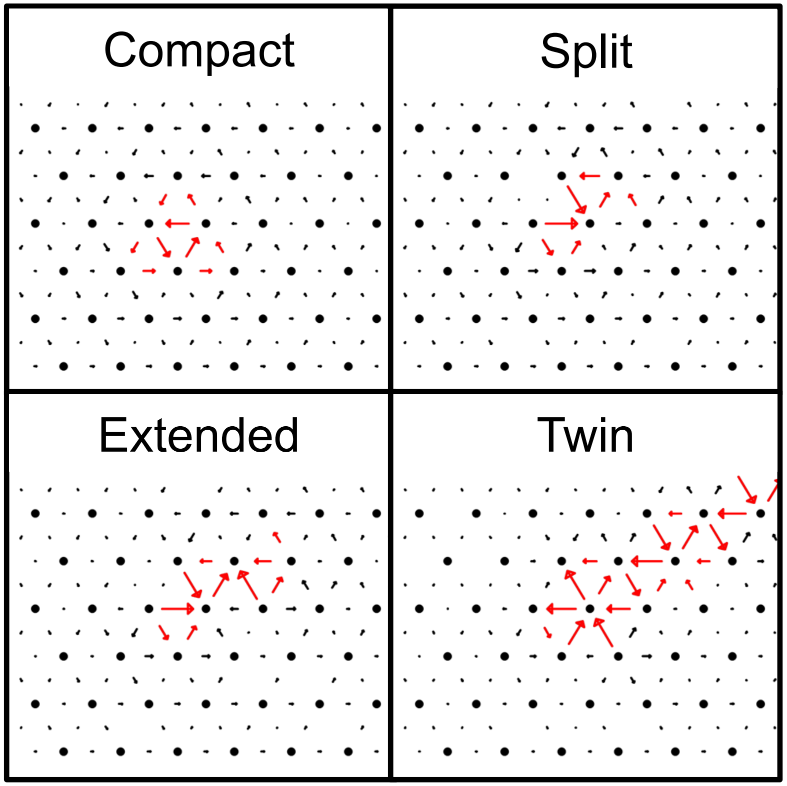


Visualization of a screw dislocation in Ta before (above) and after (right) slip

Dislocation Core Transformations

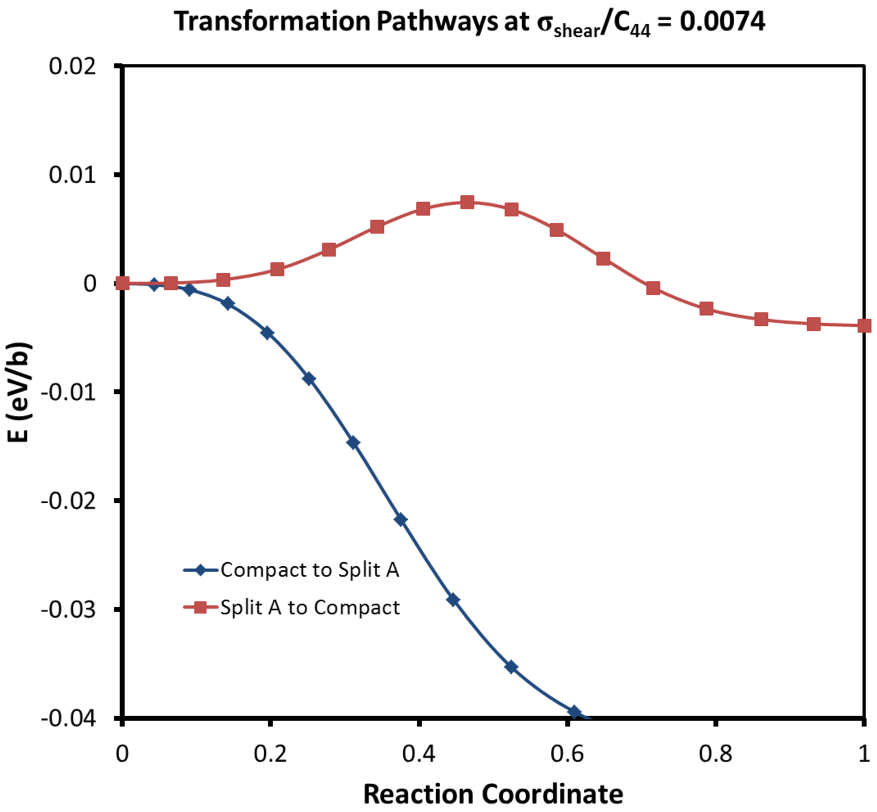
- CRSS discontinuities related to changing core structures and critical events
- Similar behavior and cores observed with 4 EAM potentials

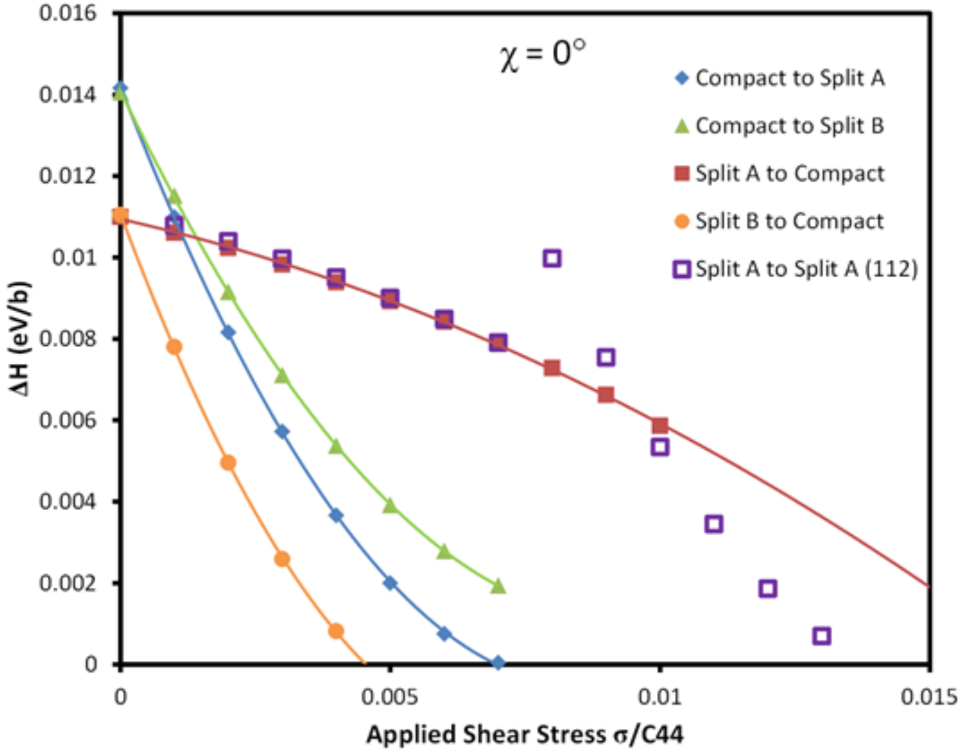




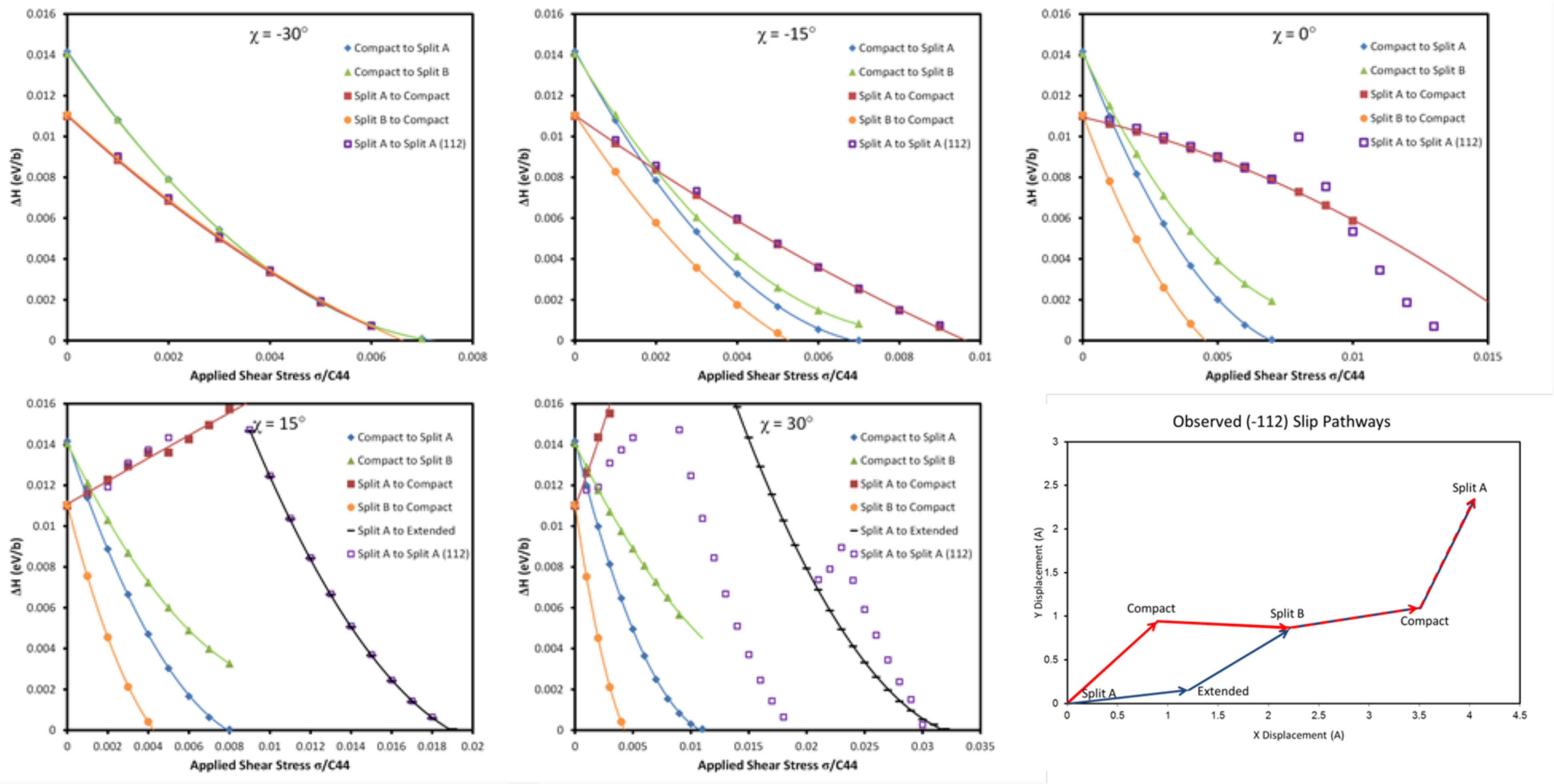
Stress Dependent Barriers

- 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 → Split A) < (Compact → Split B)!


Transformation Pathways at σ_{shear}/C_{44} = 0.0074

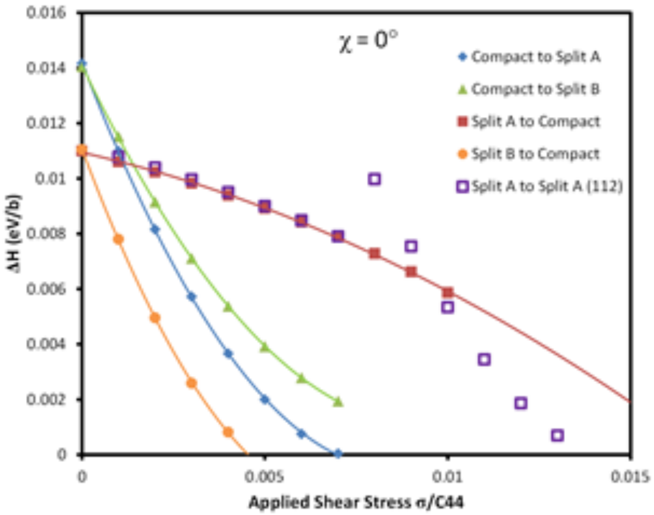


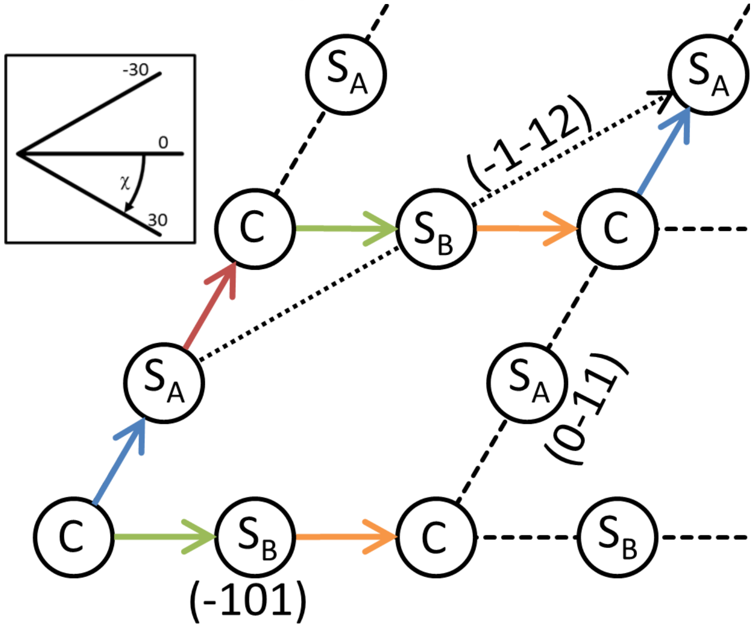
Activation Enthalpies



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

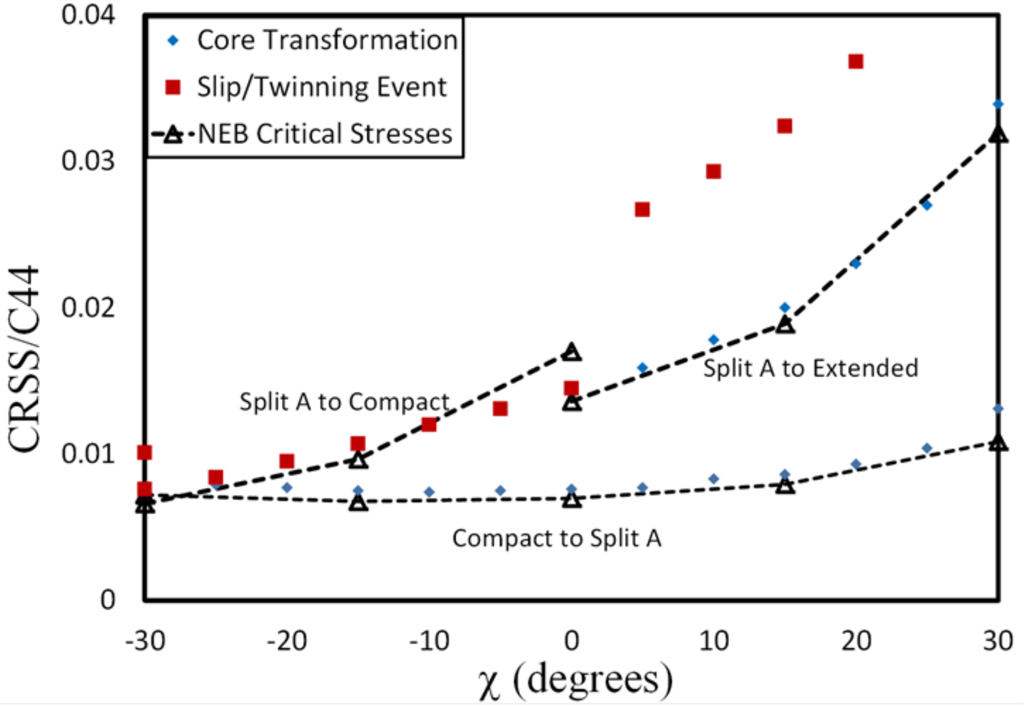
- Dislocation starts at a compact, C
- First motion depends on if critical stress for $C \rightarrow S_A$ or $C \rightarrow S_B$ is lower:
- If $C \rightarrow S_B$ is lower
  - (-101) slip will occur when $C \rightarrow S_B$ and $S_B \rightarrow C$ are activated
- If $C \rightarrow S_A$ is lower
  - 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





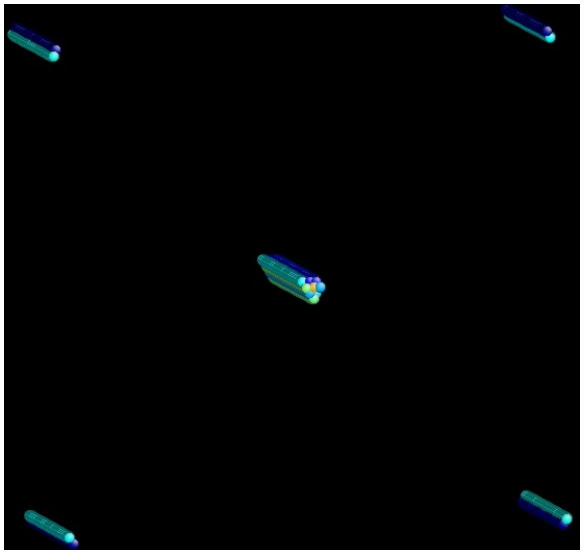
Barrier Dependent CRSS

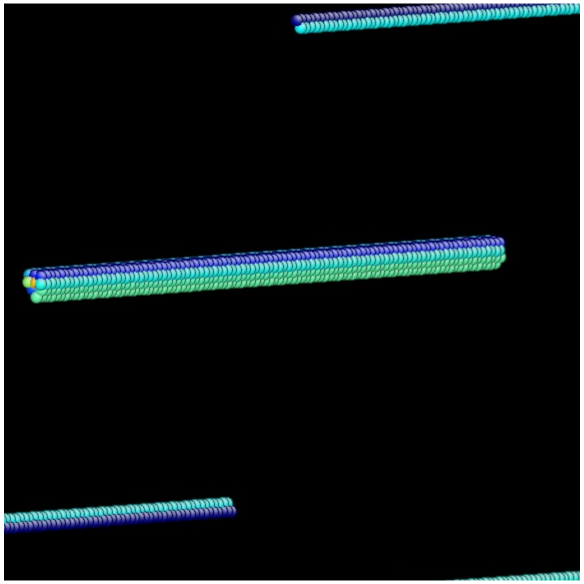
- Transformation and slip predicted by barrier critical stresses
- Barrier associated with CRSS changes with orientation
- Different critical barrier for (-101) and (-1-12) slip
- Model for slip at 0 K cannot assume only one critical barrier



Larger Simulations

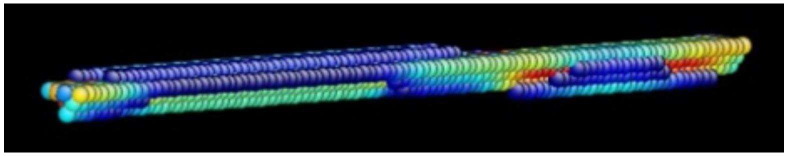
- Systems of roughly 208 Å x 208 Å x 286 Å created containing a single screw dislocation
- Surfaces in x- and y-directions free, z-direction periodic
- Shear stress added to system by adding a force in the z-direction to atoms in regions near the y surfaces
- System is updated dynamically with NVT integration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

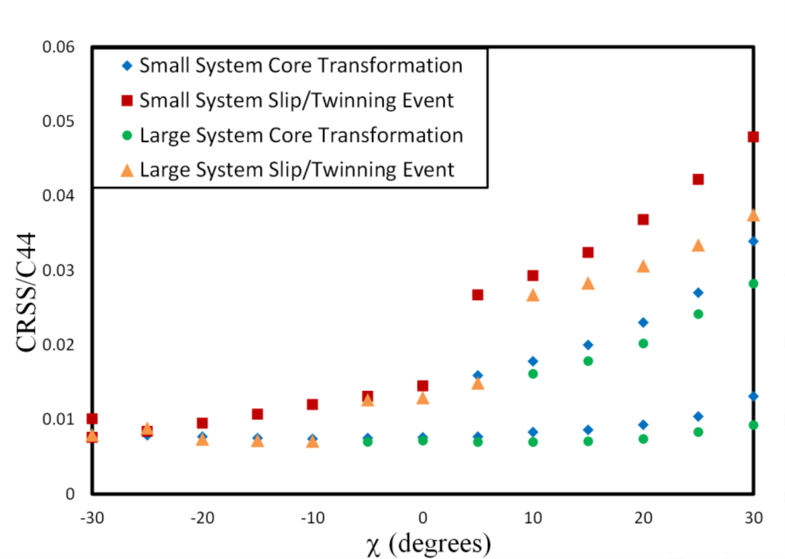


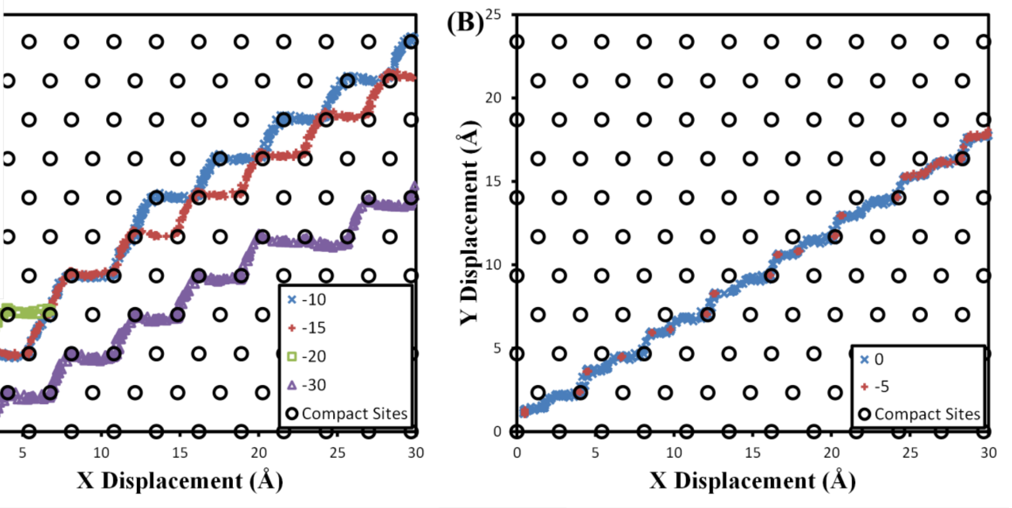


Low Temperature, High Stress

- Observed behaviors consistent with CRSS results
- Alternating {110} glide for $\chi \leq -10°$ (approximate {112})
- Exact {112} slip for $-5° \leq \chi \leq 5°$ (Extended core pathway)
- Twinning for $\chi \geq 10°$

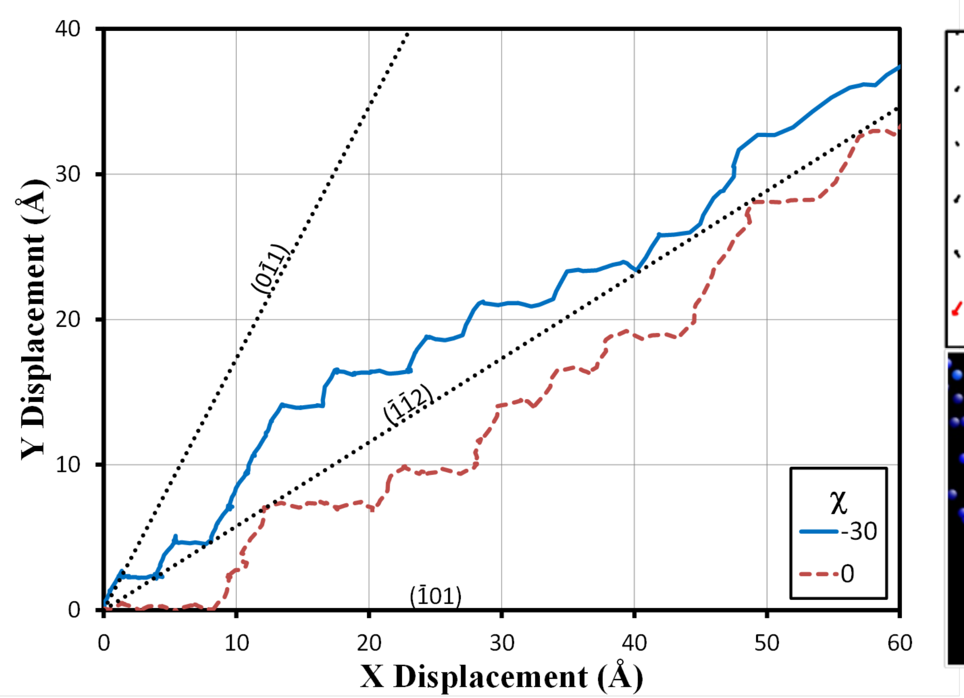


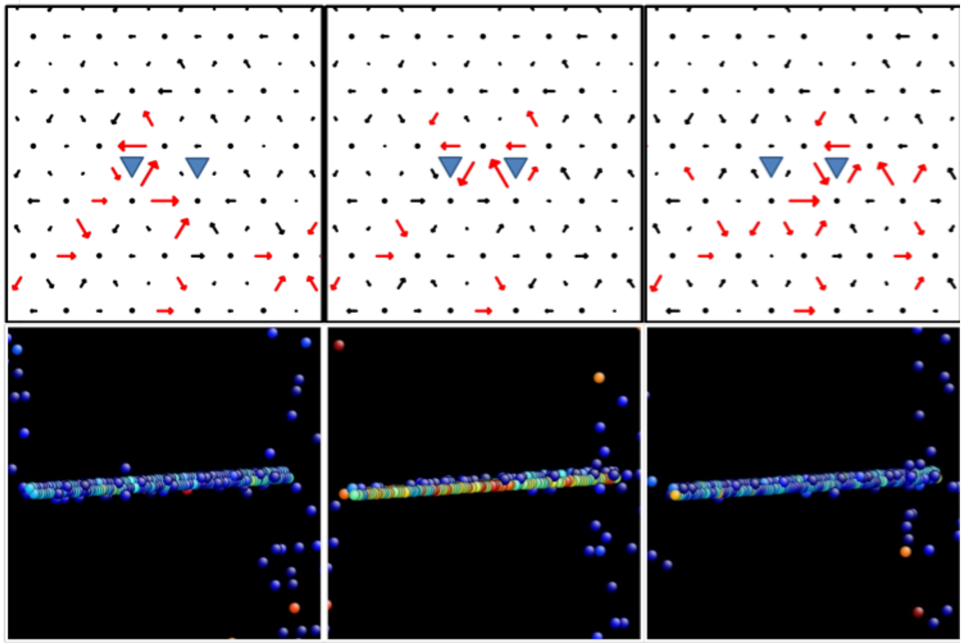




High Temperature, Low Stress

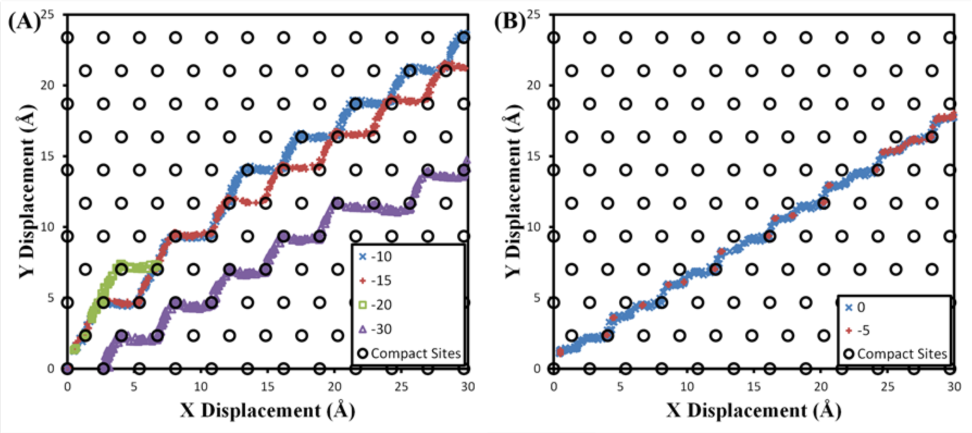
- Compact to split barriers largest
- Random activation of {110} planes
- Cumulative {112} slip for χ = -30°, 0°
- No slip for χ = 30° up to 1 GPa shear stress

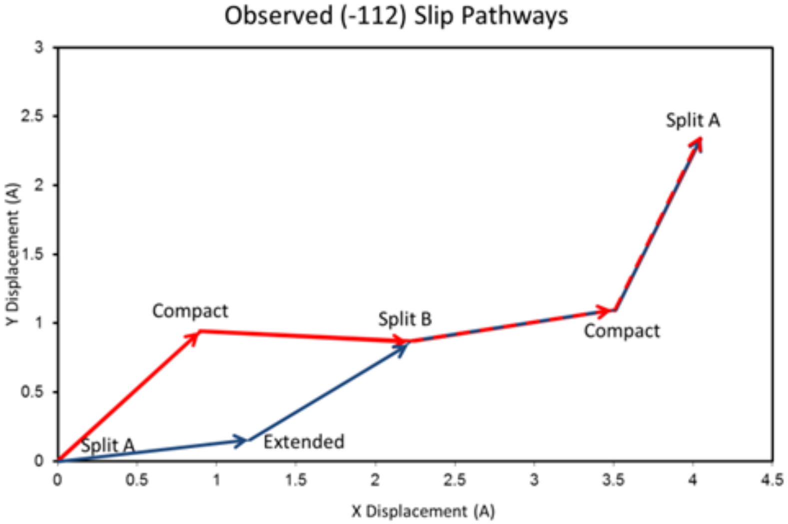




Why (-1-12)?

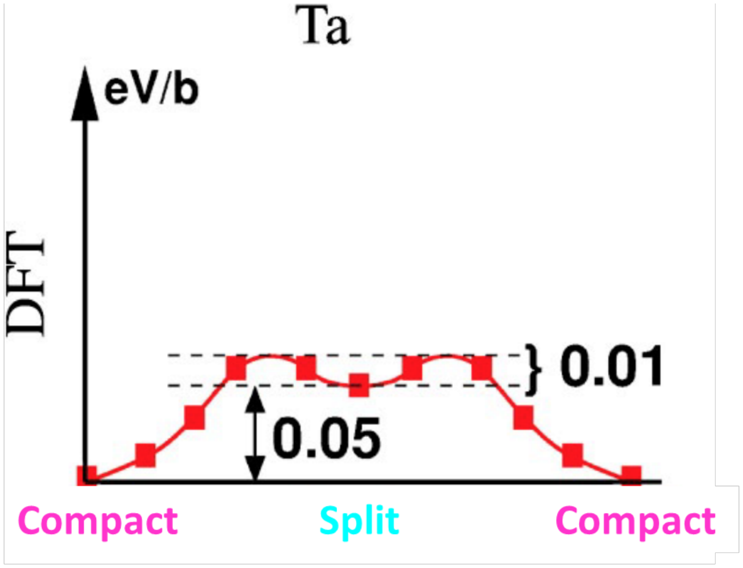
- Why does dislocation glide alternate {110} planes as opposed to remaining on one?




Observed (-112) Slip Pathways

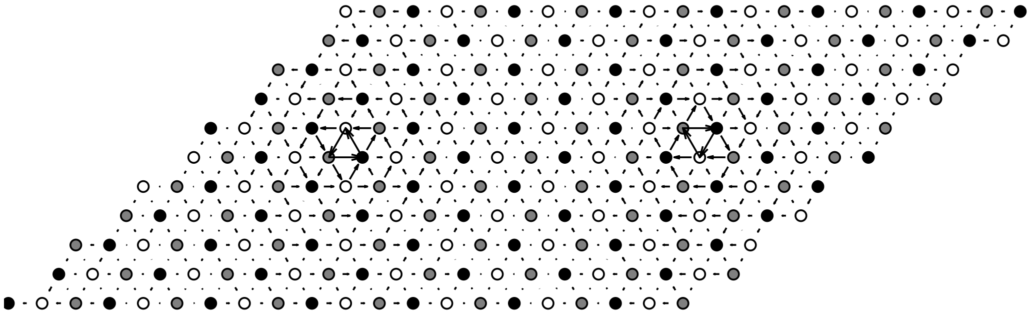
  - Finite system makes actual driving force felt by dislocation different than applied force (not likely critical here)
  - Similar activation enthalpies on both planes at low stresses allows for comparable thermal activation rates
  - Dislocation structure drives the planar switching (extended core)
  - Dislocation motion from a compact position depends on motion to that position: pathway of least resistance

DFT Simulations of Slip in Ta



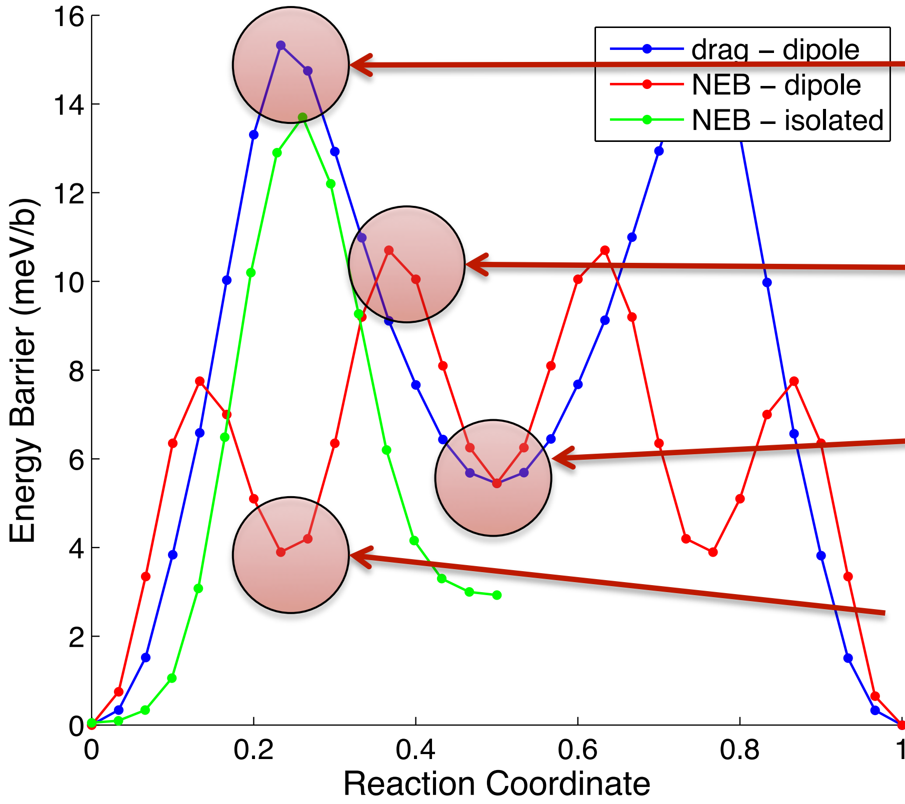
- Experiments: {110} slip
- Atomistics: {112} slip involving metastable split core
- What about DFT?
  - Segall et al.: metastable hard core and {112} slip
  - Woodward and Rao: {112} slip
  - Li et al.: {110} slip

Goal: Determine the slip planes and metastable core structures of Tantalum using DFT dipole approach using different exchange-correlation functions (LDA/PBE).



231 atom dipole simulation shows compact core structure
Homogeneous strain to obtain slip
Use NEB/drag method to determine stable core structures

Comparison of NEB/Drag using ADP



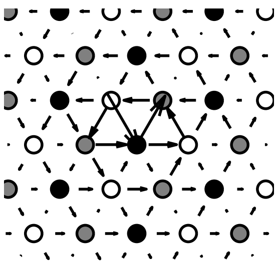
Drag method produces shapes similar to an isolated dislocation.

NEB finds lower transition states.

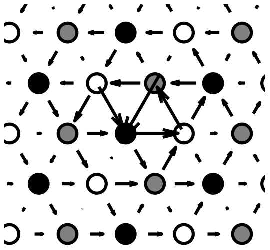
Drag & NEB find the same meta-stable hard core.

NEB finds additional metastable states.

Split Core



New Core



Conclusion: Drag method is suitable for determining the Peierls potential shape In small dipole simulations

Path Forward: Conduct drag simulations on DFT LDA/PBE dislocation dipoles. Strain dislocation dipoles until motion is observed.

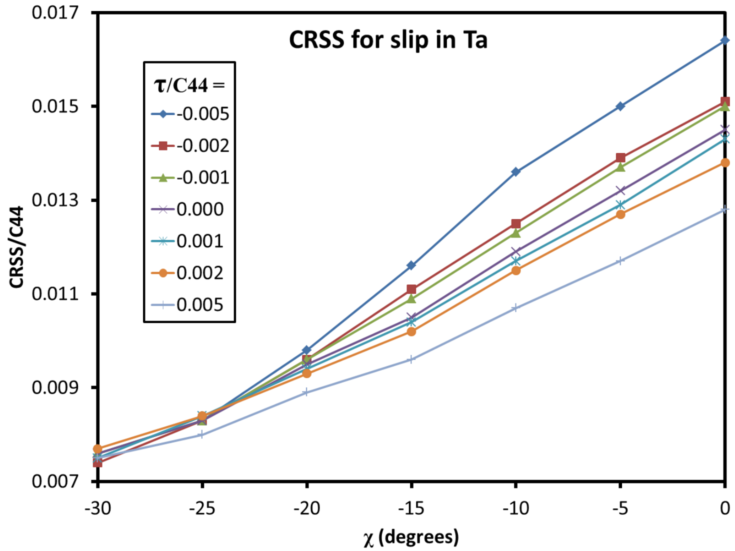
Construction of a Single-Crystal Yield Law

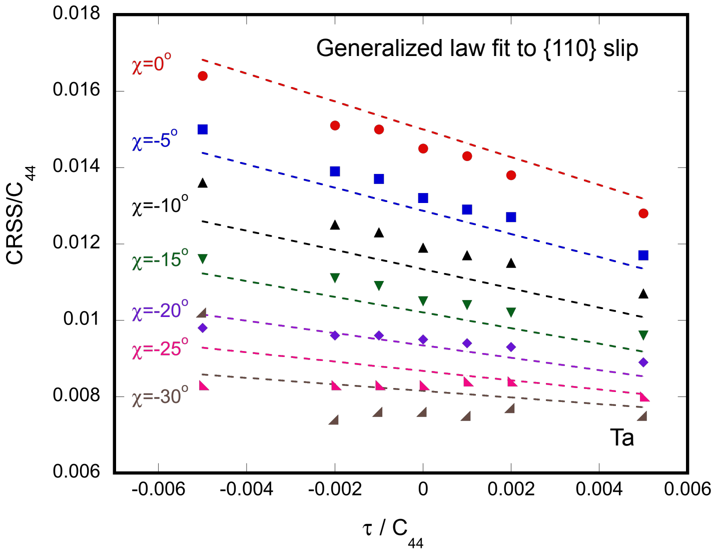
- Using atomistic simulation results quantifying critical resolved shear stress (CRSS) as a function of in-plane orientation (χ) and out-of-plane loading (τ) we have developed a linearized, generalized yield law for slip in single crystal Ta.

$$\tau_{\mathrm{cr}}^{*\alpha} = \mathbf{P}_{\mathrm{tot}}^{\alpha} : \boldsymbol{\sigma} = \mathbf{P}_{\mathrm{s}}^{\alpha} : \boldsymbol{\sigma} + \mathbf{P}_{\mathrm{ns}}^{\alpha} : \boldsymbol{\sigma}$$

Generalized Yield Laws (Linearized)

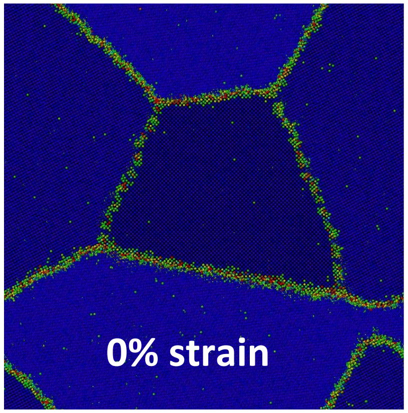
$$\mathbf{P}_{\mathrm{tot}}^{\alpha} \equiv c_0 \mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_1 \mathbf{t}^{\alpha} \otimes \mathbf{m}^{\alpha} + c_2 \mathbf{t}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_3 \mathbf{n}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_4 \mathbf{t}^{\alpha} \otimes \mathbf{t}^{\alpha} + c_5 \mathbf{m}^{\alpha} \otimes \mathbf{m}^{\alpha}$$

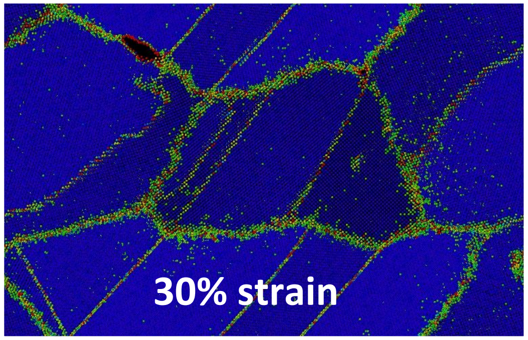


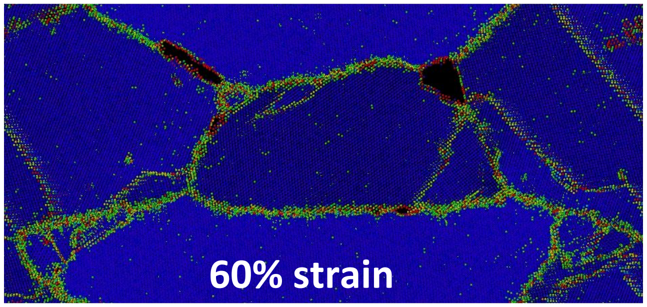


Uniaxial Tension of Nanocrystalline-Ta

- Perform room-temperature molecular dynamics (MD) simulations of uniaxial tension applied to a thin film of NC-Ta.
- Quantify how rate affects the type of defects generated and their motion in response to load.
- Apply atomistically-derived continuum metrics to characterize defects and connect their generation to locally “measured” critical stresses.

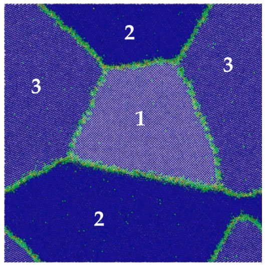




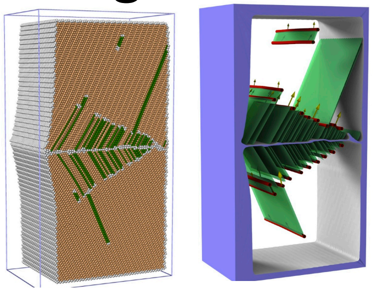


Simulation and Analysis Details

- Material model: EAM by Li *et al.* (Phys. Rev. B, 2003)
- Geometry: thin film of dimensions 34.5 nm x 34.5 nm x 7 nm
- 3 columnar grains of size 20 nm with random orientations
- Approximately 464,000 atoms
- Simulations done with LAMMPS



- Equilibration via heating to 1700K for 200 ps, then cooling to 300K for 200 ps using a Nosé-Hoover thermostat
- Uniaxial stress applied at strain rates 10^5 to 10^9 sec^{-1}
- Visualization using Ovito and ParaView

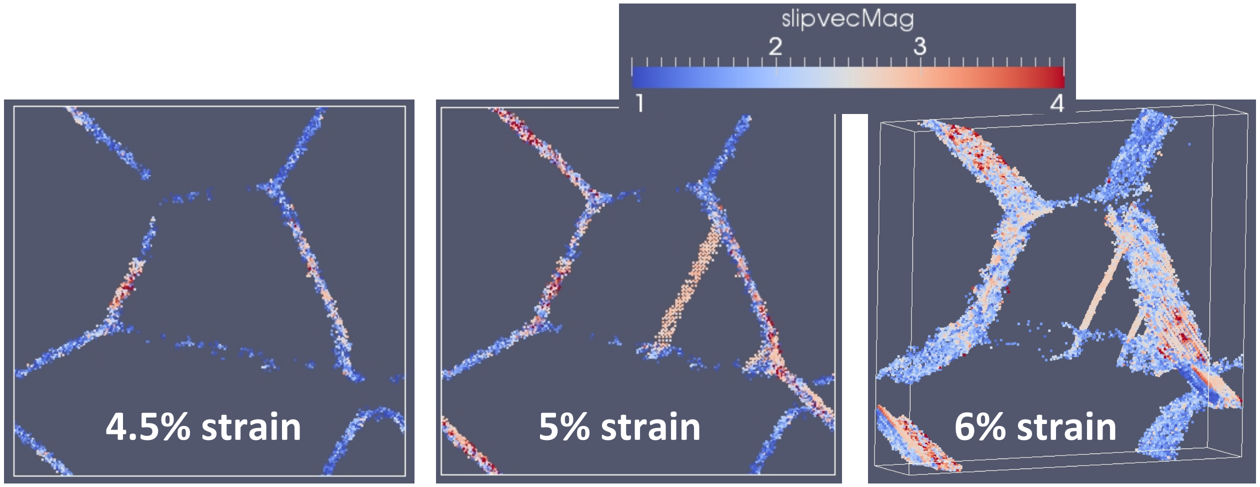


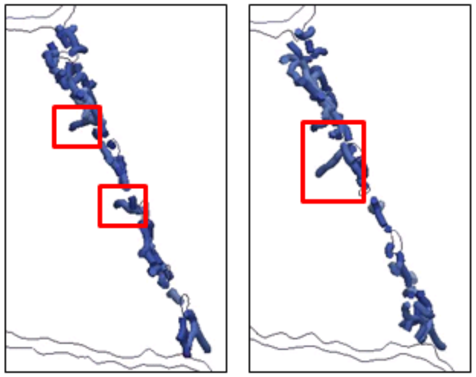
- Dislocation eXtraction Algorithm (DXA) and slip vector analysis used to identify and characterize dislocations and slip planes
- Atoms-to-Continuum (AtC) user package for LAMMPS used to evaluate local stresses

Deformation at Low Strains

$$\dot{\varepsilon} = 10^{6}\ \text{sec}^{-1}\ ,\ \varepsilon < 9\%$$

- First active mechanism is dislocation emission from grain boundaries

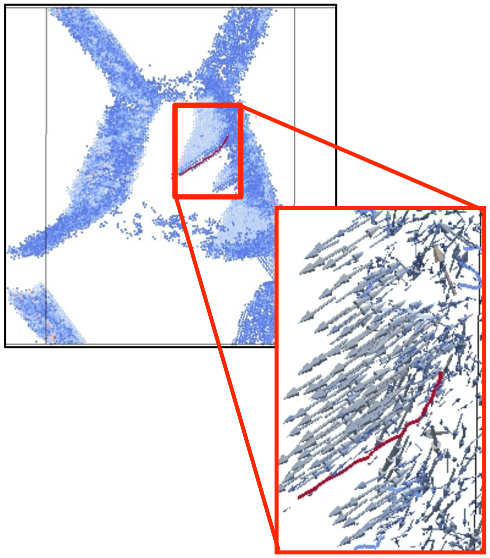




5% strain **6% strain**

$$\vec{b} = \pm\left[1.893\ 1.576\ 1.563\right]\ \text{Å} \qquad \hat{n} = \left[-0.792\ 0.455\ 0.409\right]$$

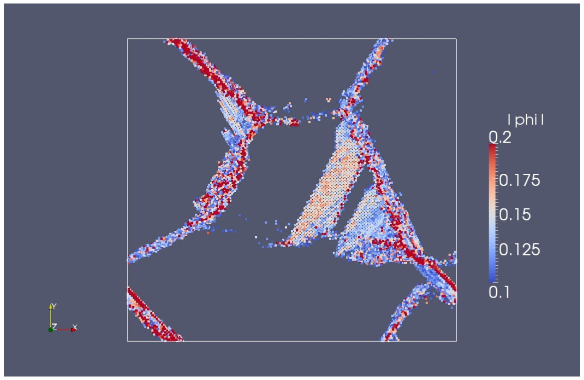
$$\left|\vec{b}\right| = 2.922\ \text{Å}\ \left(theor - 2.860\right)$$



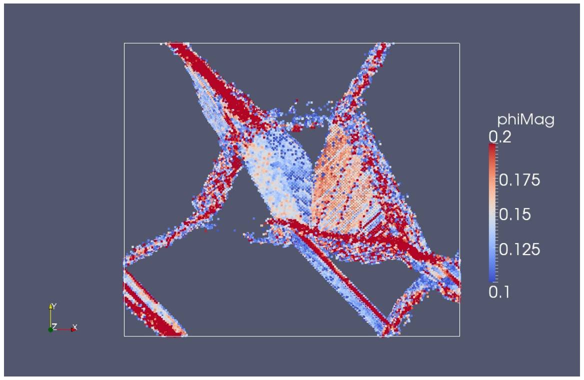
Analysis reveals initial defect is emission of a dislocation with ½<111> Burgers vector from one GB to another on a {112} plane. Combined use of DXA and slip vector analysis shows character of dislocation segment is dominantly screw.

Continuum Analysis of Atomistics

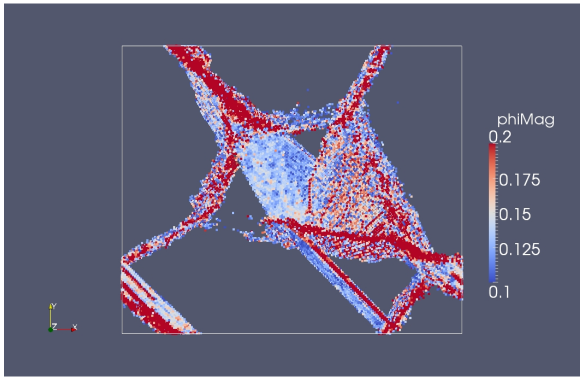
- Metrics by Zimmerman *et al*. and Tucker *et al*. are used to associate values of kinematic quantities with defects.



6% strain



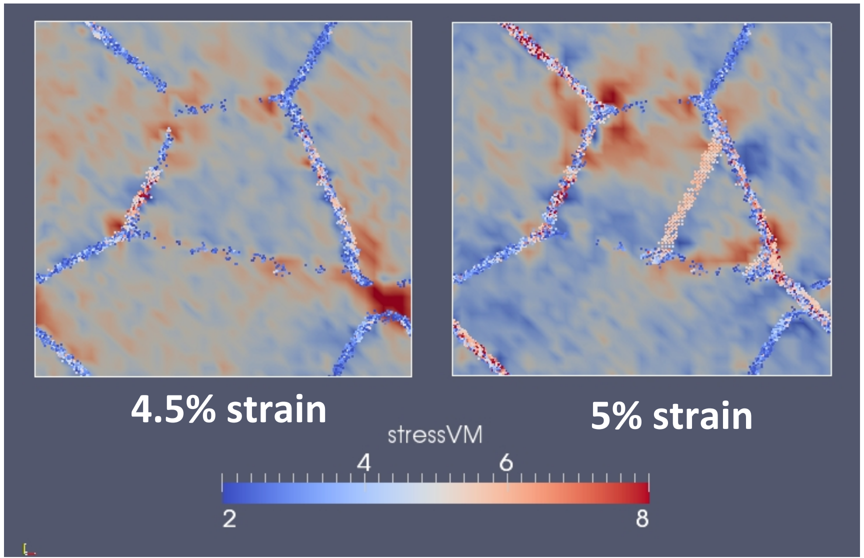
9% strain



11% strain

- Metrics by Hardy are used to correlate local evaluations of stress (resolved shear, Von Mises) with defect nucleation sites.

Stresses where first dislocations form (on GBs) are not necessarily significant. This analysis indicates ‘weak spots’ on GBs.



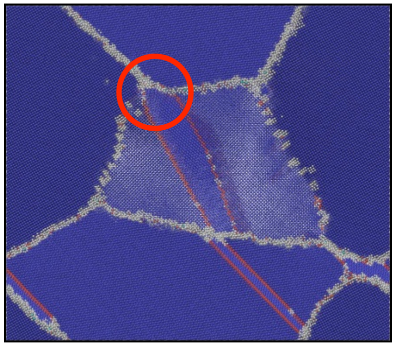
4.5% strain

5% strain

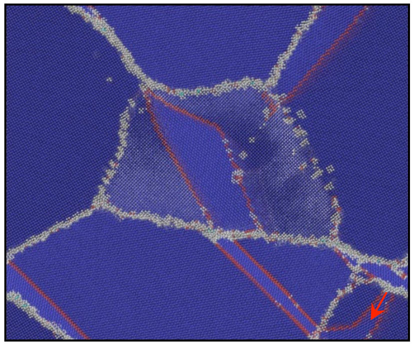
Deformation at Moderate Strains

$$\dot{\varepsilon} = 10^6 \text{ sec}^{-1}, \varepsilon \sim 9-11\%$$

- At larger strains, the formation of deformation twins occurs:

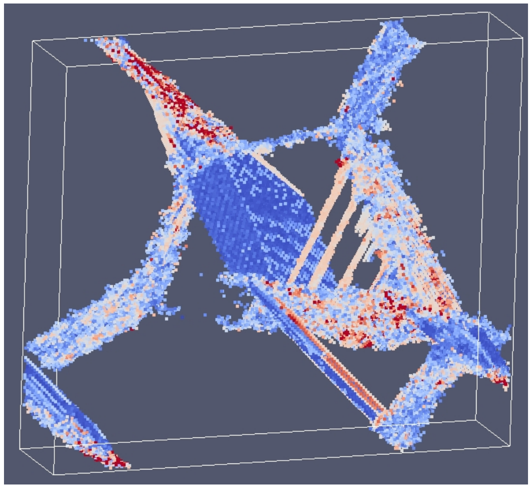


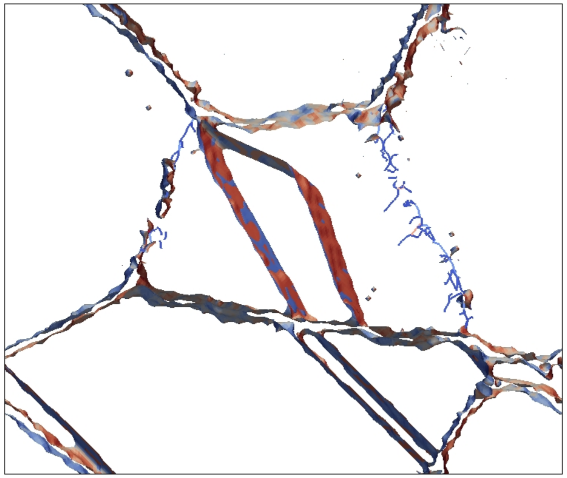
CNA showing twin formation at 9%(left) and 12% (right) strain.



Twins originate from GB junctions and expand to penetrate GBs as loading continually increases.

Slip vector and DXA analyses show that twin boundaries form on {112} planes and have ⅙<111> Burgers vector, |b| ~ 0.95 Å.

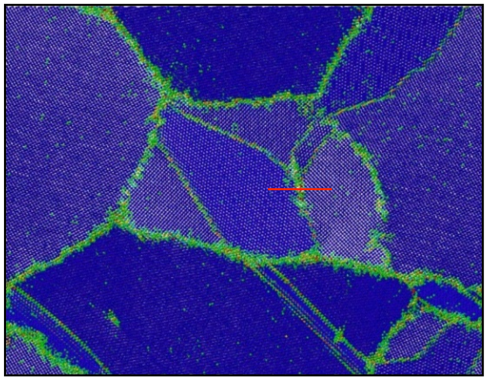




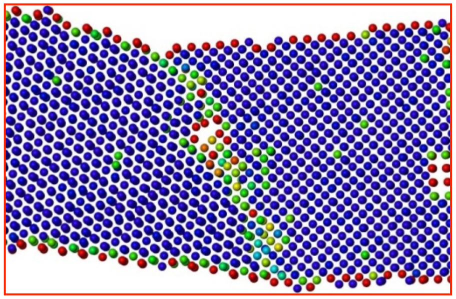
Deformation at Large Strains

$$\dot{\varepsilon} = 10^{6}\ \mathrm{sec}^{-1}\ , \varepsilon \geq 15\%$$

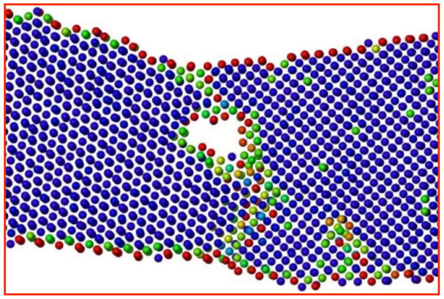
- At larger strains, we observe the formation of nano-voids at grain boundaries and GB junctions, that grow and lead to fracture of the thin film:
  - Here, nanovoid forms at the impingement between two twin boundaries. At other strain rates, fracture begins near triple junctions and in grain boundaries.
  - Fracture is consistently observed at interfaces, implying that fracture prediction models should focus on accurately capturing interfacial strengths.



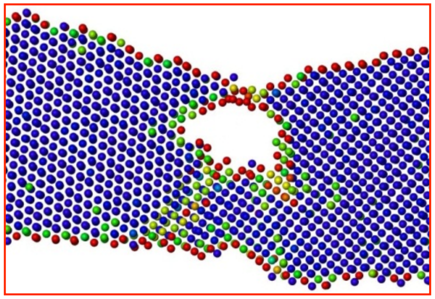
17.5% strain



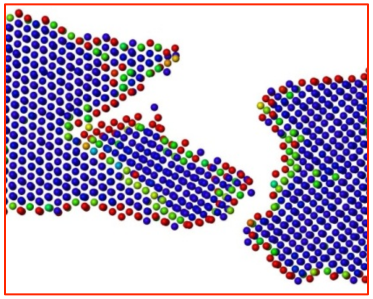
17.5% strain



20% strain



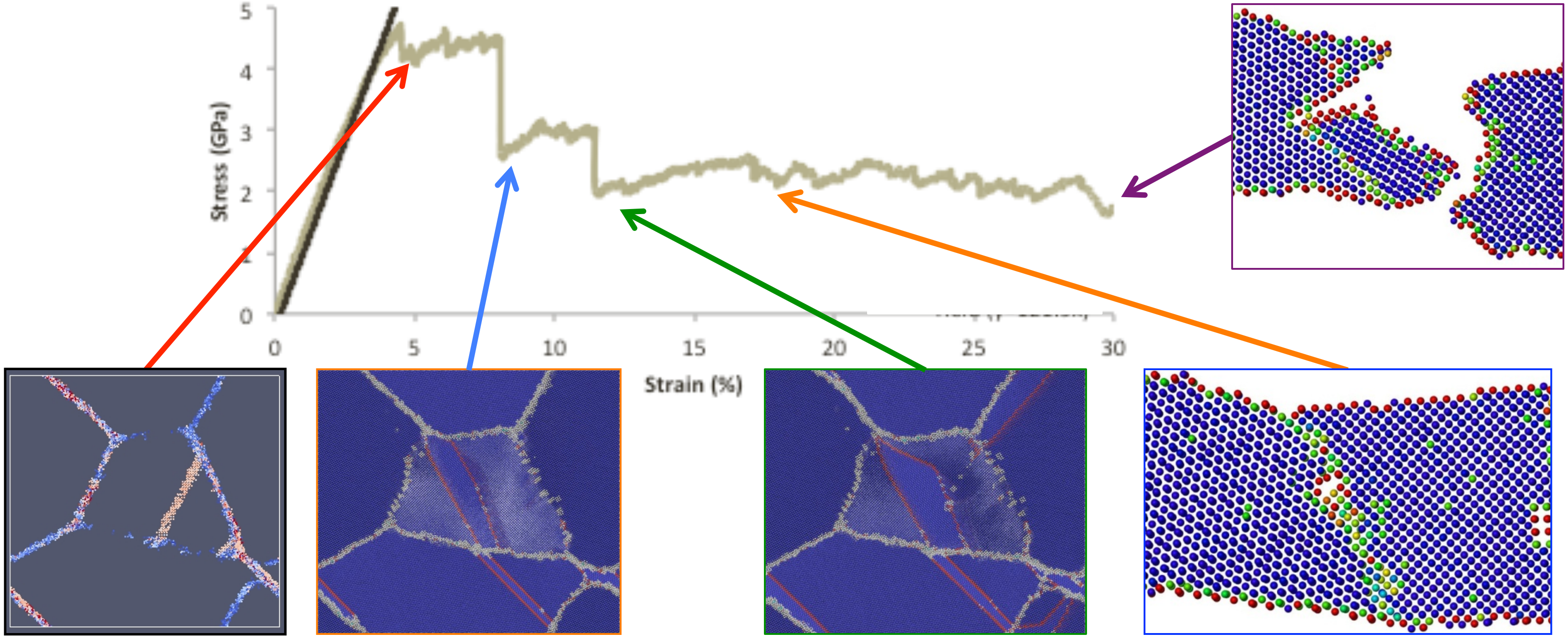
23% strain



29% strain

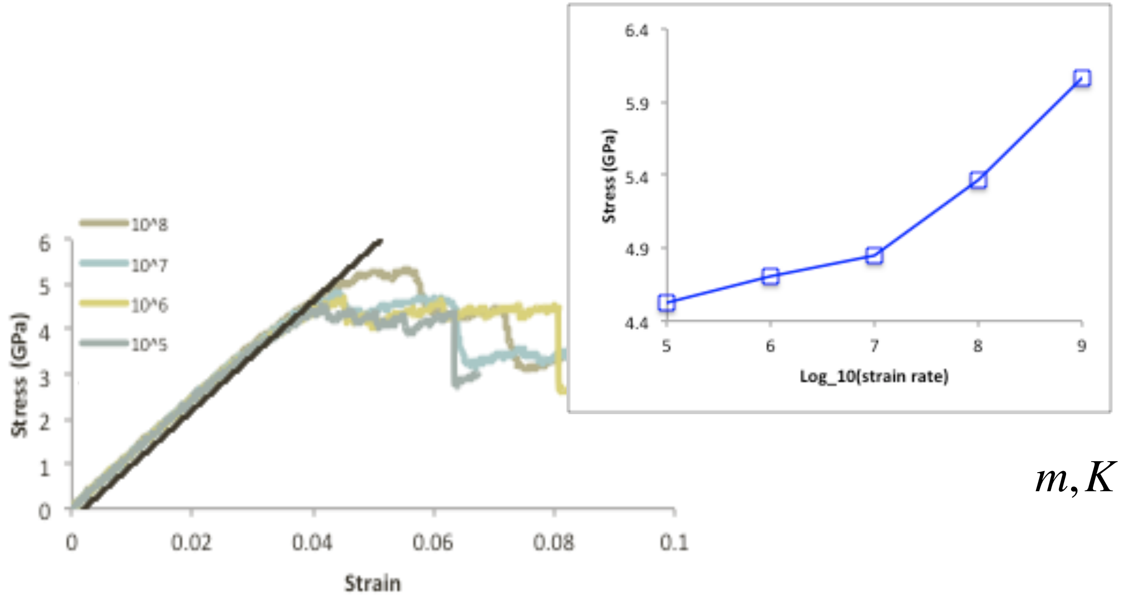
Correlating Defects with Deformation

- The mechanisms of dislocation emission, twin formation and nanovoid creation can be correlated with the system's stress-strain response:



Effects of Varying Strain Rate

- Onset of specific mechanisms varies for different strain rates, e.g. larger loading rates lead to earlier appearance of deformation twins.
- System stress response is used to quantify a strain-rate sensitivity of the nucleation stress for the first defect leading to plastic deformation.
- A strain rate sensitivity exponent was determined to be in the range 0.015 – 0.049, comparable to the range of 0.02 to 0.05 measured in experiments by Wei et al. and Cao et al. on NC materials with similar-sized grains.



$$\sigma_n = K\dot{\varepsilon}^m$$

$$\log(\sigma_n) = k + m\log(\dot{\varepsilon})$$

$$m, K = \begin{cases} 0.015\,,\ 3.81\,\text{GPa} & \text{low rate data} \\ 0.049\,,\ 2.19\,\text{GPa} & \text{high rate data} \\ 0.031\,,\ 3.06\,\text{GPa} & \text{all data} \end{cases}$$

Publications, Presentations & Symposia

- Publications
  - "Incorporating atomistic data of lattice friction into BCC crystal plasticity models" – *International Journal of Plasticity* (2012)
  - "Slip planes in BCC transition metals" – Submitted to *International Materials Review*
  - "Understanding {112} Slip in Tantalum" – In Preparation for *Physical Review B*
  - "Molecular dynamics study of the competition between slip and twinning in a tantalum nanocrystalline thin film" – In Preparation for *Acta Materialia (maybe)*
  - "Strain-rate sensitivity of deformation mechanisms in a tantalum nanocrystalline thin film" – In Preparation for *Computational Materials Science*
- Presentations
  - Plasticity 2012 (Weinberger), WCCM-2012 (Hale)
  - MS&T-12 (Zimmerman) – almost!
  - ASME/IMECE-2012 (Zimmerman, Weinberger) – Yes!
  - TMS 2013 Annual Meeting (Zimmerman, Weinberger, Hale, Smith) – TBD
- Symposia
  - ASME/IMECE-2012 – Multiscale Perspectives on Plasticity in Metals
  - MS&T-13 – Multiscale Perspectives on Plasticity in BCC Metals

Backup Slides

(-1-12) Zero Stress Slip Pathway

Nudged Elastic Band calculations of the reaction pathway and barriers

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