Atomistic Modeling of Thermally Activated Processes for Crystal Dislocations

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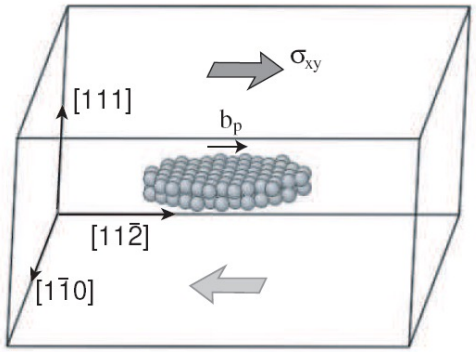
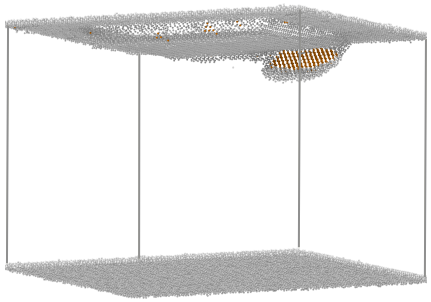
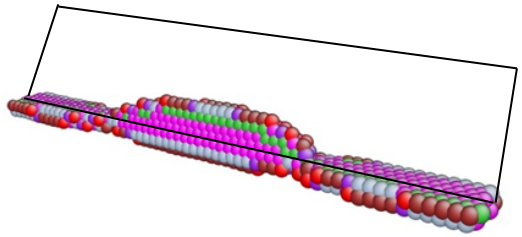
Outline







1. **Dislocation Nucleation in FCC Cu**

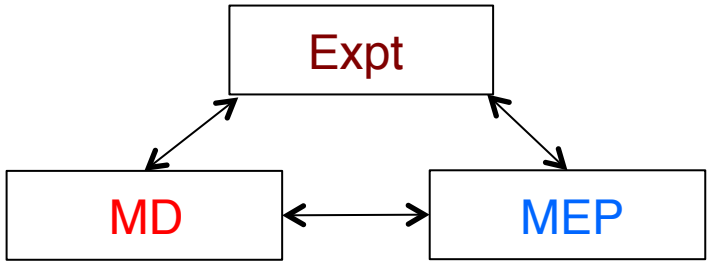
   Importance of Activation Entropy

2. Dislocation Nucleation in DC Si

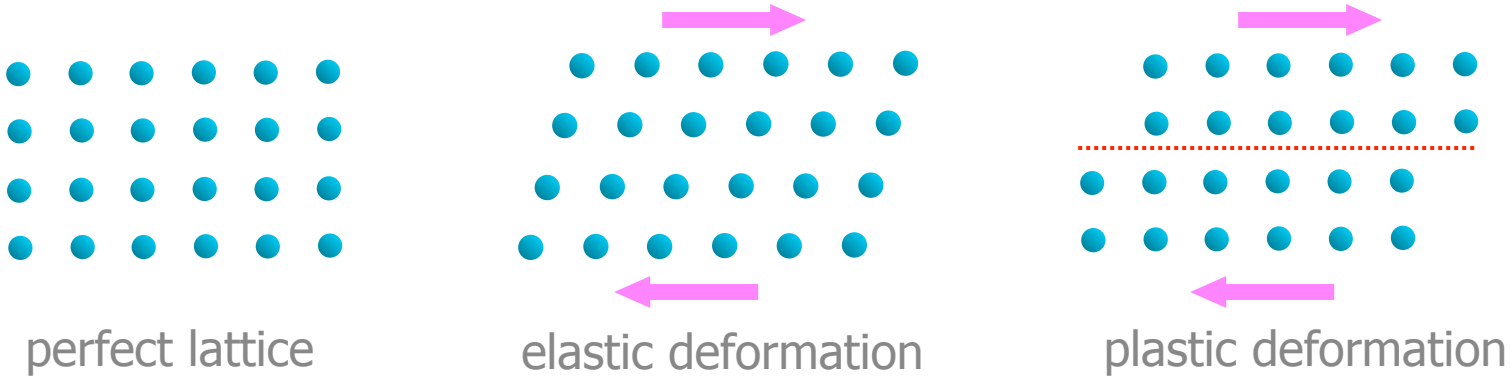
   Importance of Surface Morphology

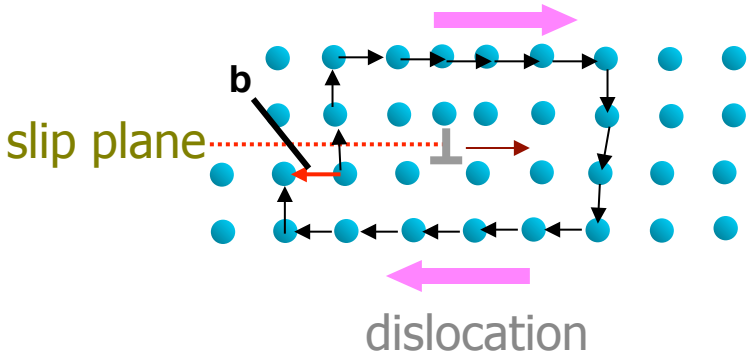
3. Cross Slip in FCC Ni

   Multiple Stress Components



Dislocations Responsible for Plastic Deformation



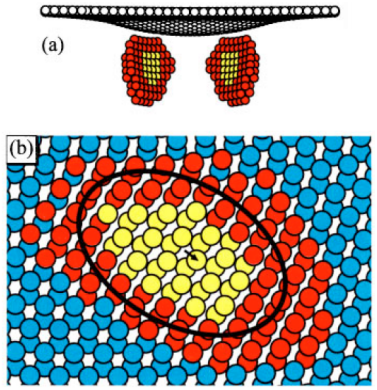


b : Burgers vector

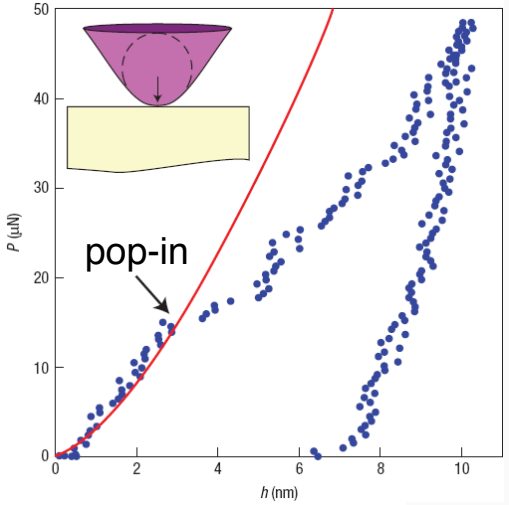
is the boundary between slipped and *un*-slipped area
Orowan, Polanyi, Taylor (1934)

Thermally Activated Dislocation Processes

Dislocation **nucleation** in nano-indentation and nano-pillar/nanowire deformation



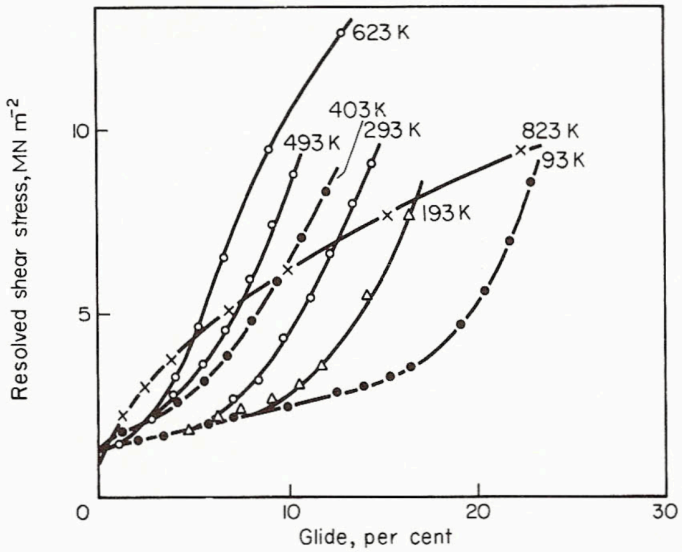
Kelchner et al.
PRB 58, 11085 (1998)



Schuh et al.
Nature Mater 4, 617 (2005)

Dislocation **cross slip** in temperature depend σ(ε) curves onset of Stage III hardening

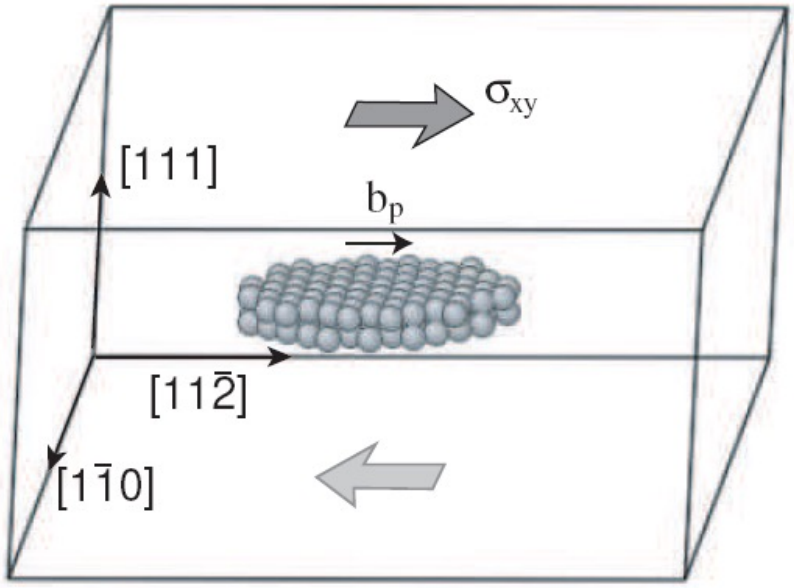
Single Crystal Cu, near [011]



R. W. K. Honeycombe (1968)
Plastic Deformation of Metals

Homogeneous Dislocation Nucleation Rate

Nucleation of *partial* dislocation under pure shear stress σ_{xy}

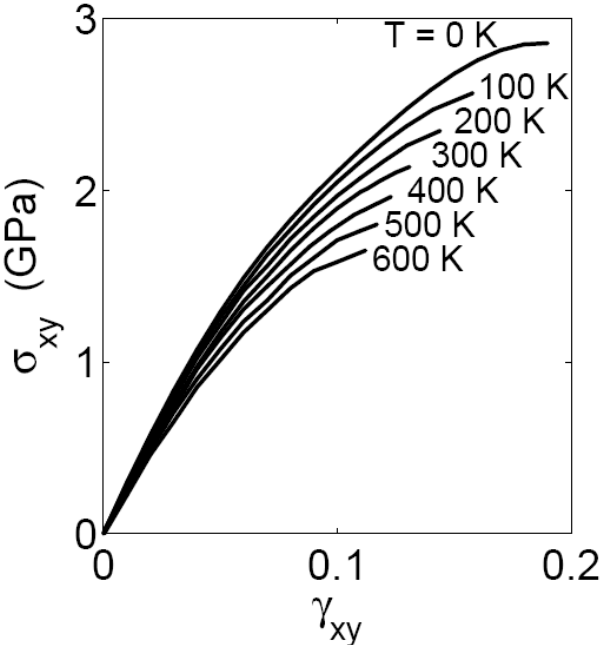


Goal:

nucleation rate $J^{\mathrm{NUC}}(\sigma, T)$

When the (finite T) ideal strength is reached, the crystal collapses by homogenous nucleation of dislocations

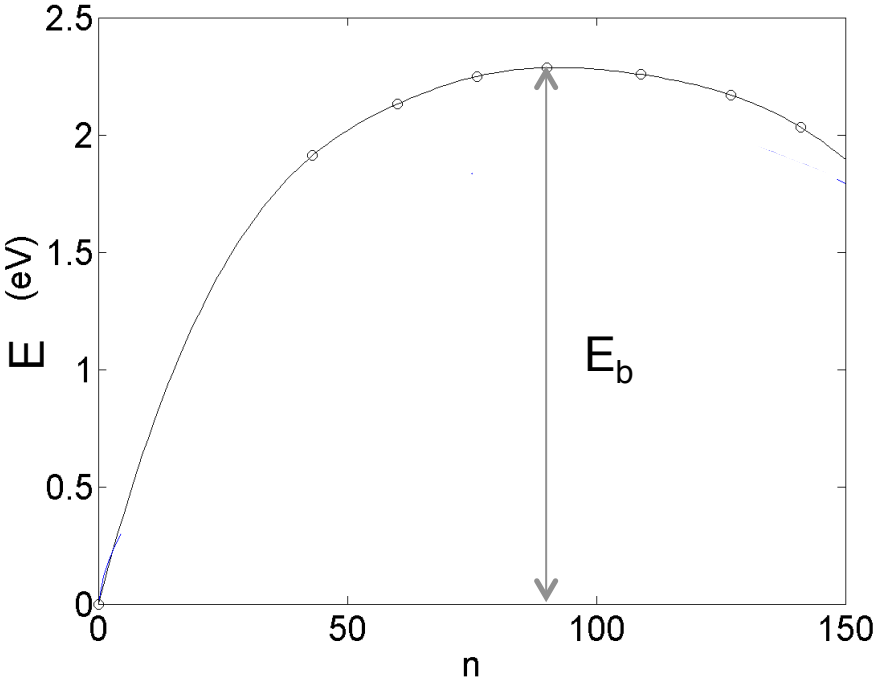
Shear stress-strain curves from MD

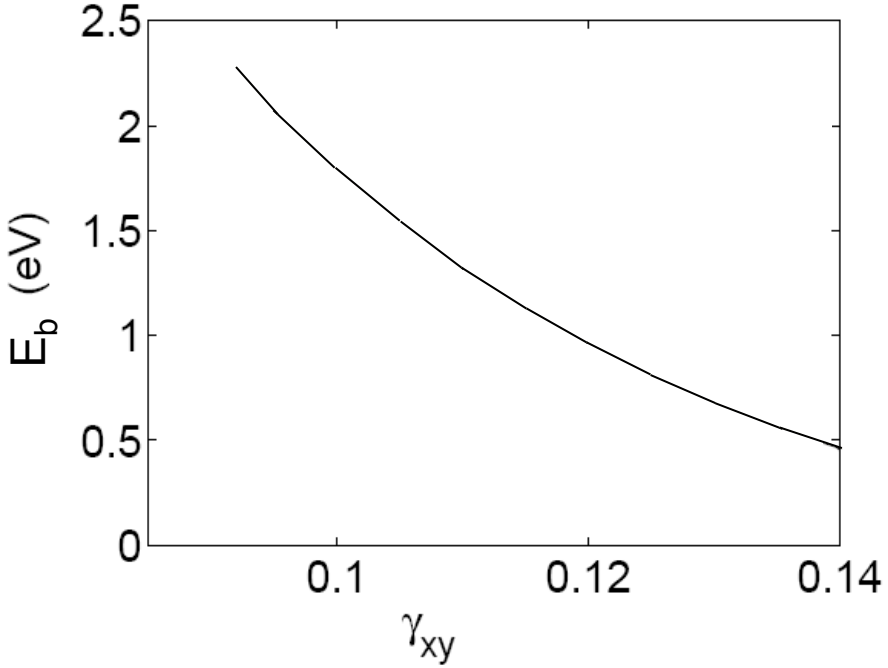


FCC Cu EAM Mishin Potential

Minimum Energy Path from String Method

at shear strain $\gamma_{xy} = 0.092$





Nucleation Rate from Classical Nucleation Theory

Becker-Döring Theory, Ann. Phys. (N.Y.) 24, 719 (1935)

$$J^{\mathrm{NUC}} = \nu_0 \exp\left(-\frac{F_c(\gamma,T)}{k_B T}\right)$$

where $F_c(\gamma,T)$ **Activation (Helmholtz) free energy** at shear strain γ

$\nu_0 = f_c^+ \Gamma$ f_c^+: nucleus fluctuation rate

Γ : Zeldovich factor (related to curvature of F(n) curve)

Transition State Theory (TST)

$$I^{TST} = \nu_0 \exp\left(-\frac{F_c(\gamma,T)}{k_B T}\right) = \nu_0 \exp\left(\frac{S_c(\gamma)}{k_B}\right) \exp\left(-\frac{E_c(\gamma)}{k_B T}\right) \qquad F_c = E_c - TS_c$$

where $\nu_0 = \frac{k_B T}{h} \approx 10^{13}\,\mathrm{s}^{-1}$ at T = 300K

Harmonic Transition State Theory (HTST)

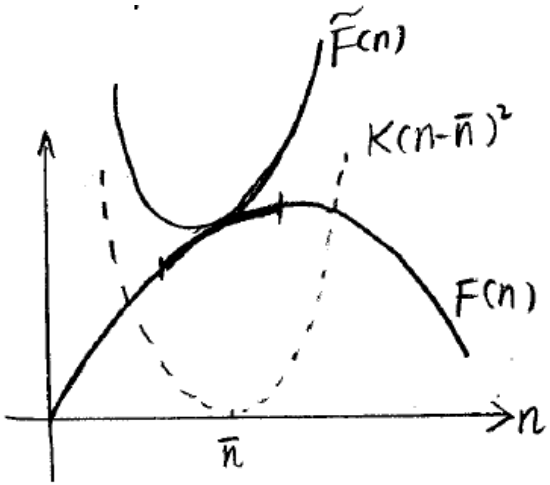
metastable state

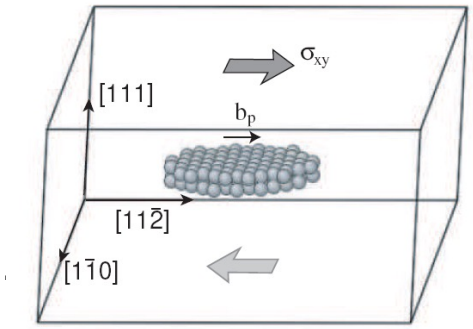
$$I^{HTST} = \frac{\prod_{i=1}^{N} \nu_i^m}{\prod_{i=1}^{N-1} \nu_i^a} \exp\left(-\frac{E_c(\gamma)}{k_B T}\right) \approx \nu_D \exp\left(-\frac{E_c(\gamma)}{k_B T}\right)$$

activated state

where $\nu_D \approx 10^{13}\,\mathrm{s}^{-1}$ (Debye frequency)

Umbrella Sampling (Monte Carlo) for Free Energy Barrier





$$U^{new}(\{r_i\}) = U^{EAM}(\{r_i\}) + K \cdot (n(\{r_i\}) - \bar{n})^2$$

original potential

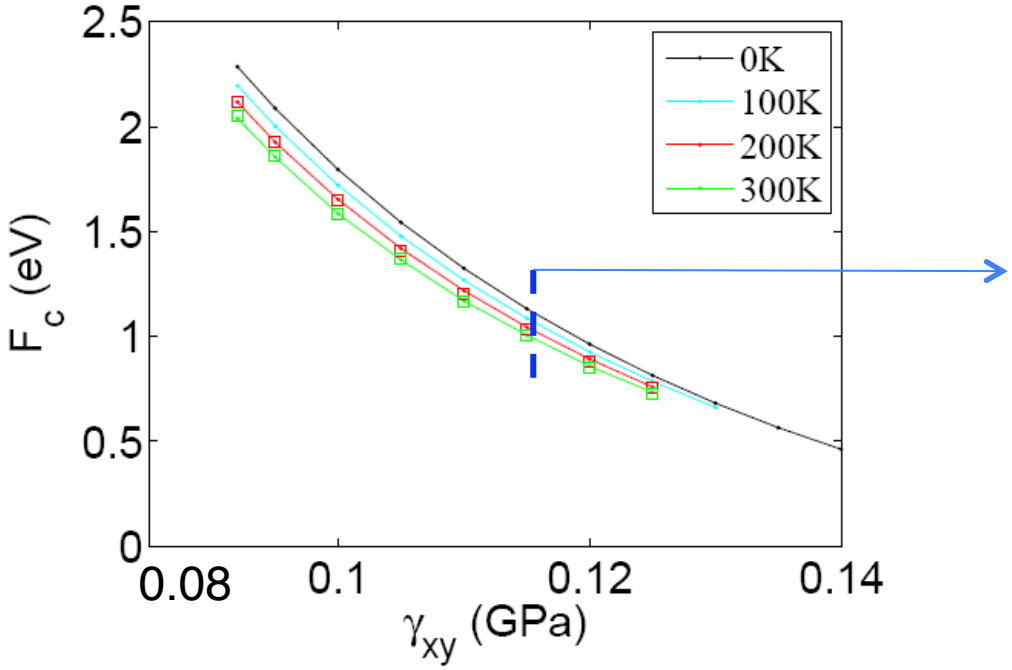
bias potential

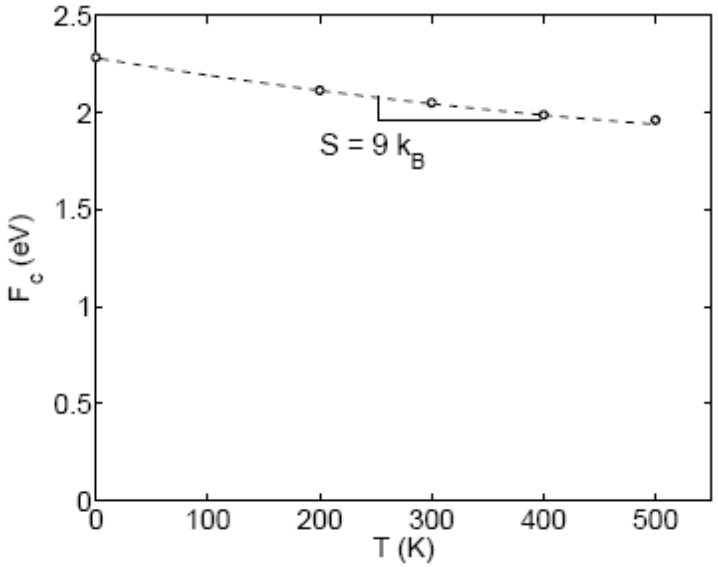
Order parameter: $n(\{r_i\})$ is the number of atoms enclosed by the dislocation loop

1. For each atom i, if $\max_j (|r_{ij} - r_{ij}^0|) > d_c$ atom i is labeled as "slipped"
2. "Slipped" atoms closer to each other than r_c are grouped into one cluster.
3. $n(\{r_i\})$ is the number of atoms in the largest cluster

Similar order parameter used in
Zuo, Ngan, Zheng, PRL, 94, 095501 (2005)

Activation Helmholtz Free Energy $F_c(\gamma, T)$





Activation entropy at const γ

$$S_c(\gamma) \equiv -\left.\frac{\partial F_c(\gamma,T)}{\partial T}\right|_{\gamma}$$

describes how fast F_c decreases with T *at constant* γ

at $\gamma = 0.092$

$S_c(\gamma) = 9\ k_B$

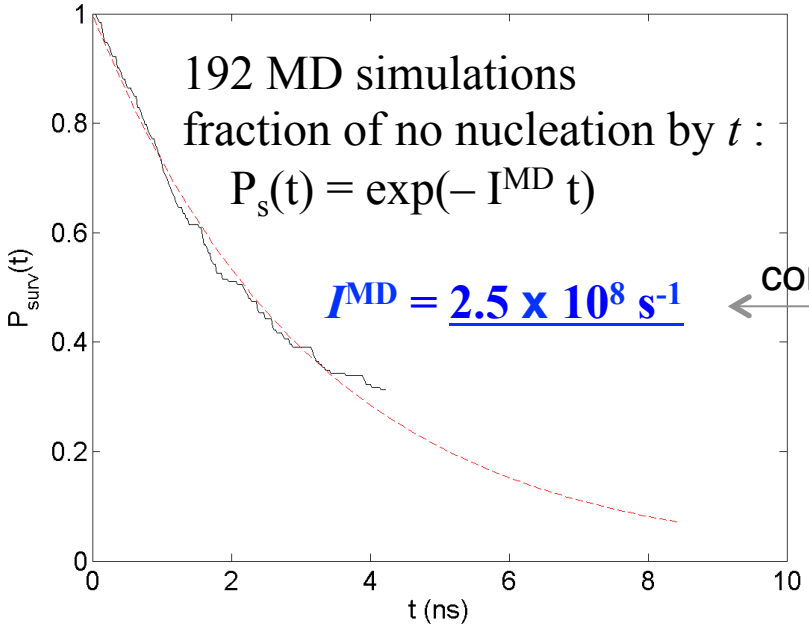
$\exp(\ S_c(\gamma)/k_B\ ) \sim 10^4$

Ryu, Kang, Cai, PNAS, 108, 5174 (2011); J Mater Res 26, 2335 (2011)

Testing Becker-Döring Theory for Dislocation Nucleation

Benchmark from brute-force MD

$\gamma_{xy} = 0.135$ $\sigma_{xy} = 2.16$ GPa T = 300 K



consistent

Prediction from Becker-Döring Theory

$$I^{BD} = f_c^+ \Gamma \exp\left(-\frac{F_c(\gamma,T)}{k_B T}\right)$$

rate per nucleation site

$F_c(\gamma=0.135, T=300K) = 0.53$ eV

$f_c^+ \Gamma = 3 \times 10^{13}$ $s^{-1} \sim \nu_D$

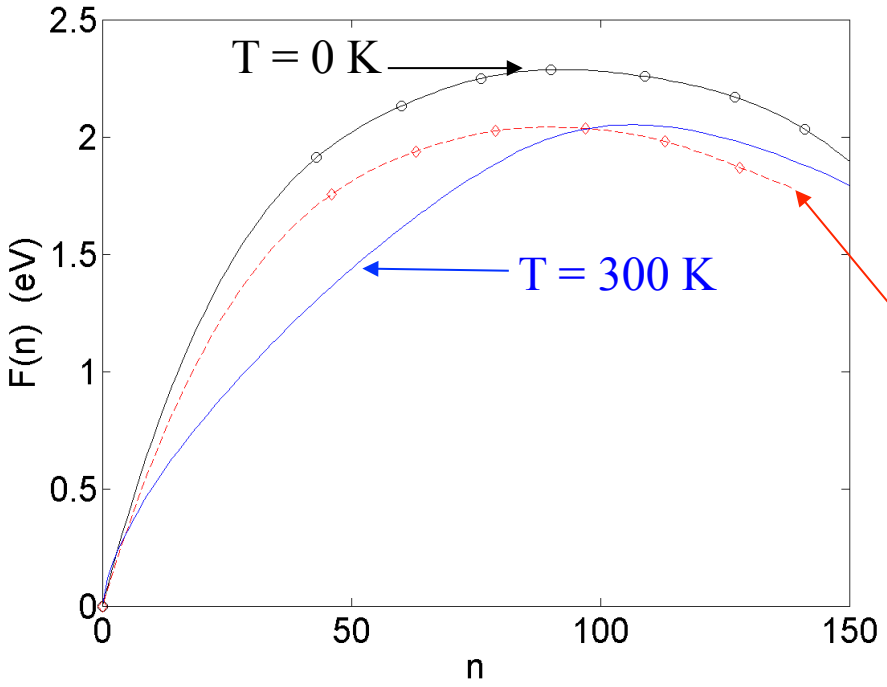
$N_{tot} = 14976$ (atoms)

$N_{tot}\, I^{BD} = 5.5 \times 10^8$ s^{-1}

MD ↔ MEP E_c $-TS_c$

Ryu, Kang, Cai, PNAS, 108, 5174 (2011); J Mater Res 26, 2335 (2011)

Origin of Activation Entropy $S_c(\gamma)$



Thermal expansion (anharmonic effect)

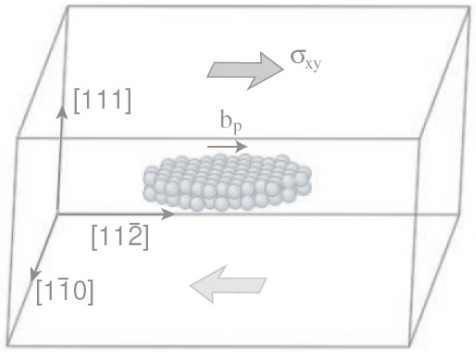
Increasing Temperature:

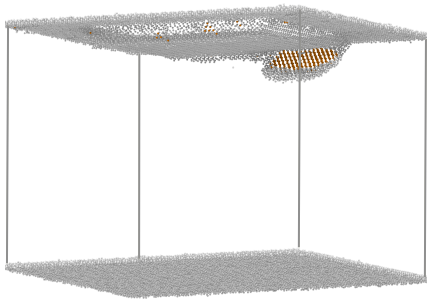
- atoms separated further
- interaction becomes weaker
- crystal is easier to shear

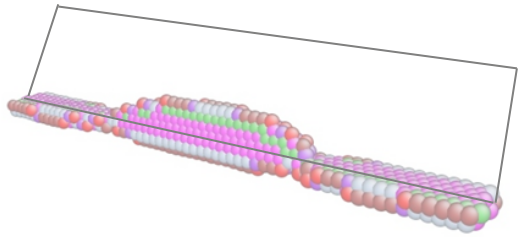
T = 0 K but hydrostatically strained to match thermal expansion at 300 K
(Cu CTE: $\alpha = 16.5 \times 10^{-6}\ K^{-1}$)

Ryu, Kang, Cai, PNAS, 108, 5174 (2011); J Mater Res 26, 2335 (2011)

Outline







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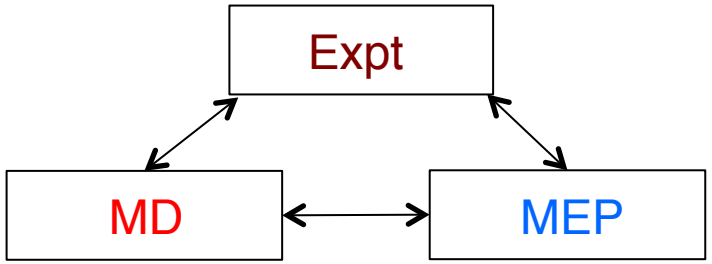
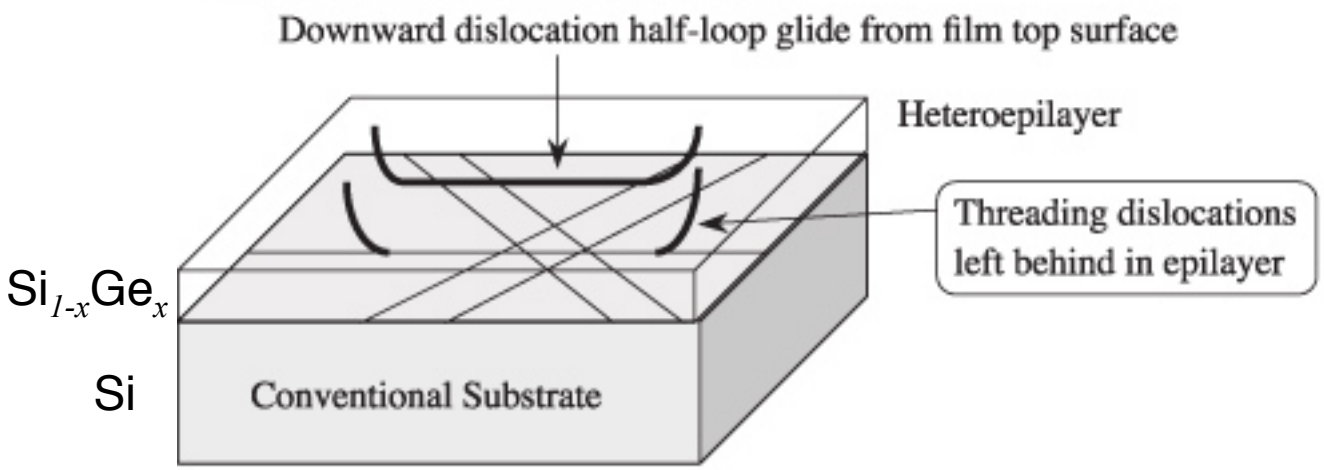


Dislocation Nucleation on SiGe/Si Film during Annealing

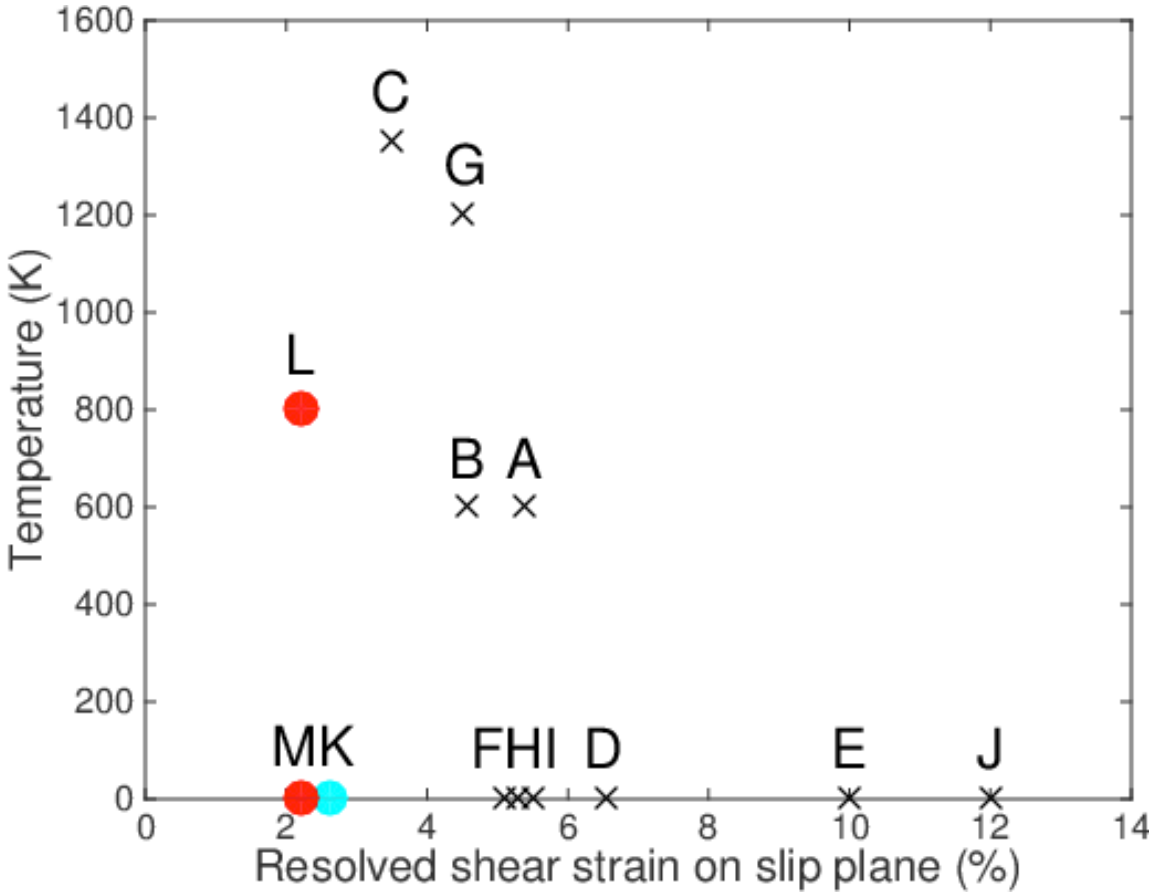
Maximum misfit (normal) strain $x = 1$ (between Ge and Si) : 4%, shear strain 2%

misfit (normal) strain at $x = 0.5$ (between $Si_{0.5}Ge_{0.5}$ and Si) : 2%, shear strain 1%



Dislocation nucleation from Si under applied compression as a model

Previous Predictions Require Too High Strain



A: surface step, shuffle set, tension
B: surface step, shuffle set, compression
C: surface step, glide-set, tension [3]
D: bulk corner, shuffle-set [4]
E: glide-set [5]
F: bulk corner, shuffle-set [4]
G: crack tip [6]
H: 2d ledge, shuffle-set [7]
I: surface step, glide-set, ab initio [8]
J: homogeneous, glide-set [5]

This work:
K: Pit shuffle-set,
L/M: Pit shuffle-glide complex MD/NEB

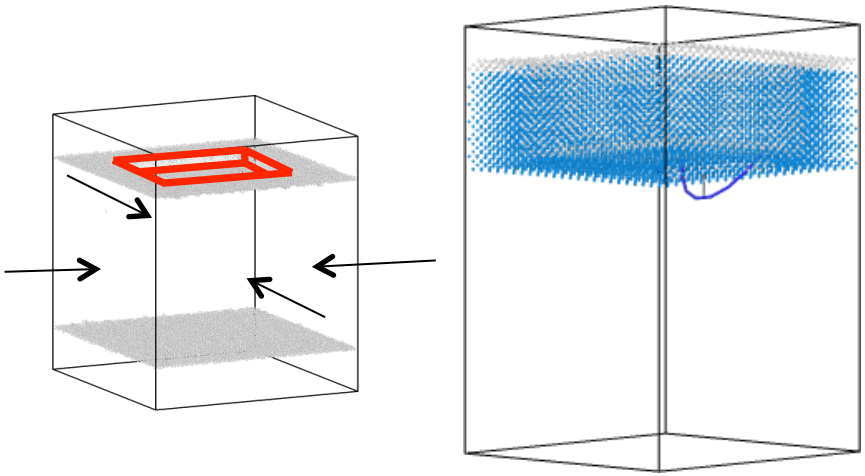
(references in notes)

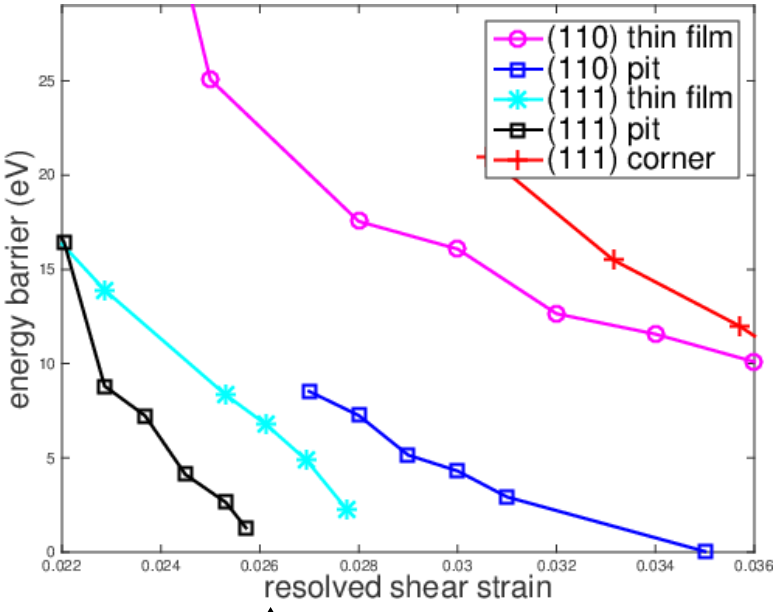
Energy Barrier for Nucleation from Surface Pit

flat surface

step/corner

surface pit



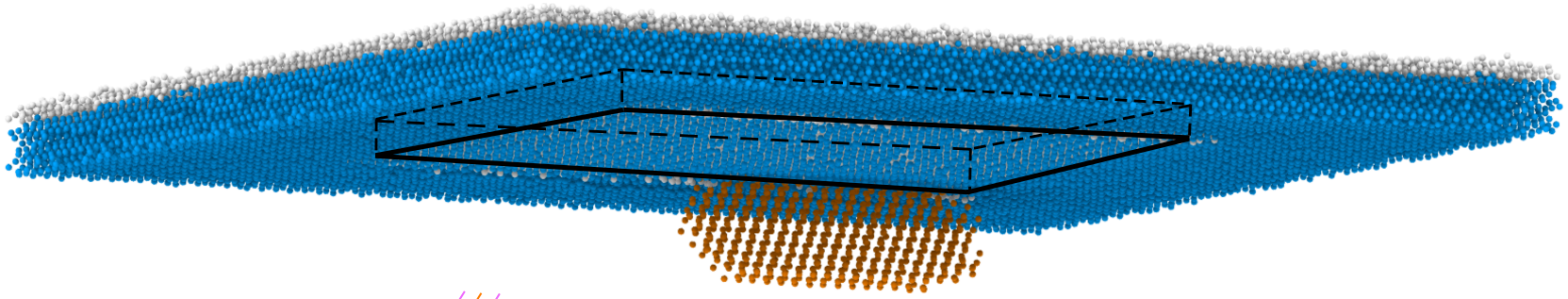


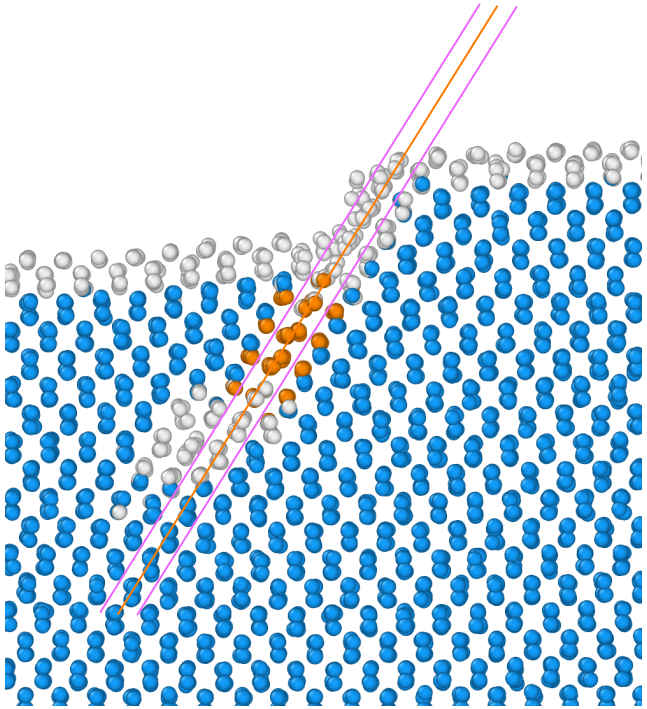
(K)

shuffle-set perfect dislocation

zero temperature prediction

Finite Temperature MD Predicts a Different Mechanism

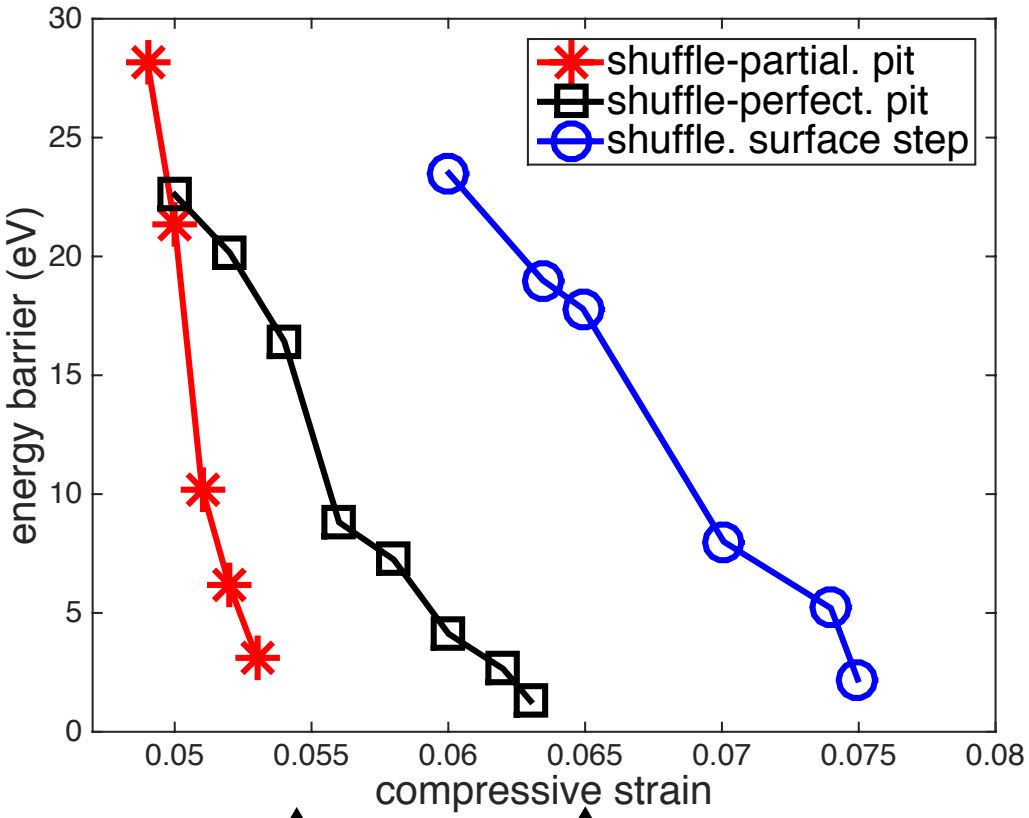




Findings:

1. Dislocation encloses a stacking fault !
2. So it cannot be shuffle-set perfect dislocation
3. It is not a glide-set partial dislocation either
4. It is a dislocation complex spanning one glide-set plane + two shuffle-set planes

Shuffle-Glide Complex Has Even Lower Energy Barrier

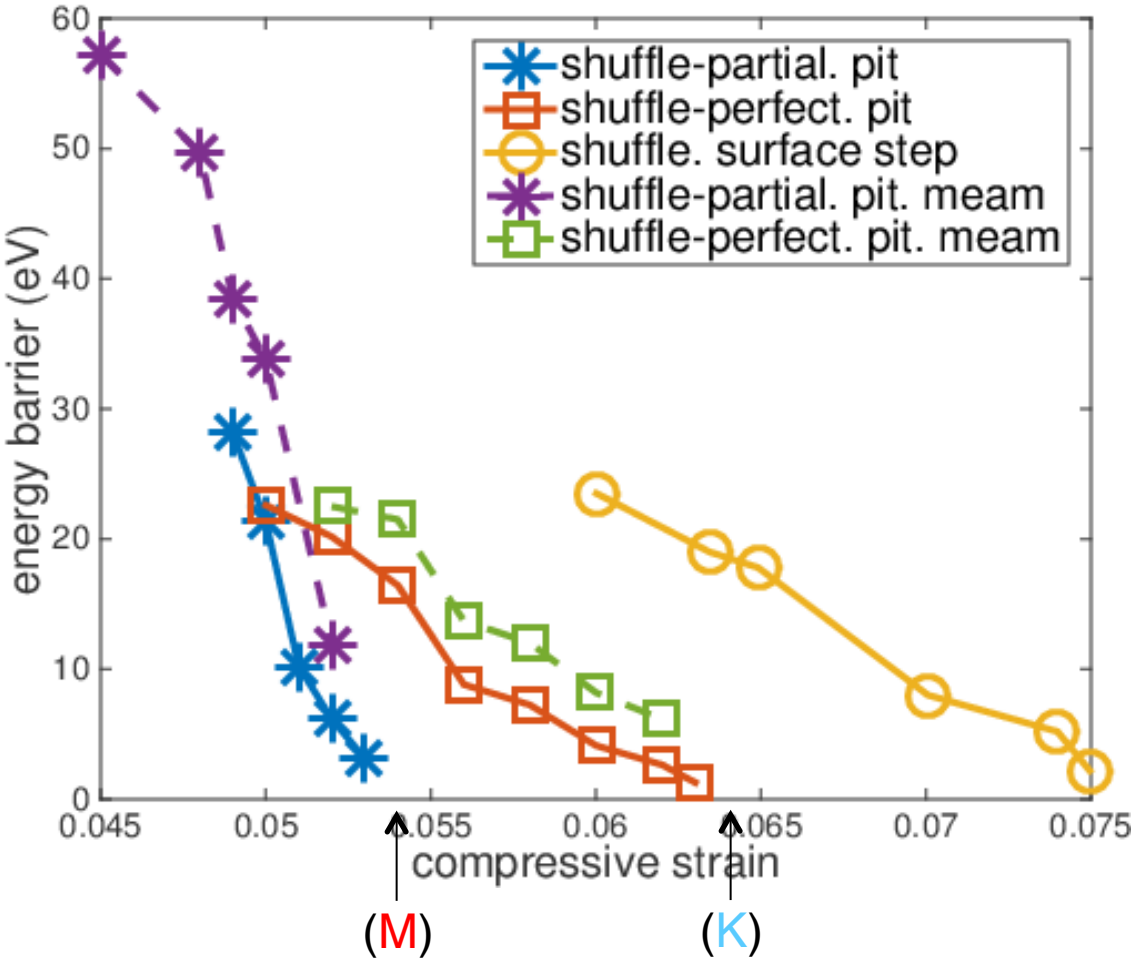


Stillinger-Weber (SW) potential

(M)
shuffle-glide complex
zero temperature prediction

(K)
shuffle-set perfect dislocation
zero temperature prediction

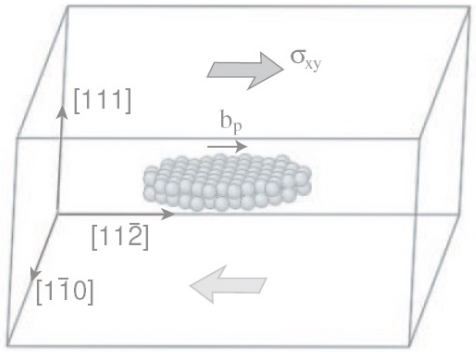
Effect of Interatomic Potential

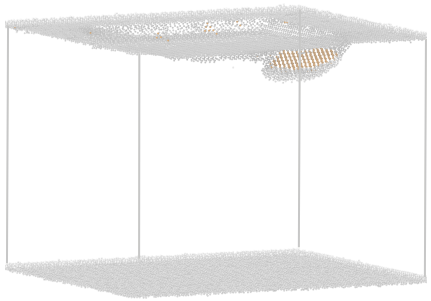


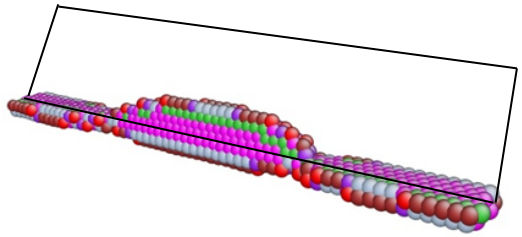
SW: solid lines
MEAM: dashed lines

- MEAM predicts higher energy barrier than SW
- Shuffle-glide complex still has lower barrier than other dislocations
- MD ←→ MEP consistent
- Inconsistency between MD/MEP and Expt probably due to **surface irregularity** and/or **new dislocation** types

Outline







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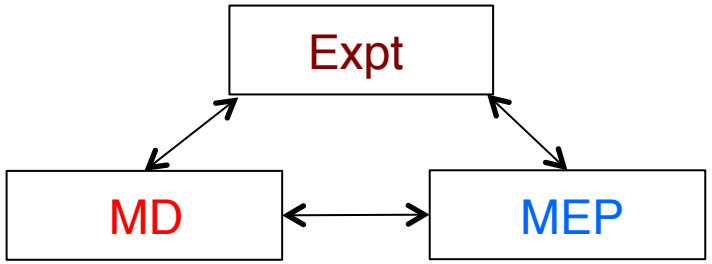
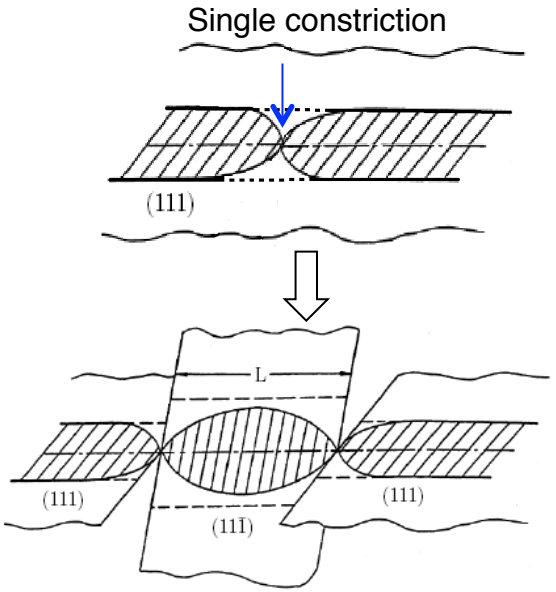
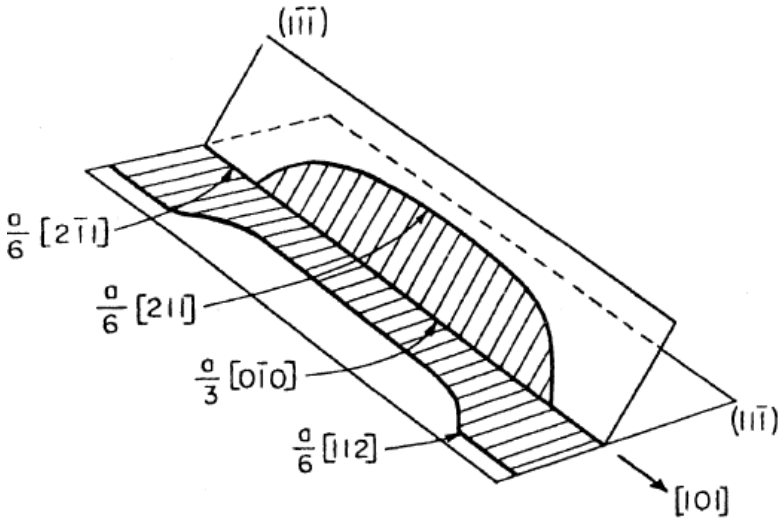


Proposed Mechanisms of 'Homogeneous' Cross Slip





Friedel-Escaig (FE)

1. Constriction forms on glide plane
2. Re-dissociates on cross-slip plane

Favorable at high T, low stress

Fleischer

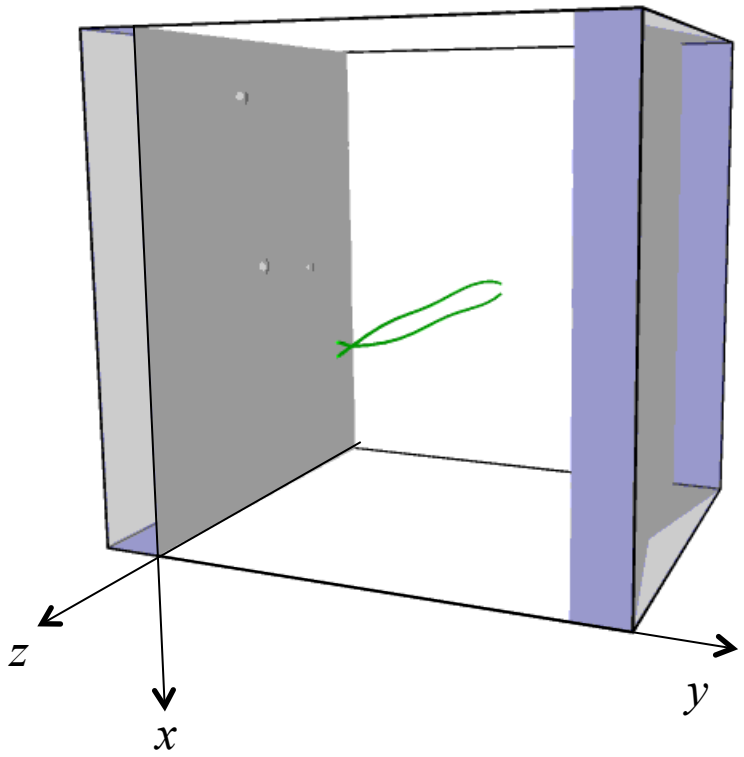
1. No constriction
2. 3D stacking fault structure

Favorable at low T, high stress

Which stress component?

Review by Puschl, Prog. Mater. Sci. 47, 415 (2002)

MD Simulation of 'Homogeneous' Cross Slip

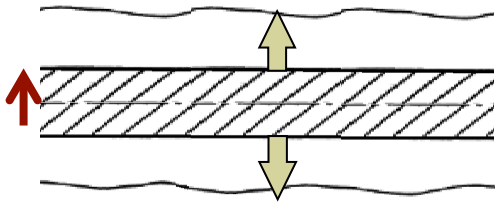


T = 550 K
σ_{yz} = 800 MPa,
σ_{zz}=-1944 MPa, σ_{yy}=1944 MPa,
σ_{xz}=1062 MPa

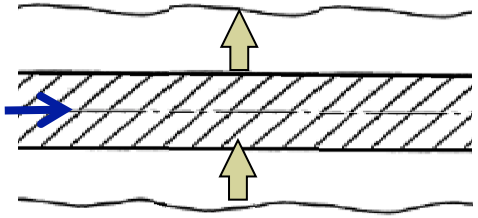
MD simulation (by MD++)
Dislocation extracted by Ovito/DXA

Various Stress Components

Escaig stress



Schmid stress



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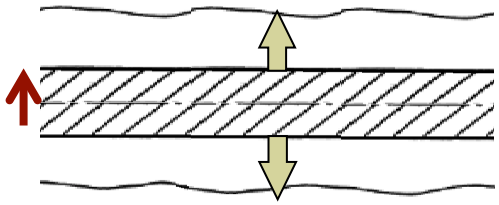

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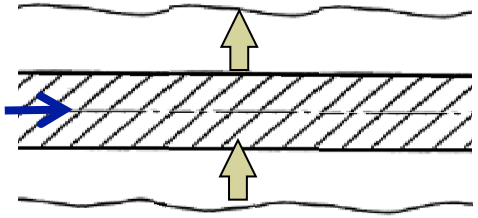
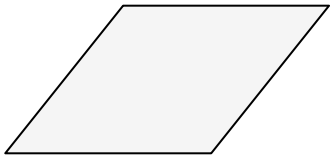
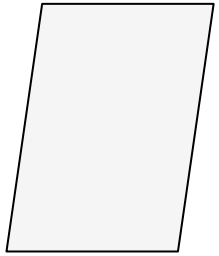


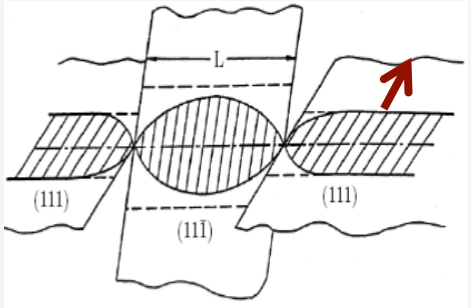
glide plane



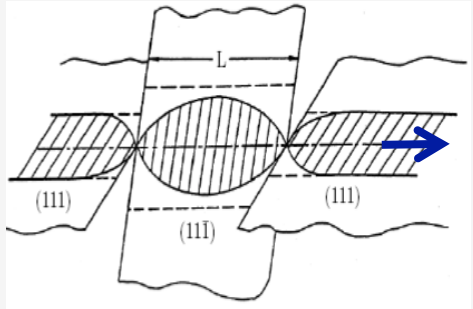
cross slip plane



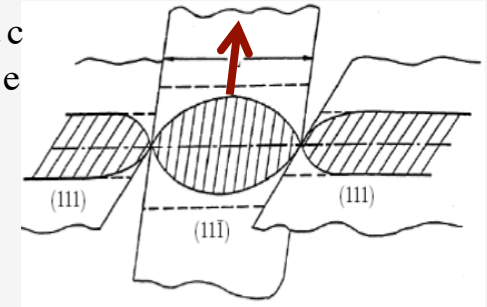
σ_e^g



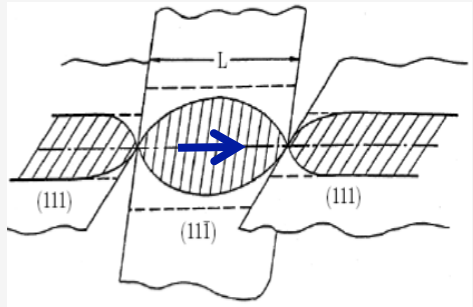
σ_s^g



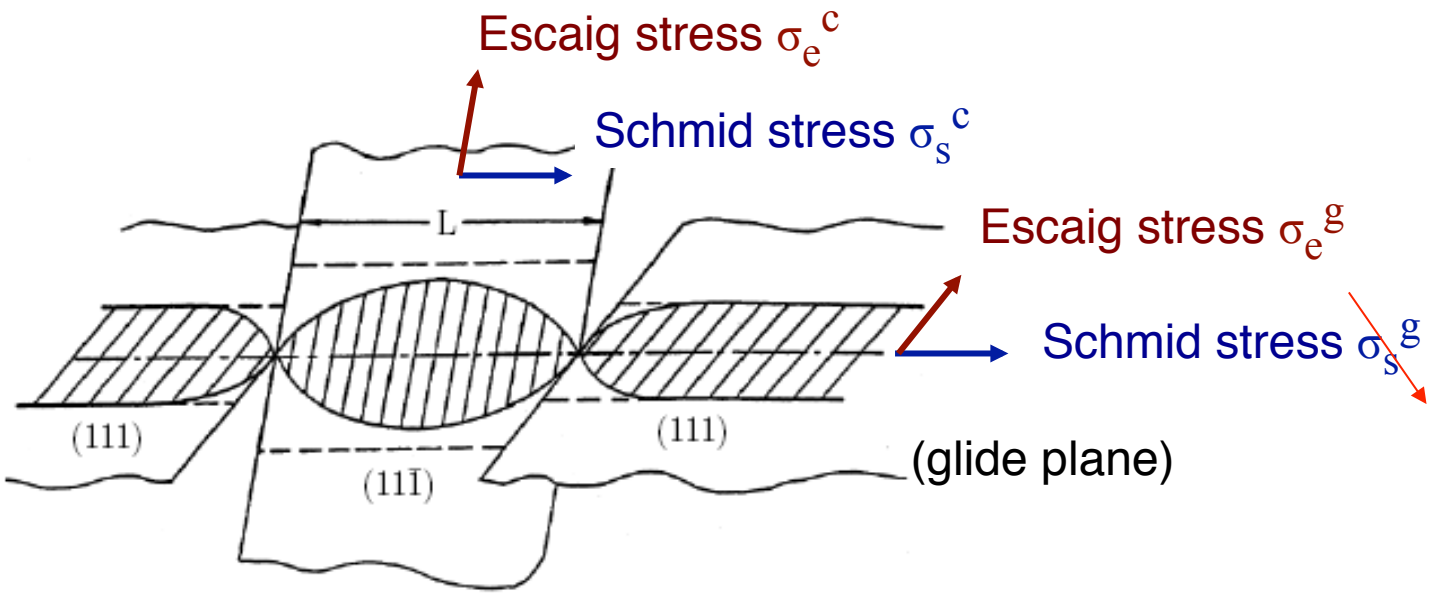
σ_e^c



σ_s^c



Effects of Multiple Stress Components

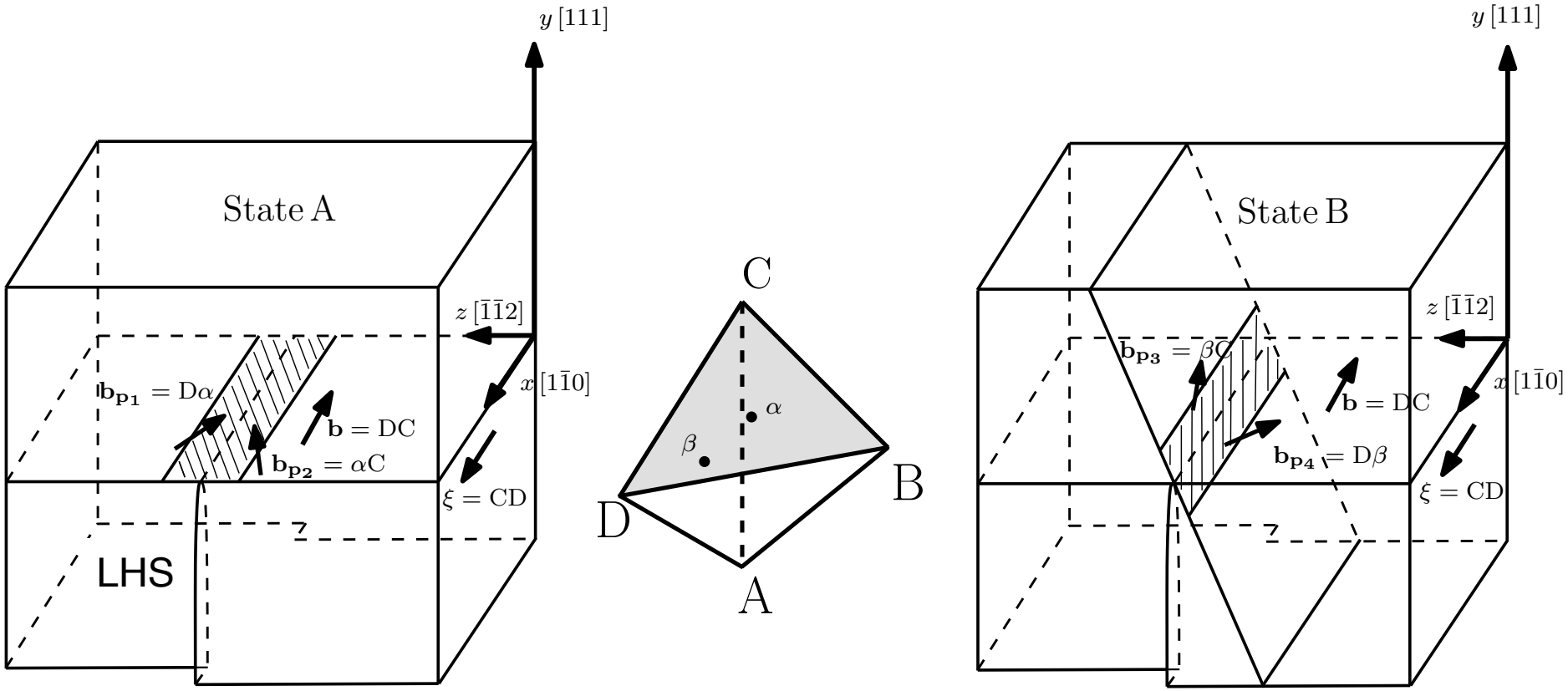


$$E_b(\sigma_s^g, \sigma_e^g, \sigma_s^c, \sigma_e^c)$$

No study has included effects of **all** relevant stress components

assume 0 (for now), i.e. dislocation not moving

Simulation Cell Set-up (skip)

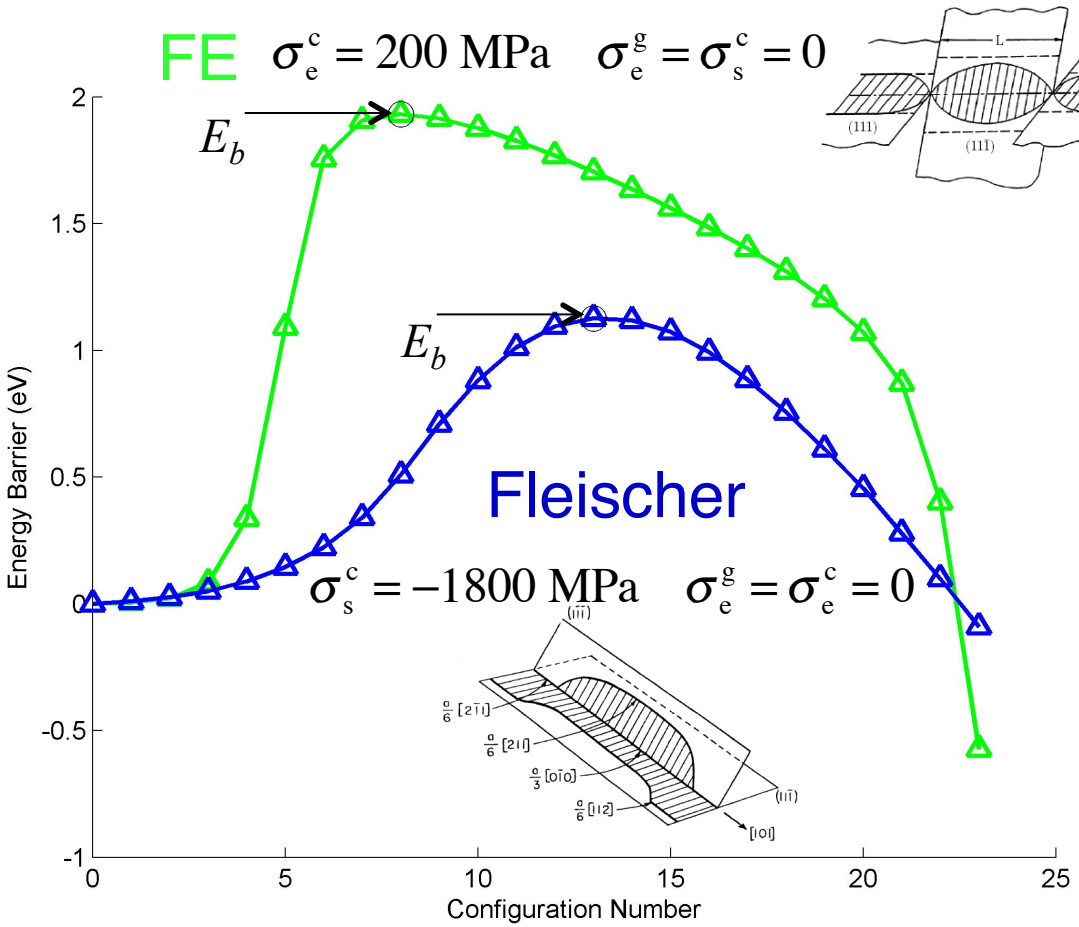


30[1 -1 0] × 30[1 1 1] × 20[-1 -1 2],
345600 atoms

PBC along x, z; free surface along y

Ni **EAM** potential 'vnih' used by S. Rao et al. Philos. Mag. A 79, 1167 (1999)
γ_{SF} (119 mJ/m^2) in good agreement with expt (125-128 mJ/m^2)

Converged minimum energy paths



What we need:

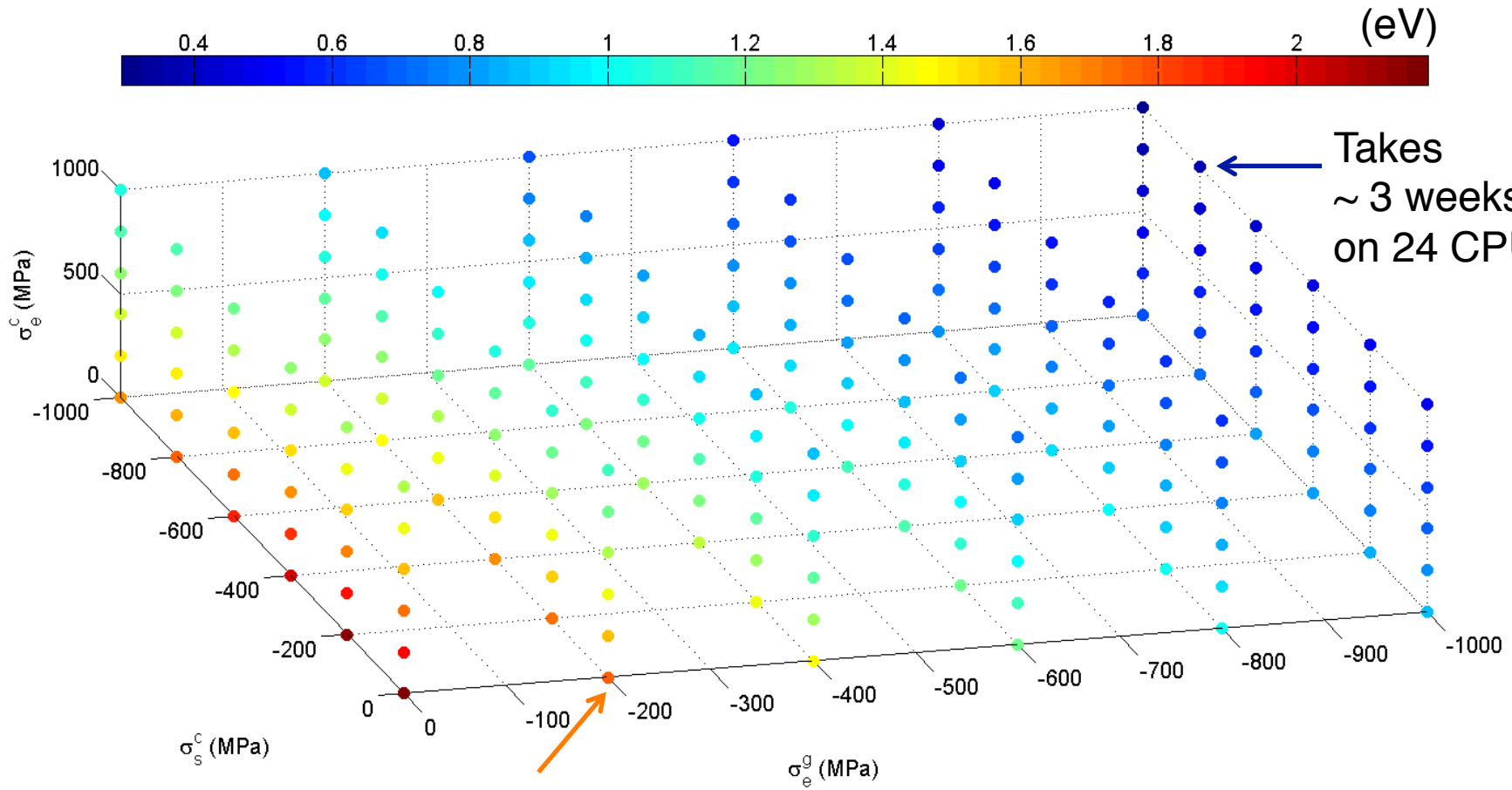
$-\sigma_e^g = 0,200,...,1000$ MPa

$\sigma_e^c = 0,200,...,1000$ MPa

$-\sigma_s^c = 0,200,...,1000$ MPa

$6 \times 6 \times 6 = 216$ stress states!

Atomistic Data: E_b for FE Mechanism

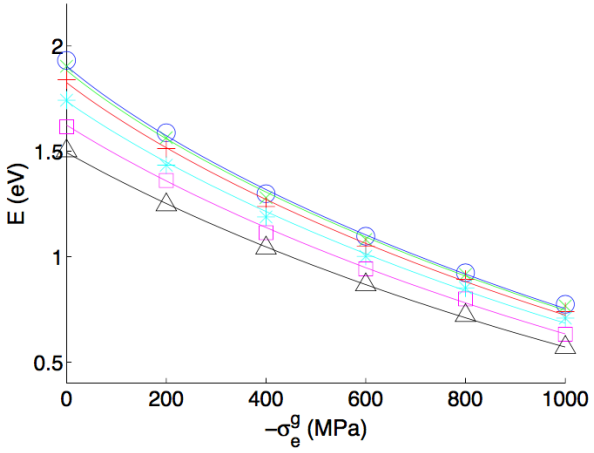


Takes
~ 3 weeks
on 24 CPU

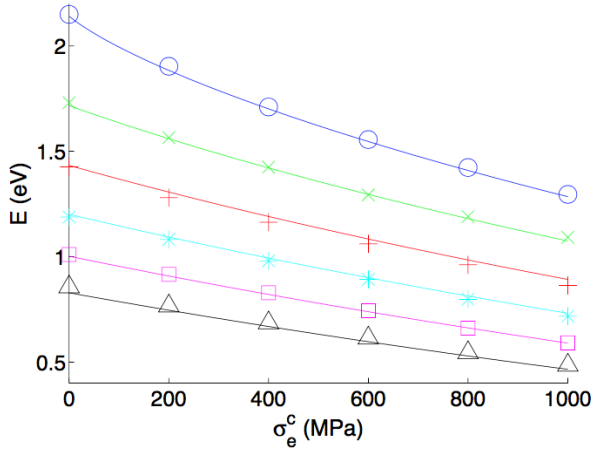
Takes
~ 1 week
on 24 CPU

W. Kuykendall, PhD Thesis,
Stanford University (2015)

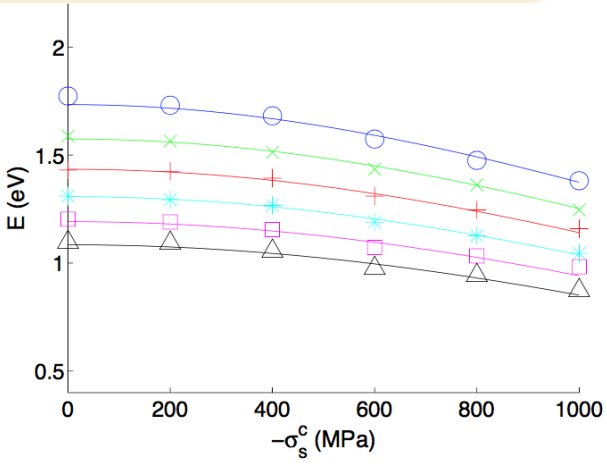
Effect of different stress components on E_b



(a) $E_b(\sigma_e^g)$ at $\sigma_e^c = 200$ MPa



(b) $E_b(\sigma_e^c)$ at $\sigma_s^c = -200$ MPa



(c) $E_b(\sigma_s^c)$ at $\sigma_e^g = -200$ MPa

E_b decreases most rapidly with $-\sigma_e{}^g$ (reduce spreading on glide plane)

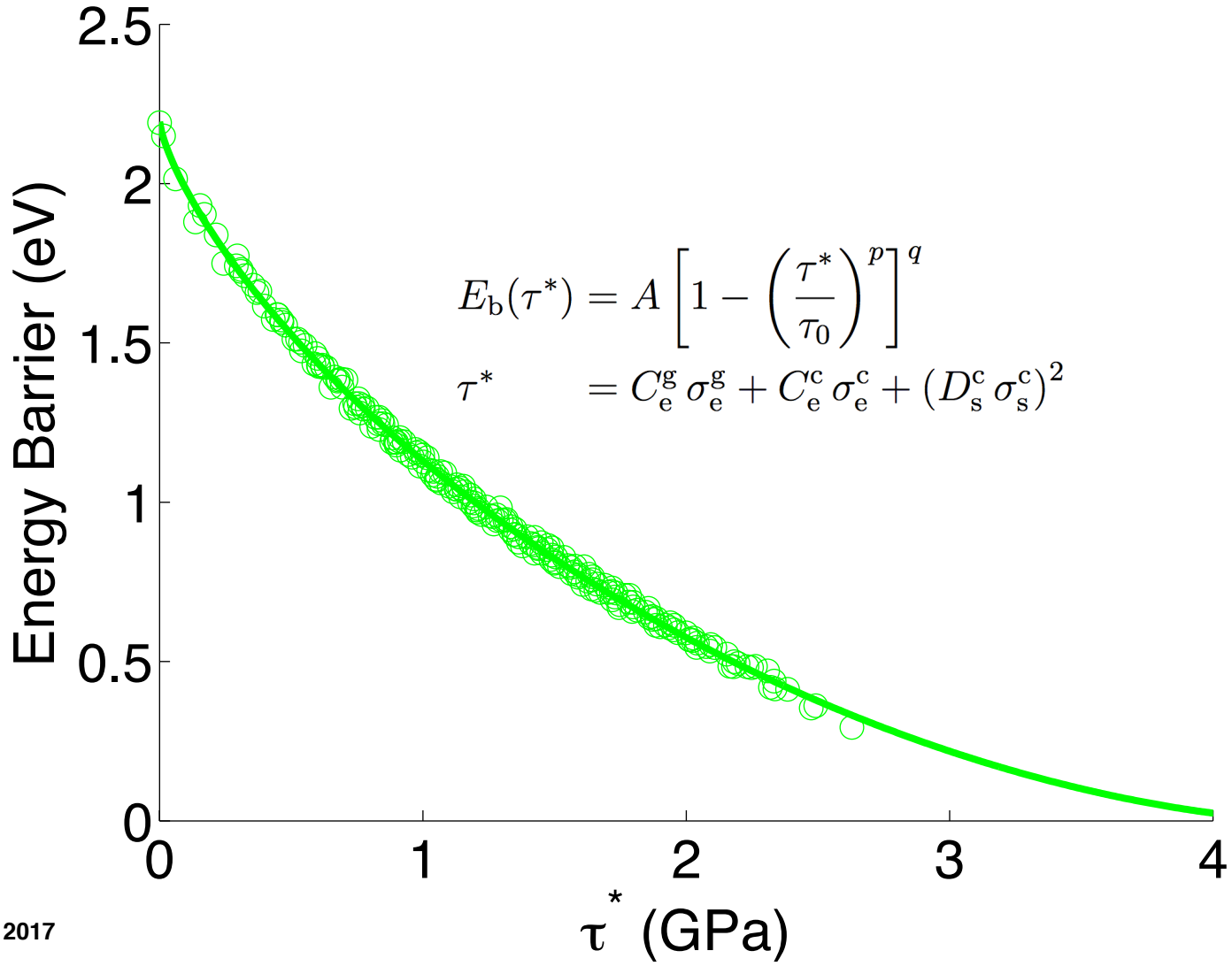
(increase spreading on cross-slip plane)

E_b is an even function of $\sigma_s{}^c$ (bow out on cross-slip plane)

$$E_b(\tau^*)$$

effective stress $\tau^* = C_e^g \sigma_e^g + C_e^c \sigma_e^c + (D_s^c \sigma_s^c)^2$

Express energy barrier function analytically



Are MEP results consistent with MD?

Cross slip rate

$$I^{CS} = A\frac{l}{l_0}\exp\left(-\frac{E_b(\sigma)}{k_B T}\right)$$

Kubin et al. Solid State Phenomena 1992

Frequency prefactor $\nu(l) = A\frac{l}{l_0}$

~ vibrational frequency of dislocation line
<< Debye frequency $\nu_D \sim 10^{13}$ s^{-1}

MD simulations:

20 runs, 25 ps each run, at T = 450 K, l = 15 nm

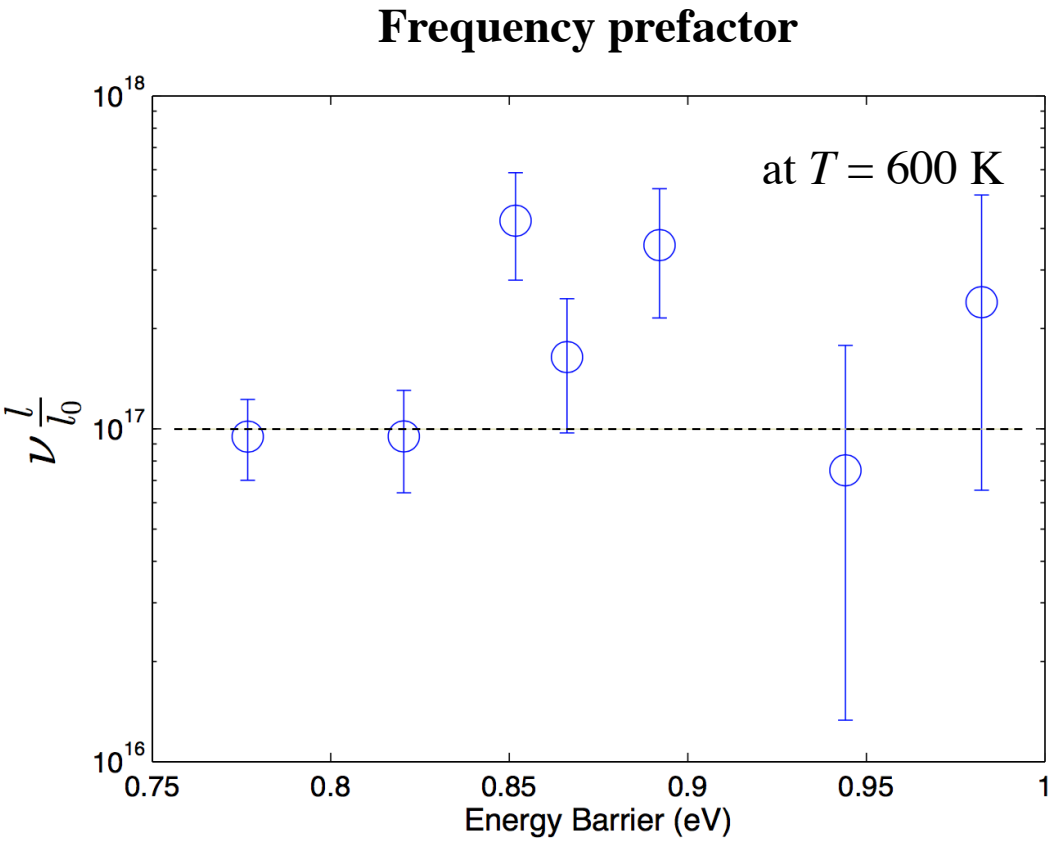
σ_{yz} = 0.8 GPa, σ_{zz} = -1.944 GPa, σ_{yy}=1.944 GPa, σ_{xz}=1.062 GPa

τ^* = 2.64 GPa, $E_b(\tau^*)$ = 0.52 eV, k_BT = 0.0388 eV, $\exp(E_b/k_BT) \sim 1.5\text{x}10^{-6}$
(cross slip not expected to occur under this stress at MD time scale)

Yet ~ 40% of MD runs show cross slip → $I^{cs} \sim 1.6\text{x}10^{10}$ s^{-1}

Frequency prefactor $A\, l/l_0 \sim 10^{16}$ s^{-1} >> ν_D

Cross slip: Are MEP results consistent with MD?



	Frequency prefactor $A\ l/l_0$
T = 450 K	10^{16} s^{-1}
T = 600 K	10^{17} s^{-1}

$A\ l/l_0 >> \nu_D \sim 10^{13}$ s^{-1}

Activation entropy?

William Kuykendall, PhD Thesis, Stanford University, 2015

Summary

- **Dislocation Nucleation in FCC Cu**

  activation entropy needed to bring consistency between
  MD ←→ MEP

- **Dislocation Nucleation in DC Si**

  surface features/ new dislocation may bring consistency between
  experiment ←→ MD/MEP

- **Dislocation Cross Slip in FCC Ni**

  activation entropy needed again to bring consistency between
  MD ←→ MEP (?)