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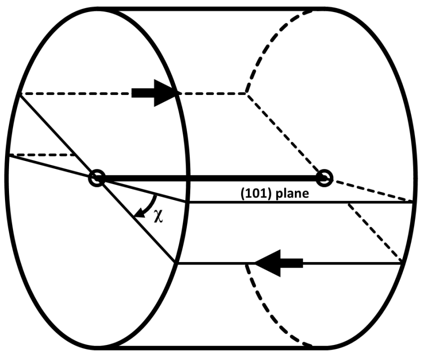

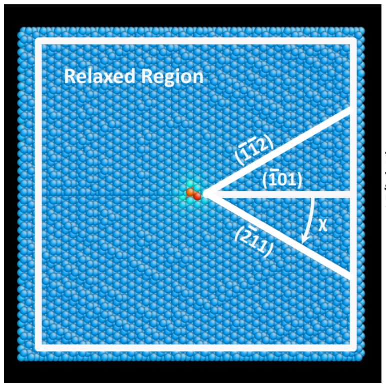

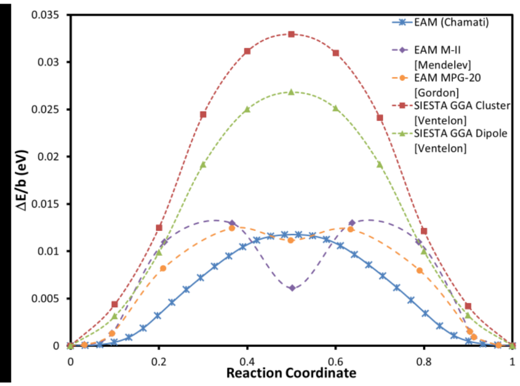

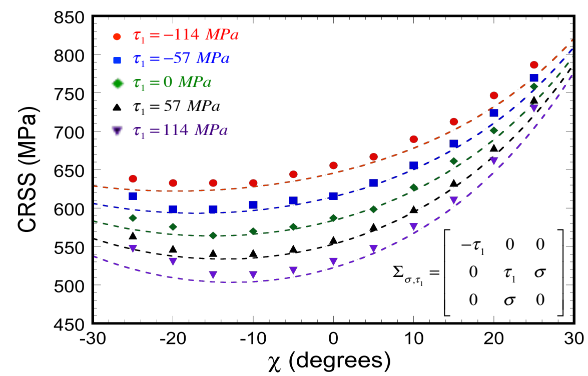

Atomistic Modeling of Dislocation Slip in α-Fe

Jon Zimmerman, Lucas Hale – Mechanics of Materials
Hojun Lim, Chris Weinberger – Computational Materials & Data Science

U.S. DEPARTMENT OF ENERGY   NNSA National Nuclear Security Administration

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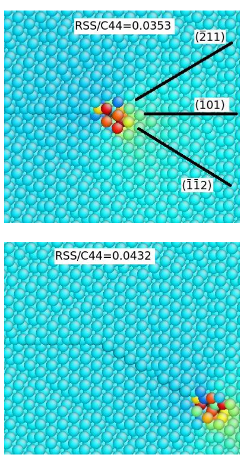
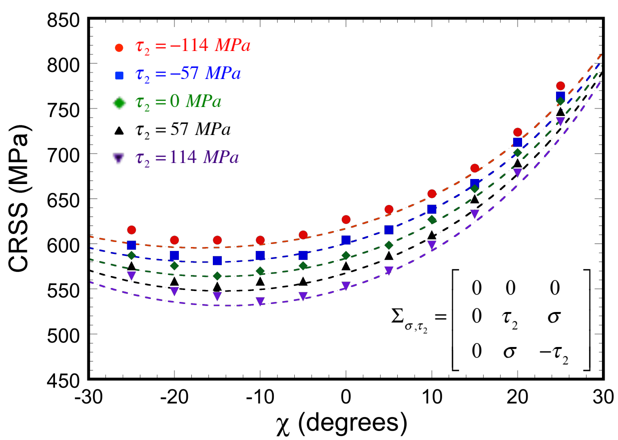
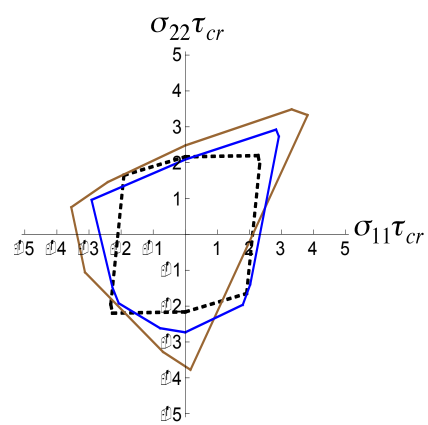
Motivation

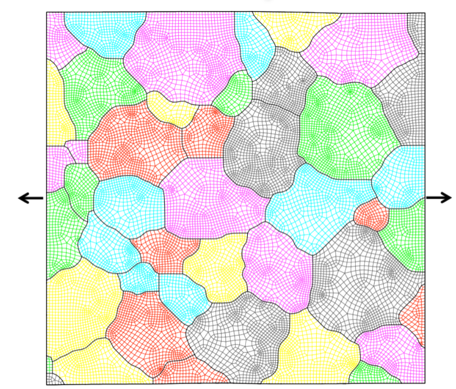
- Gain a fundamental understanding on the atomic-level mechanisms and dominant defects relevant to incipient plastic deformation and ductile fracture of BCC metals.
- Dislocation slip in BCC metals is orientation and stress-state dependent, producing "non-Schmid" single crystal yield.
- Use atomistic simulation to quantify these dependencies, then map onto grains in polycrystal geometries to predict overall mechanical response.

Atoms-up: Develop physics-based models to provide scientific insight



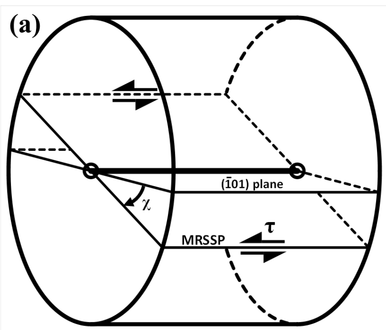


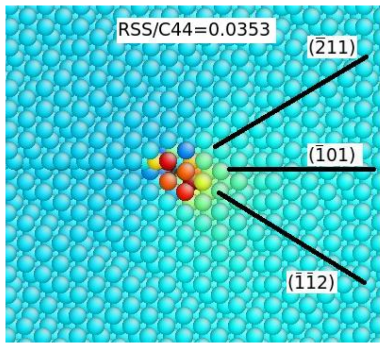


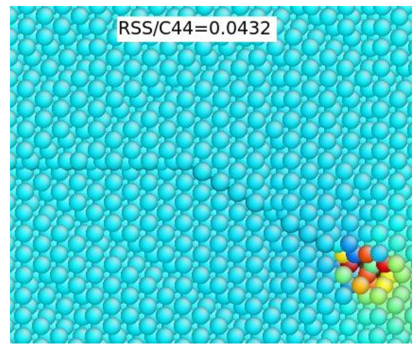


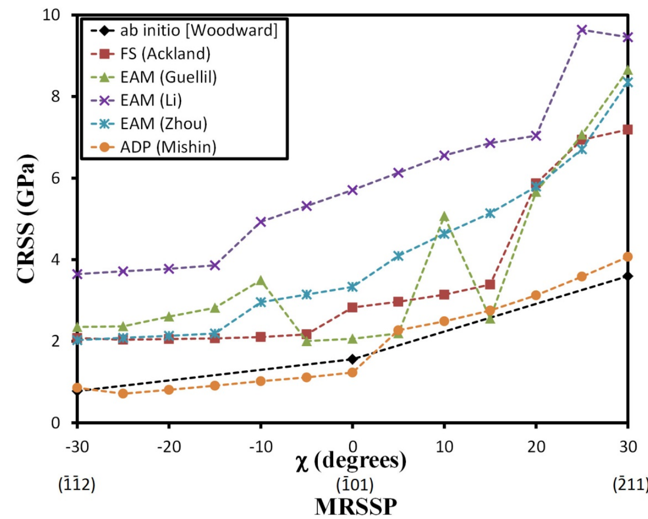
Motivation

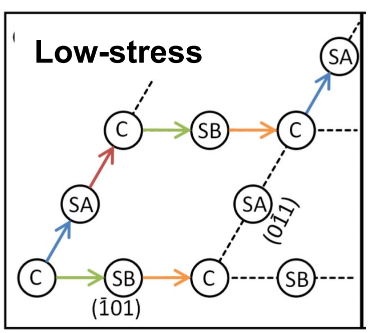
- FY11-13 atomistic simulations to establish the fundamental slip planes of BCC Ta showed {112} dominant for a variety of inter-atomic potentials and conditions.

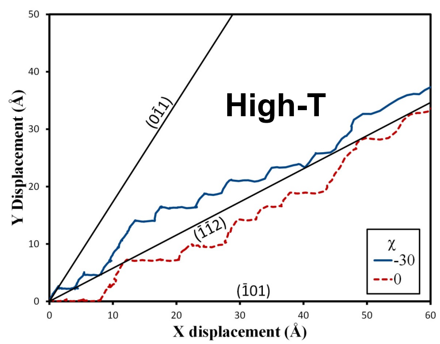


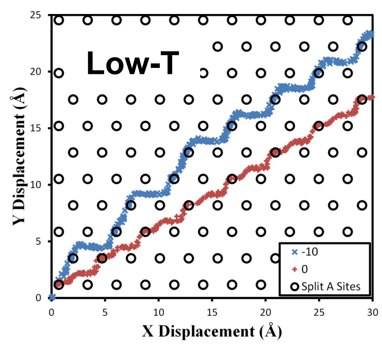


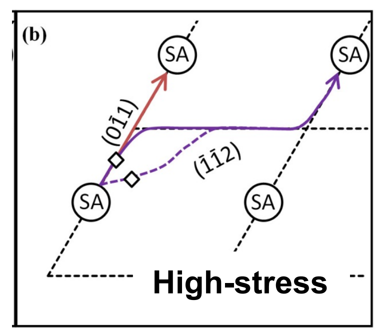












Stability of split-core structure causes {112} slip

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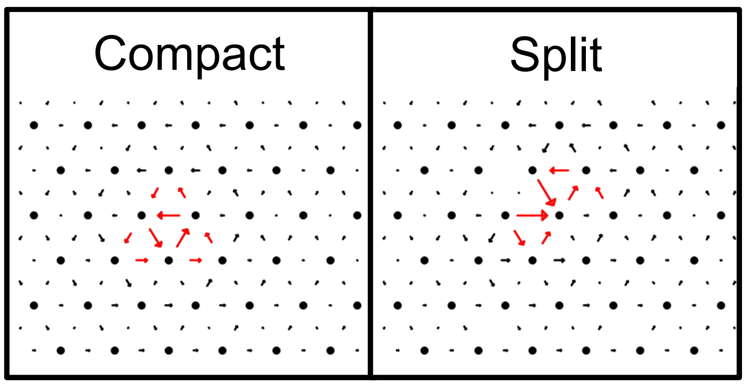
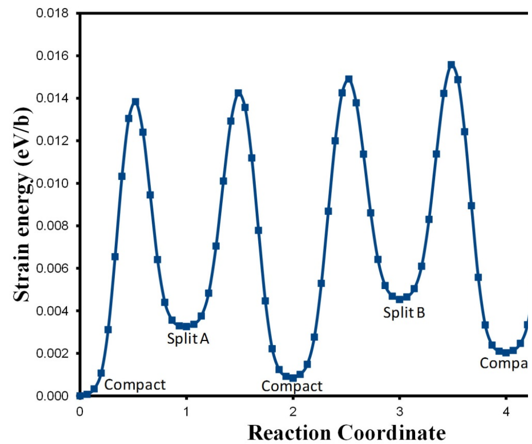
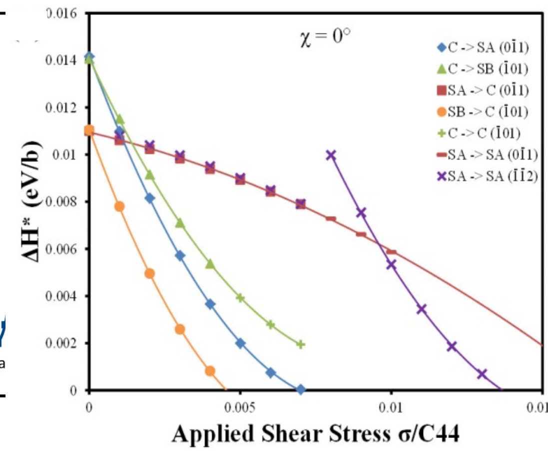
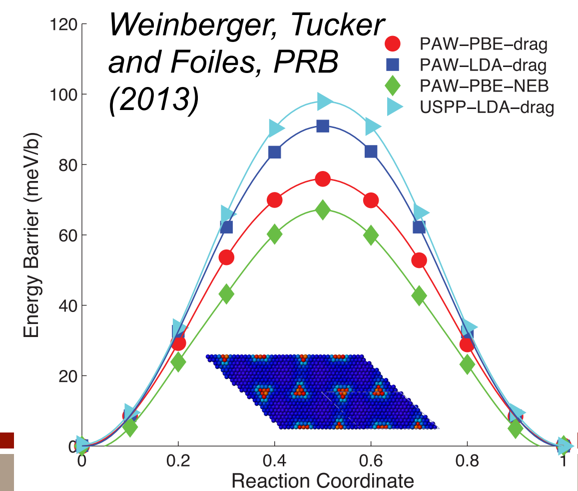
- The split-core structure has a sufficiently low energy to be a preferred state once stress is applied.
- The barrier between compact and split-core structures is sufficiently low to ensure that this is the dominant transition.





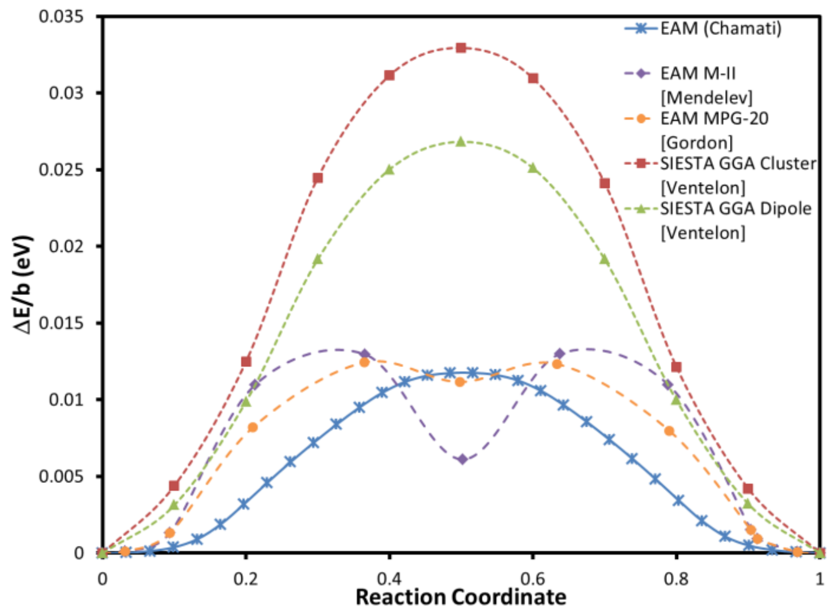


- Experimental work found in the literature, and done by PPM-Task 1 staff show {110} slip actually occurs (especially at low temperatures).
- DFT calculations confirm that the Peierls potential should be camel hump-shaped, indicating a compact-to-compact transition.



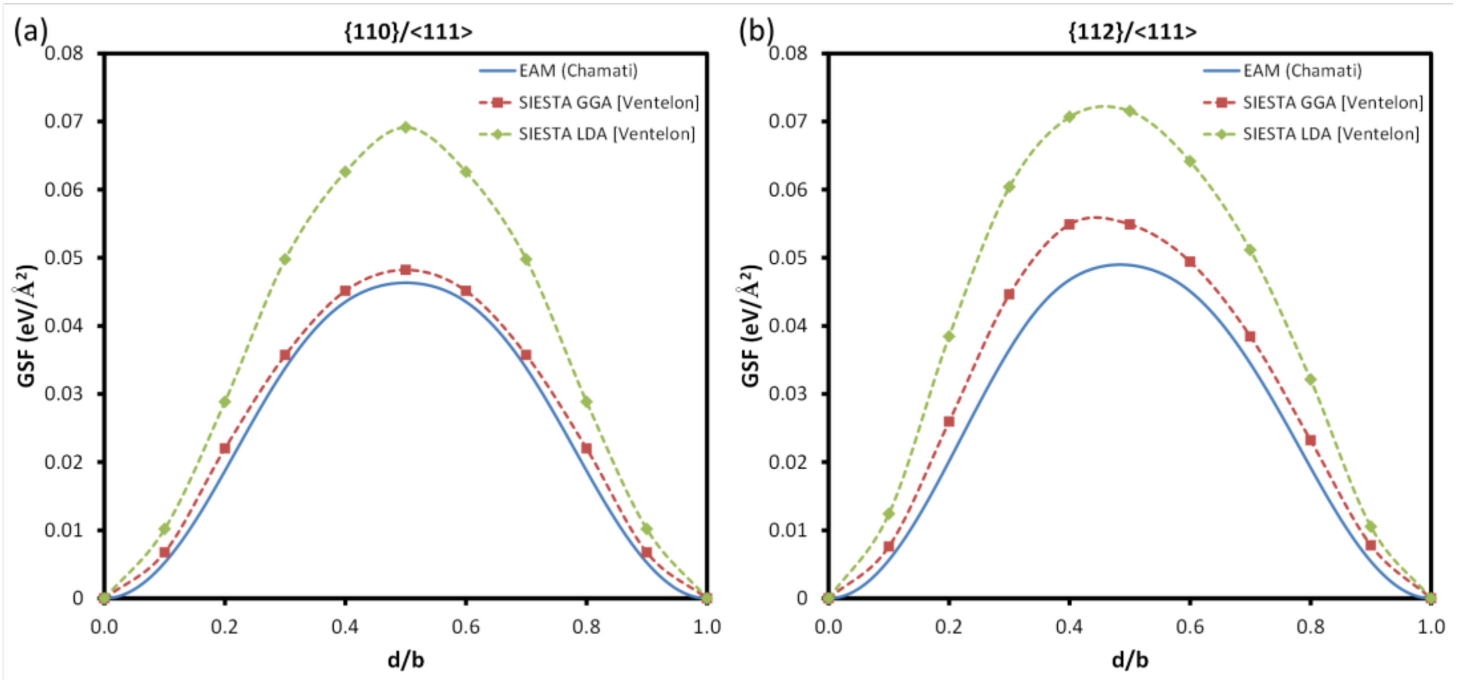
Paths for FY13

- Find/develop an inter-atomic potential for Ta that shows the correct Peierls potential behavior.
  - SNAP (Spectral Neighbor Analysis Potential) under development in LDRD by A. Thompson; some theoretical issues and large computational cost.
  - MGPT (Model of Generalized Pseudopotential Theory) being developed by LLNL; potential not yet released and large computational cost.
- As PPM is also interested in Fe (i.e. ferrite phases in austenitic stainless steels), can we find a suitable Fe potential that displays the correct dislocation core structure and slip behavior? Yes – Embedded Atom Method potential by Chamati *et al.*, *Surface Science* (2006).



Characterization of Fe potential

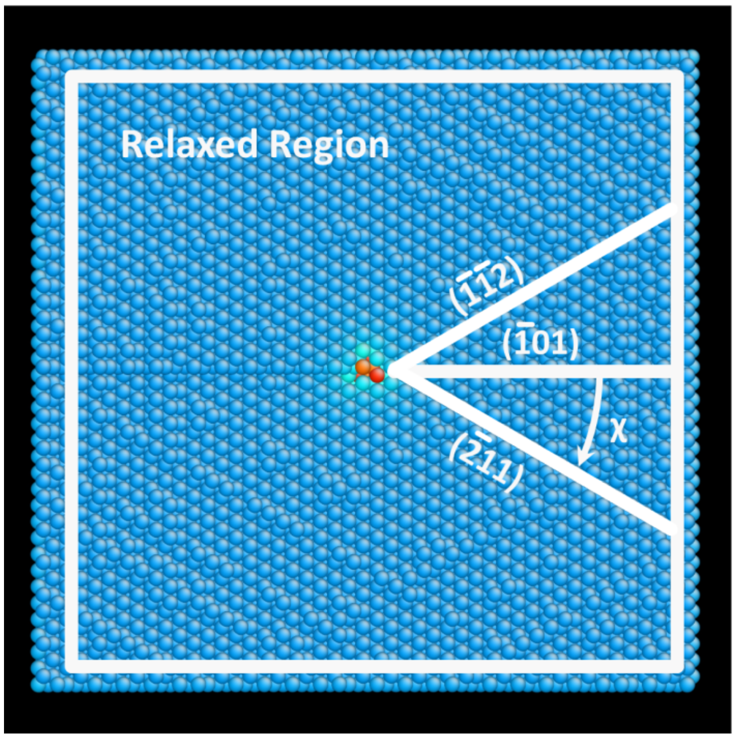
- We computed the generalized stacking fault curves for {110} <111> and {112}<111> shearing and compared with DFT by Ventelon and Willaime (*Philos. Mag.*, 2010).

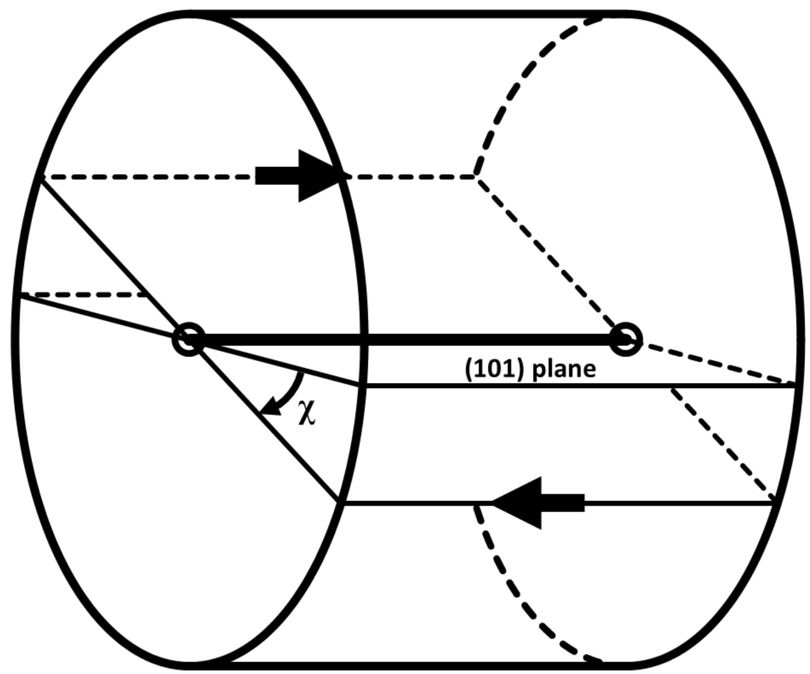


- Potential agrees qualitatively with DFT calculations, and quantitatively close to GGA-type calculations.

Calculation of CRSS

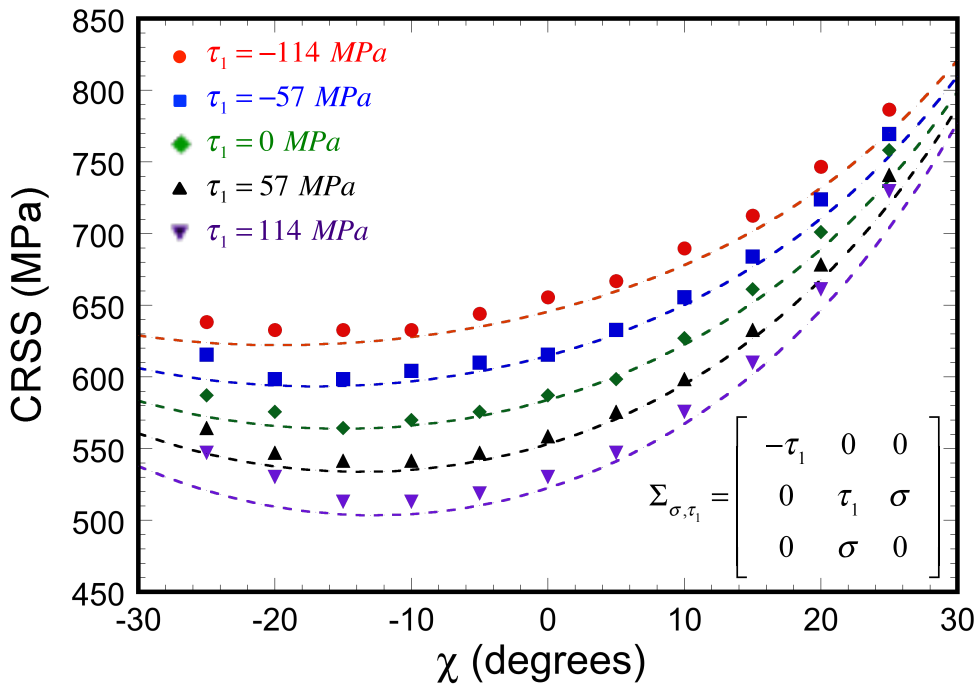
- Single dislocation in 168 Å x 162 Å x 20/238 Å systems
- Strain applied according to anisotropic elasticity solution
- Middle of system relaxed with a force minimization





Calculation of CRSS

- Values of critical resolved shear stress (CRSS) estimated using both quasi-static simulations showing the onset of slip, and from Nudged Elastic Band (NEB) calculations extrapolated to the zero energy barrier case.

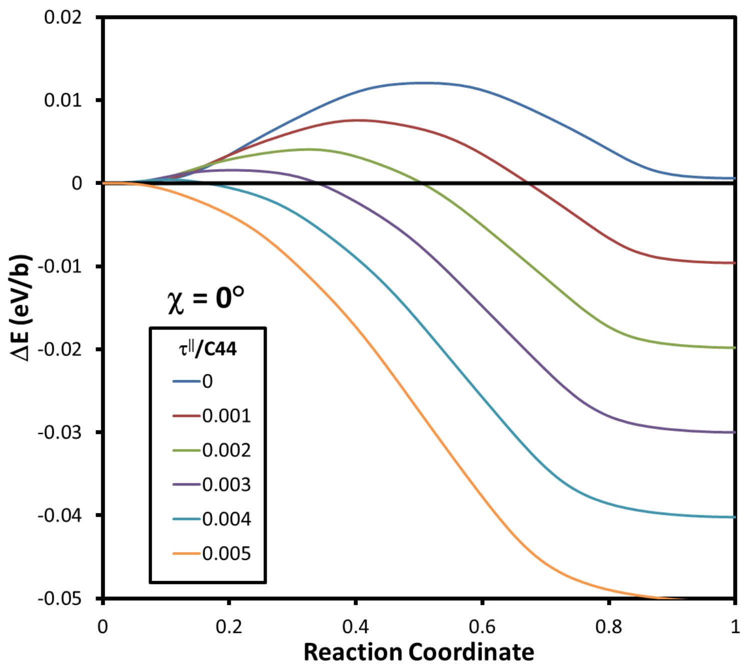


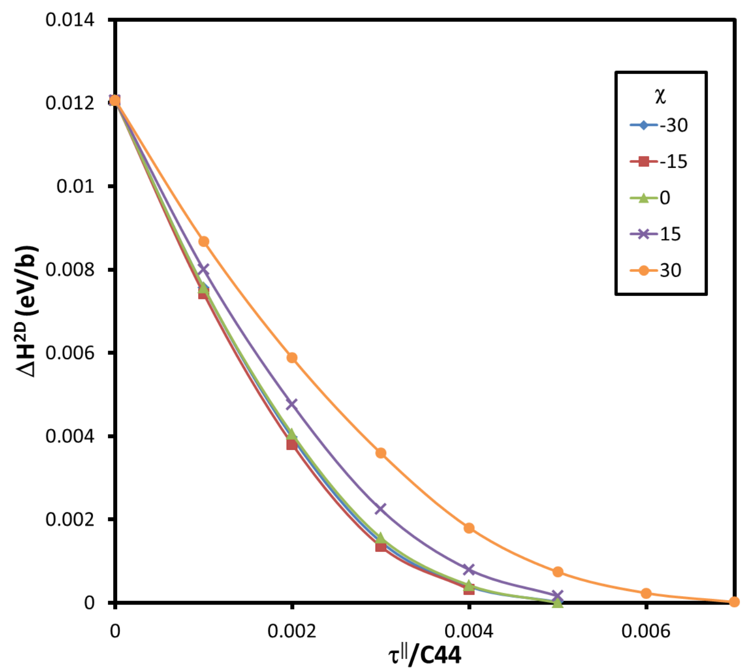
Atomistic simulations show dislocation slip that is always fundamentally on {110} planes.

{112} slip occurs only when resolve shear aligns with {112} planes (and even then, slip is resolvable as alternating {110} slip on two different planes).

Exploration of Energy Landscape

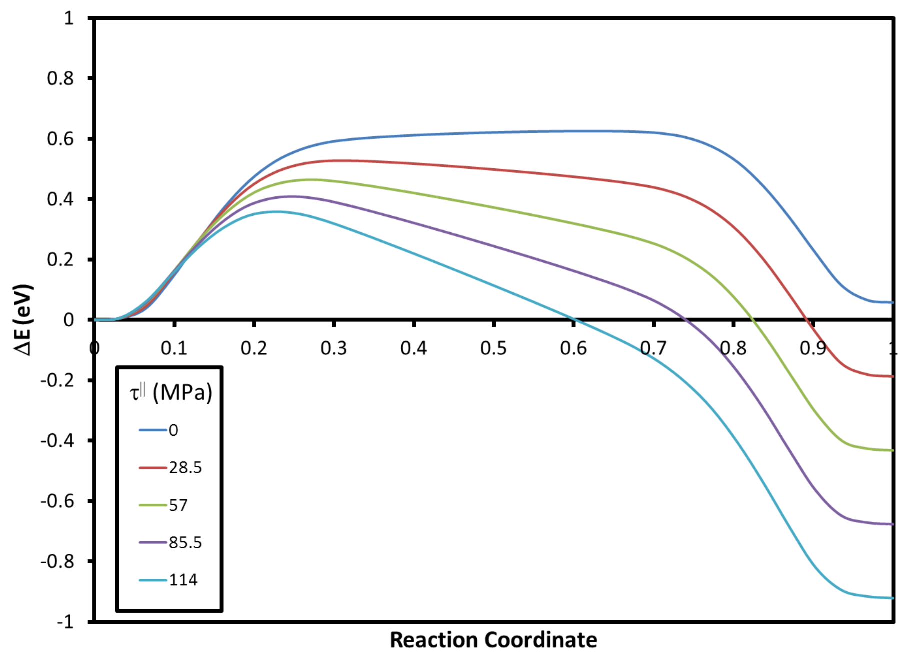
- NEB calculations for a 2D slip pathway show no evidence of the metastable/split core, even at high stress.
- 2D activation enthalpy is a single curve for a given loading orientation.





Activation enthalpy for slip via kinks

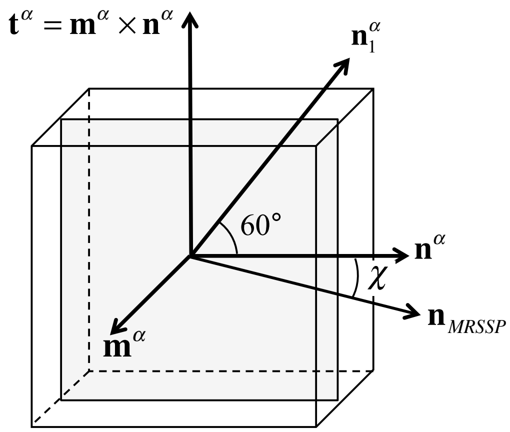
- NEB calculations show that activation enthalpy for stressed systems is associated with the formation of kinks. Once formed, the stress naturally drives the kinks to easily move.

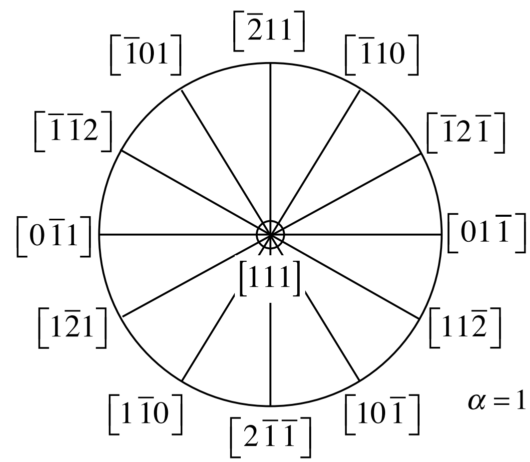


Generalized Non-Schmid Yield Criteria

$\mathbf{m}^{\alpha}$: slip direction

$\mathbf{n}^{\alpha}$: slip plane normal





The resistance to slip on a slip system α:

$$\tau_{\mathrm{cr}}^{\alpha} = \mathbf{P}_{\mathrm{tot}}^{\alpha} : \boldsymbol{\sigma} = \underbrace{\mathbf{P}_{\mathrm{s}}^{\alpha} : \boldsymbol{\sigma}}_{\text{Schmid}} + \underbrace{\mathbf{P}_{\mathrm{ns}}^{\alpha} : \boldsymbol{\sigma}}_{\text{Non-Schmid}}$$

$$\mathbf{P}_{\mathrm{s}}^{\alpha} = c_0 \frac{1}{2} \left(\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} + \mathbf{n}^{\alpha} \otimes \mathbf{m}^{\alpha} \right)$$

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

If yield function is independent of hydrostatic stress, $c_3 + c_4 + c_5 = 0$

$$\mathbf{P}_{\mathrm{ns}}^{\alpha} = c_1 \mathbf{t}^{\alpha} \otimes \mathbf{m}^{\alpha} + c_2 \mathbf{t}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_3 \mathbf{n}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_4 \mathbf{t}^{\alpha} \otimes \mathbf{t}^{\alpha} - (c_3 + c_4) \mathbf{m}^{\alpha} \otimes \mathbf{m}^{\alpha}$$

Fitting on non-Schmid constants

$$\mathbf{P}^{\alpha}_{\text{tot}} = c_0 \frac{1}{2} \left(\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} + \mathbf{n}^{\alpha} \otimes \mathbf{m}^{\alpha} \right) + c_1 \mathbf{t}^{\alpha} \otimes \mathbf{m}^{\alpha} + c_2 \mathbf{t}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_3 \mathbf{n}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_4 \mathbf{t}^{\alpha} \otimes \mathbf{t}^{\alpha} + c_5 \mathbf{m}^{\alpha} \otimes \mathbf{m}^{\alpha}$$

$$\Sigma_{\sigma} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma \\ 0 & \sigma & 0 \end{bmatrix} \qquad \mathbf{CRSS}(\chi) = \frac{\tau^{*}_{\text{cr}}}{\cos\ \chi - c_1 \sin(\chi)}$$

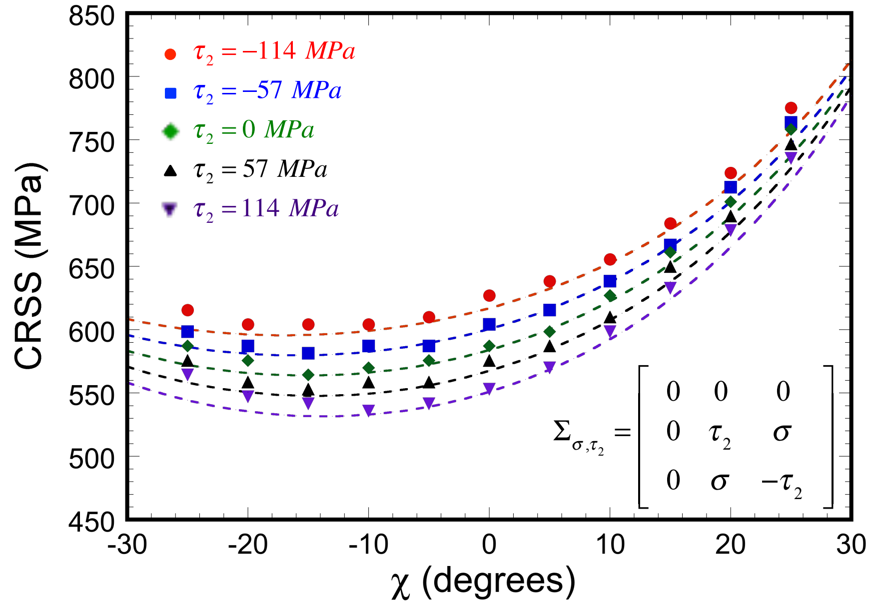
$$\Sigma^{1}_{\tau,\sigma} = \begin{bmatrix} -\tau & 0 & 0 \\ 0 & \tau & \sigma \\ 0 & \sigma & 0 \end{bmatrix} \qquad \mathbf{CRSS}(\chi, \tau) = \frac{\tau^{*}_{\text{cr}} - \tau(-c_2 \sin\ 2\chi + (c_3 - c_4)\cos 2\chi)}{\cos\ \chi - c_1 \sin(\chi)}$$

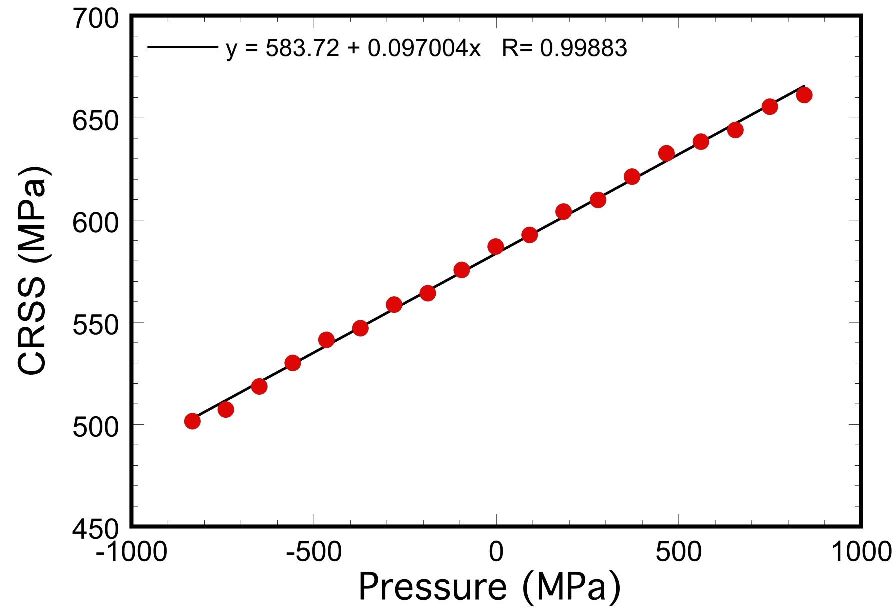
$$\Sigma^{2}_{\tau,\sigma} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \tau & \sigma \\ 0 & \sigma & -\tau \end{bmatrix} \qquad \mathbf{CRSS}(\chi, \tau) = \frac{\tau^{*}_{\text{cr}} - \tau(-c_2 \sin\chi \cos\chi + c_3 \cos^2\chi + c_4 \sin^2\chi - c_5)}{\cos\ \chi - c_1 \sin(\chi)}$$

$$c_3 + c_4 + c_5 = 0.097$$

τ_{cr} *(MPa)*	c_1	c_2	c_3	c_4	c_5
584	0.27	0.15	0.31	-0.23	0.02

Dependence on non-resolved shear and normal stresses





- CRSS shows dependencies on shear stresses along planes perpendicular to the slip direction, and on the system pressure.
- Comparison shows fitted model possesses same trends as atomistic data.

Normalization of activation enthalpy

- Given this dependency, we questioned underlying assumptions used for the Kocks model in relating activation enthalpy to shear stress: $\Delta H = H_0\left(1-\Theta^p\right)^q$
- In classic slip theory (for fcc metals), the ratio Θ represents the ratio of resolved shear stress to a known resistance:

$$\Theta = \frac{\tau^\alpha}{\tau_R^\alpha} = \frac{\mathbf{P}_s^\alpha : \sigma}{\tau_R^\alpha}$$

This expression does not incorporate non-Schmid yield, i.e. this known stress-dependence for bcc metals. Thus, we considered 3 alternative possibilities for Θ:

$$\Theta = \frac{\mathbf{P}_s^\alpha : \sigma + \mathbf{P}_{ns}^\alpha : \sigma}{\tau_{cr}} \qquad \Theta = \frac{\mathbf{P}_s^\alpha : \sigma}{\tau_{cr} - \mathbf{P}_{ns}^\alpha : \sigma} \qquad \Theta = \frac{\tau^{MRSSP}}{CRSS\left(\chi,\sigma\right)}$$

Interpretation of the 3rd expression

- τ^{MRSSP} is the maximum resolved shear stress that can be found on any plane, acting in the slip direction. It can be simply represented by the expression: $\tau^{MRSSP} = \left|\sigma \cdot \mathbf{m}\right|$

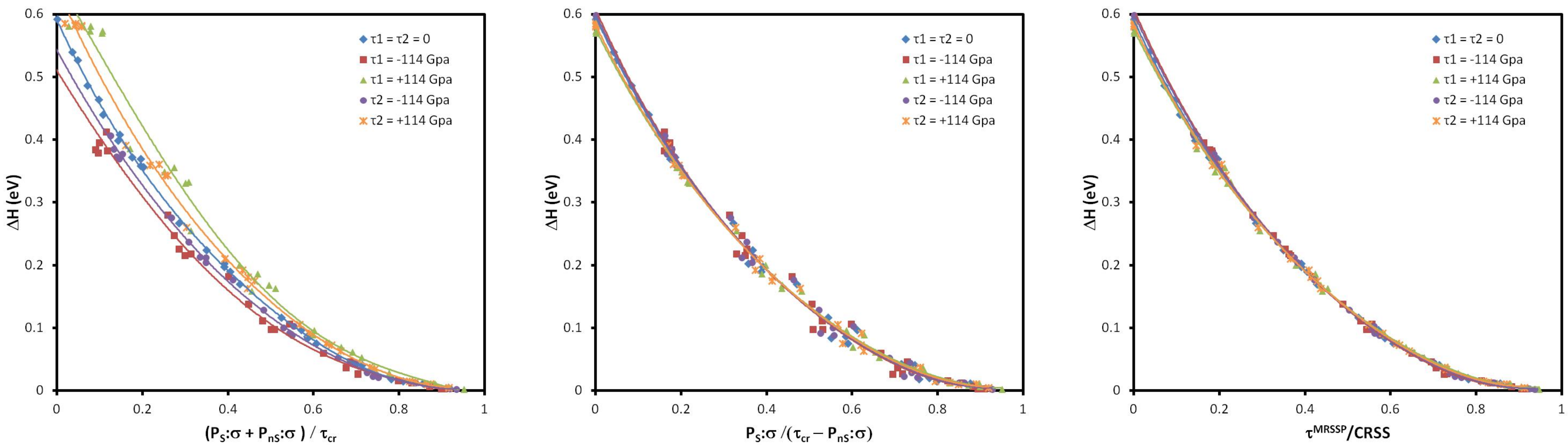
- $CRSS$ is the critical value of τ^{MRSSP} that activates slip. To ensure that it is independent of τ^{MRSSP}, we use relationships between τ^{MRSSP} and the Schmid and non-Schmid Projectors to arrive at the expression:

$$CRSS\left(\chi,\sigma\right) = \frac{\tau_{cr} - c_2\mathbf{P}_{ns}^{tn} : \sigma - c_3\mathbf{P}_{ns}^{nn} : \sigma - c_4\mathbf{P}_{ns}^{tt} : \sigma - c_5\mathbf{P}_{ns}^{mm} : \sigma}{\cos\left(\chi\right) + c_1 \sin\left(\chi\right)}$$

- Using these expressions, the ratio Θ can be simplified to:

$$\Theta = \frac{\mathbf{P}_s : \sigma + c_1\mathbf{P}_{ns}^{mt} : \sigma}{\tau_{cr} - c_2\mathbf{P}_{ns}^{tn} : \sigma - c_3\mathbf{P}_{ns}^{nn} : \sigma - c_4\mathbf{P}_{ns}^{tt} : \sigma - c_5\mathbf{P}_{ns}^{mm} : \sigma}$$

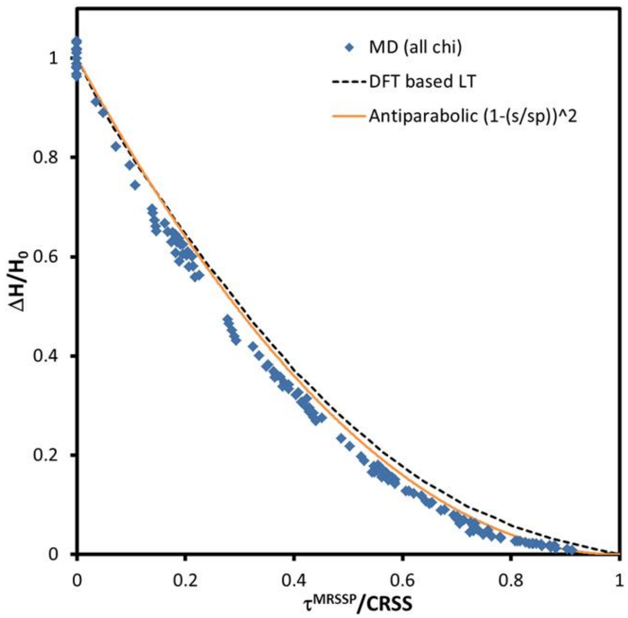
Comparison of stress ratios

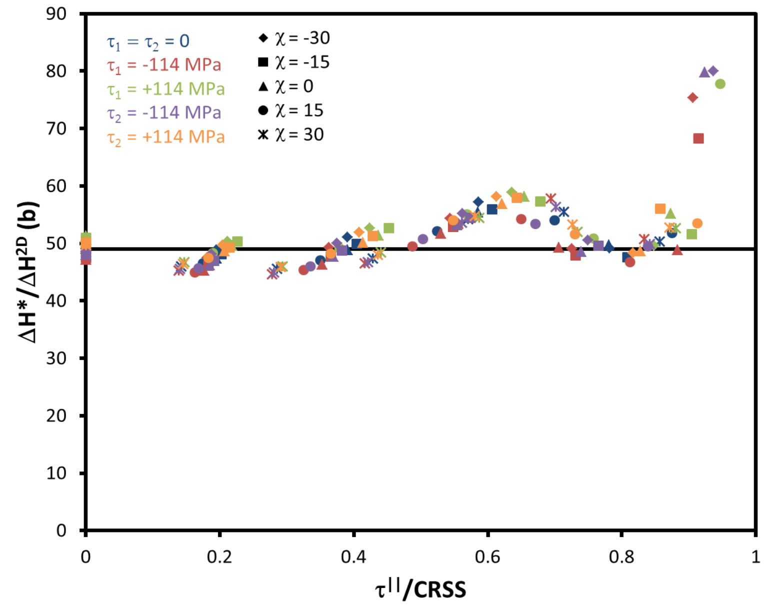


- Our simulation results for all orientations and combinations of stress show that our 3rd expression offers the best agreement with data as a normalization ratio for the activation enthalpy.
- This result also indicates that it is the total driving force acting on the dislocation that predicts slip activation, a conceptually different description of slip than the traditional slip system concept. This conclusion is consistent with the high temperature observation of pencil glide.

Activation enthalpy for 3D kinks

- Similar behavior of enthalpy for thick system with (3D) kinks as compared with thin (2D) system.
- Activation enthalpy curve falls close to both anti-parabolic (p = 2, q = 1) and DFT-based line tension models.
- Ratio of 3D-to-2D shows that, to a first approximation, the 3D can be represented by a scaled 2D.





Publications, Presentations & Symposia

- Publications
  - "Understanding {112} Slip in Tantalum" – In Review, *Computational Materials Science*
  - "Molecular dynamics study of deformation and fracture in a tantalum nano-crystalline thin film." – In Review, *Modell. Simul. Mater. Sci. Eng.*
  - *"Insights on Activation Enthalpy for Non-Schmid Slip in BCC Metals"* – In Preparation for *Physical Review Letters*
  - *"*A Multi-scale Model of Dislocation Plasticity in Alpha-Iron: Incorporating Temperature, Strain Rate and Non-Schmid Effects" – In Preparation for *International Journal of Plasticity*
- Presentations
  - ASME/IMECE-2012 (Zimmerman, Weinberger)
  - TMS 2013 Annual Meeting (Zimmerman, Weinberger, Hale, Smith)
  - 2013 LAMMPS Workshop (Zimmerman)
  - MS&T'13 (Zimmerman, Hattar, Buchheit)
  - ASME/IMECE-2013 (Zimmerman)
- Symposia
  - ASME/IMECE-2012 – Multiscale Perspectives on Plasticity in Metals
  - USNCCM12 – Continuum Theories for Modeling Atomic Scale Physics
  - MS&T'13 – Multiscale Perspectives on Plasticity in BCC Metals
  - TMS 2014 Annual Meeting – Algorithm Developments in Computational MS&E

FY14 focus: dislocation-defect interactions

- Dislocation interactions with other types of crystal defects, including voids and grain boundaries.
- Includes validation of atomistic models of GBs using TEM data by Medlin and Hattar.