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Case Studies of the Temperature Dependence of Grain Boundary Mobility

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TMS '15 Symposium:
Polycrystalline Materials: Bringing Together experiments, Simulations, and Analytic Theories

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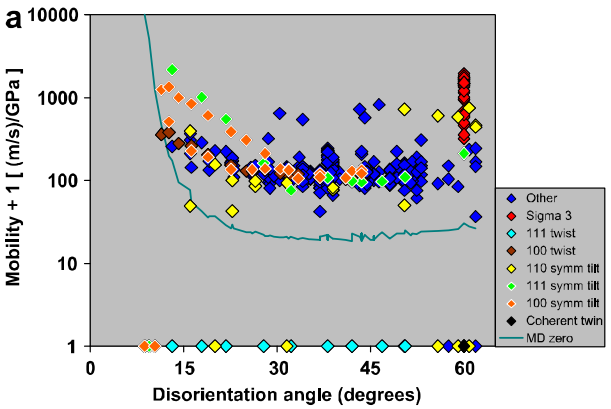
Grain Boundary Mobility

- Conventional wisdom is that thermally activated GB motion is described by a single *activation energy*
- Recent work regarding mobility shows the great variety of temperature (in)dependent behavior
  - Olmsted, *et al. (2009)*, calculated GB mobility for a set of 388 boundaries at 1400K
  - Homer, *et al. (2013)*, classified their temperature dependent mobility into categories based on the **shape** of their Arrhenius mobility plot

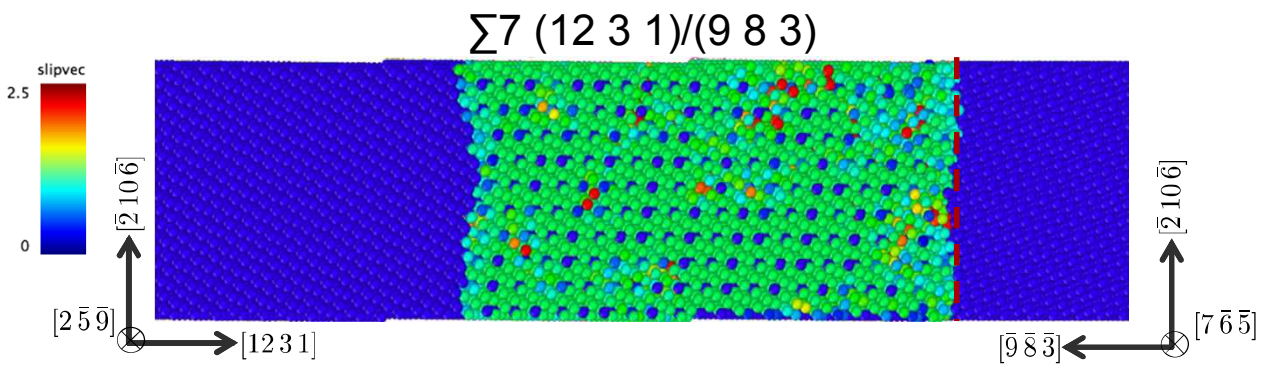
I. Thermally Activated (~57%)
II. Non-thermally Activated (~20%)
III. Mixed Modes: Transition between two regions at a temperature (~14%)
IV. Unclassifiable or Immobile (~9%)

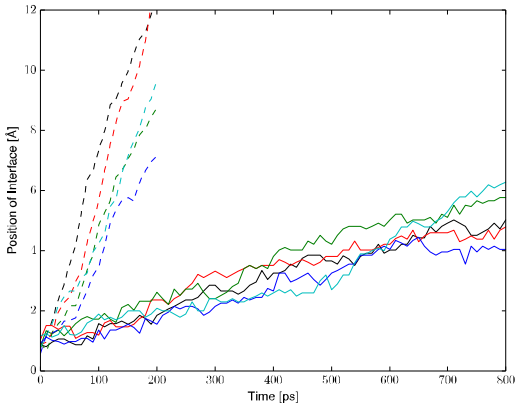


D.L. Olmsted, E.A. Holm, and S.M. Foiles, Acta Mater. 57, 3704 (2009)
E.R. Homer, E.A. Holm, S.M. Foiles, and D.L. Olmsted, JOM 66, 6 (2013)

Simulated GB Motion is Caused by an Orientation–dependent Driving Force

- None of the boundaries examined exhibit shear coupling
- GBs are planar and driven by orientation dependent driving force†
  - Implemented as ‘fix orient/fcc’ in LAMMPS
- Mobility is defined as: M = $v \cdot p$
  - Velocity is determined by averaging many boundary velocities
  - Pressure is determined by thermodynamic integration of driving force
- Atoms are colored by slip-vector‡





†K.G.F. Janssens, D. Olmsted, E.A. Holm, S.M. Foiles, S.J. Plimpton, and P.M. Derlet, Nat. Mater. 5, 124 (2006)
‡G.J. Tucker, J.A. Zimmerman, and D.L. McDowell, Int. J. Eng. Sci. 49, 11 (2011).

Arrhenius Plots of Mobility for Selected GBs

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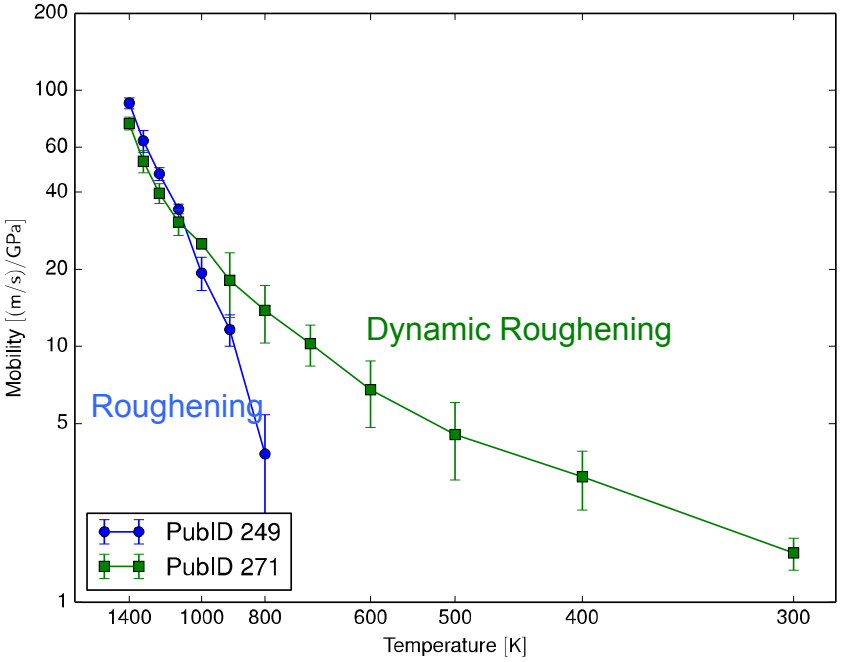
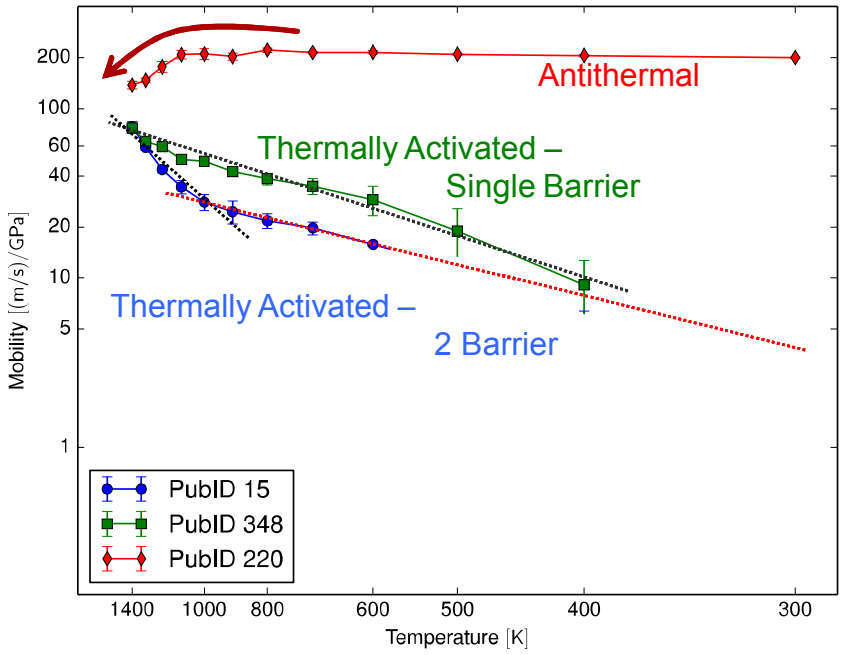
I. Thermally Activated
   1. Single Activation Energy
      ∑15 (12 5 1)/(12 5 $\bar{1}$)
   2. Two Activation Energies
      ∑5 (2 1 1)/(2 1 1)
   3. Roughening Transitions
      1. Dynamic ∑9 (5 4 2)/(2 1 0)
      2. Static ∑5 (13 1 0)/(11 7 0)

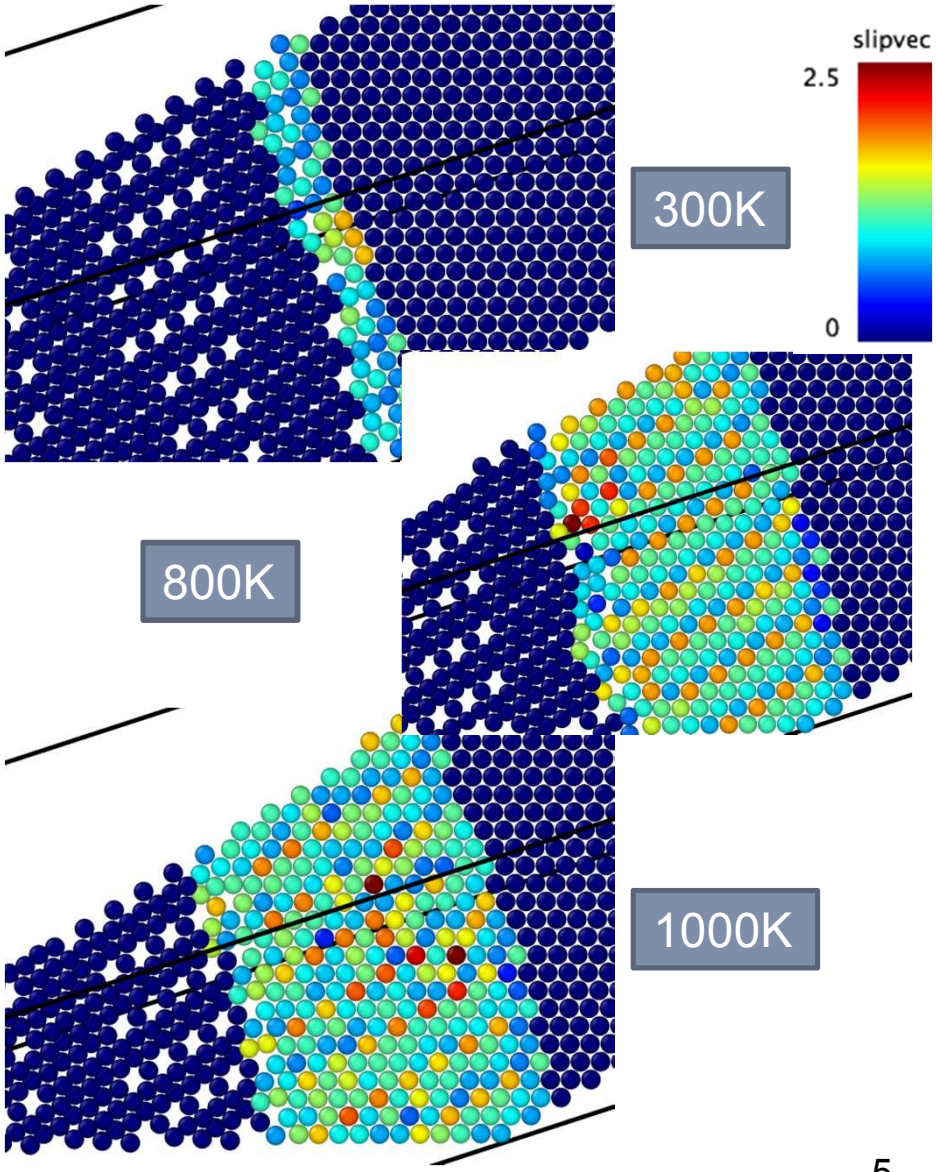
II. Non-Thermal
   1. Antithermal
      ∑7 (12 3 1)/(9 8 3)





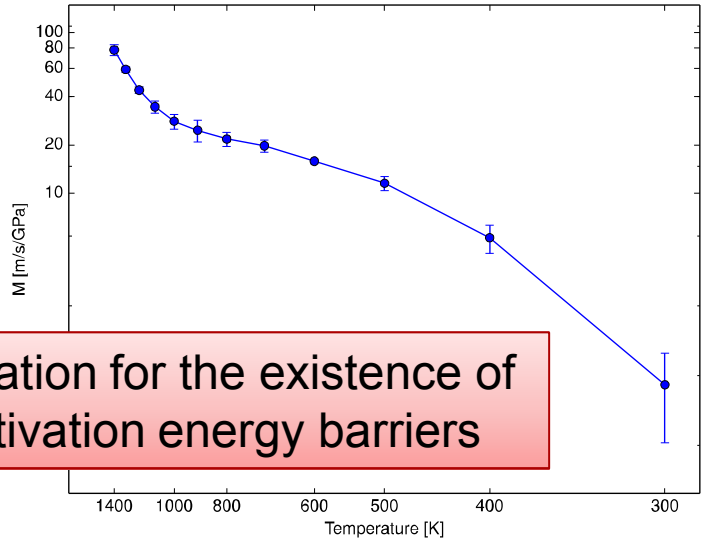
Straight-forward case of a Linear Arrhenius plot

- Slip-vector analysis shows regular pattern affected by the motion of dislocations
- Pattern is disrupted by fluctuations at higher temperatures

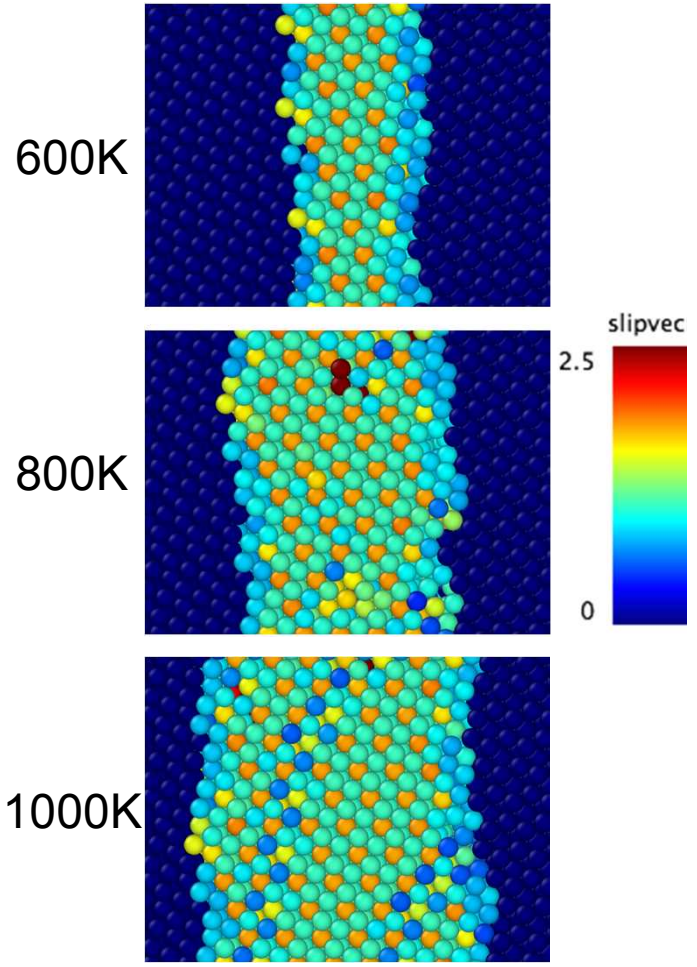


Is the 2-activation energy barrier an artifact of the plot?

- If two barriers exist, then we should see a difference in the propagation mechanism at ~800K
- Slip-vector analysis does not indicate a difference between mechanism above or below 800K



No indication for the existence of two activation energy barriers

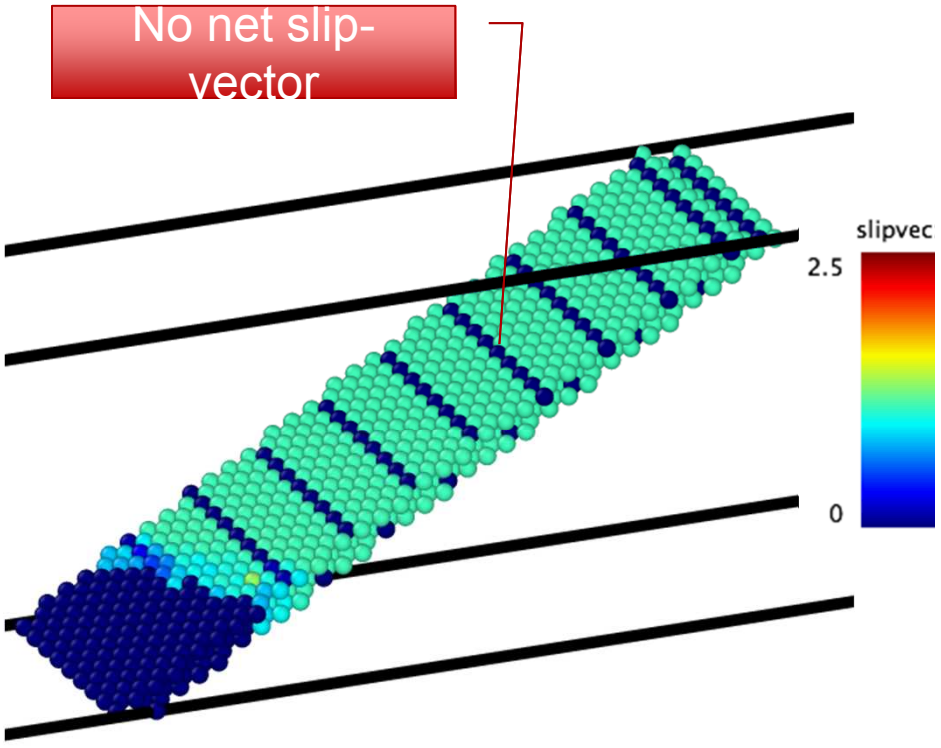


Antithermal Boundary

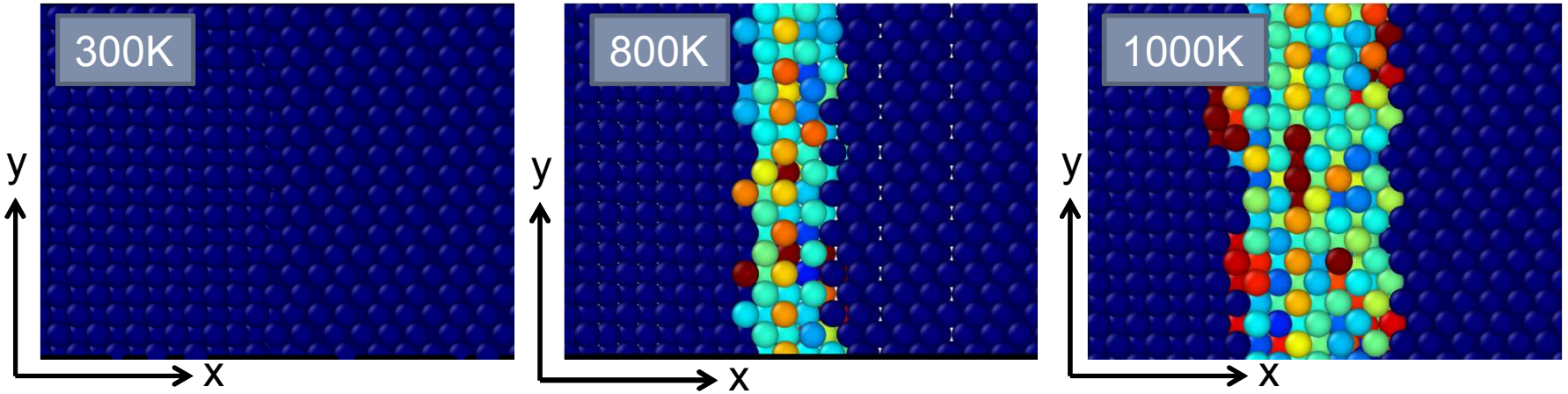
- Extremely high mobility boundary
- Cooperative motion is evident
- Mobility *decreases* with increasing temperature T ≥ 1000K

Hypothesis:

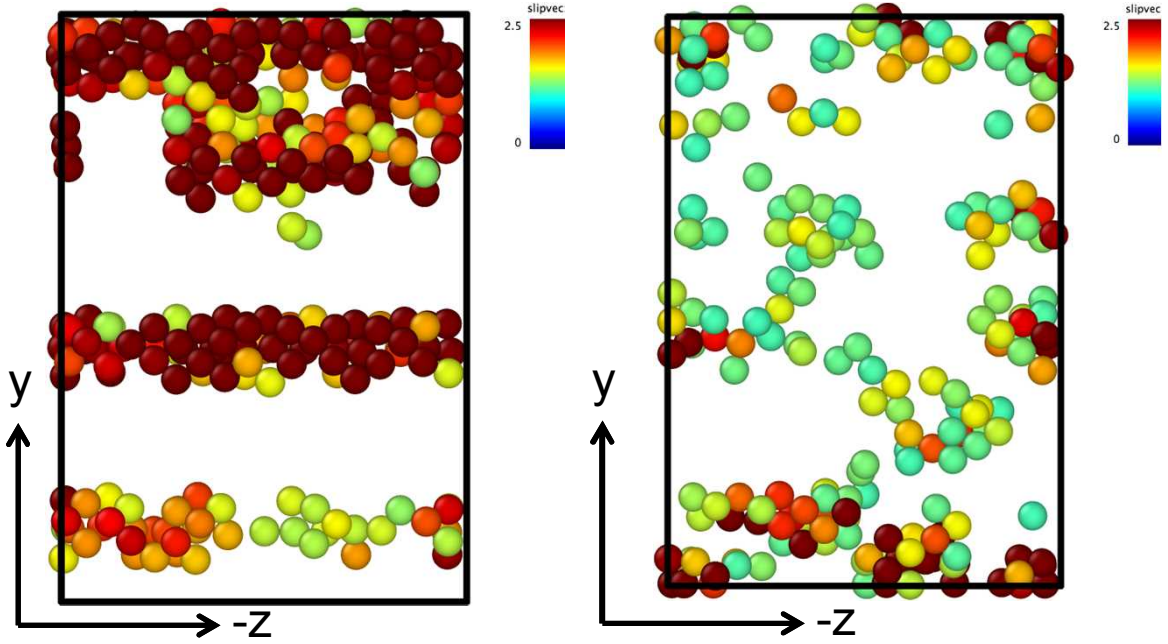
- Increasing temperature makes returning the slipped atoms to their original position increasingly less efficient



Motion mechanisms of GBs with Roughening Transitions



- Roughening boundaries are only mobile above the roughening temperature
- GB migration is blocked at 800K by formation of bands
- At 1000K the boundary moves by the nucleation and growth of islands



Dynamic Roughening Behavior is Driving Force Dependent

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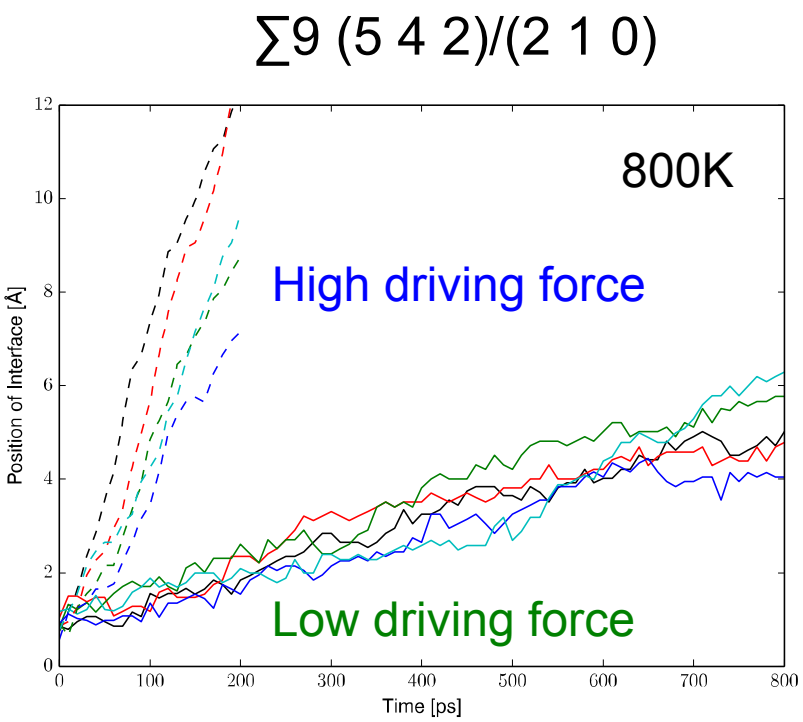

- Driving force dependence occurs below T_R
  - Mobility plot does not show a transition at T_R, but inspection of atomistic configurations does
  - Small migration distances lead to large deviation of mobility values
- Migration Mechanism
  - Nucleation and growth of islands†
  - Driving force governs nucleation rate

†C.P. Race, J. von Pezold, and J. Neugebauer, Phys. Rev. B 89, 214110 (2014).

Driving Force affects a noticeable change in nucleation mechanism at T_R

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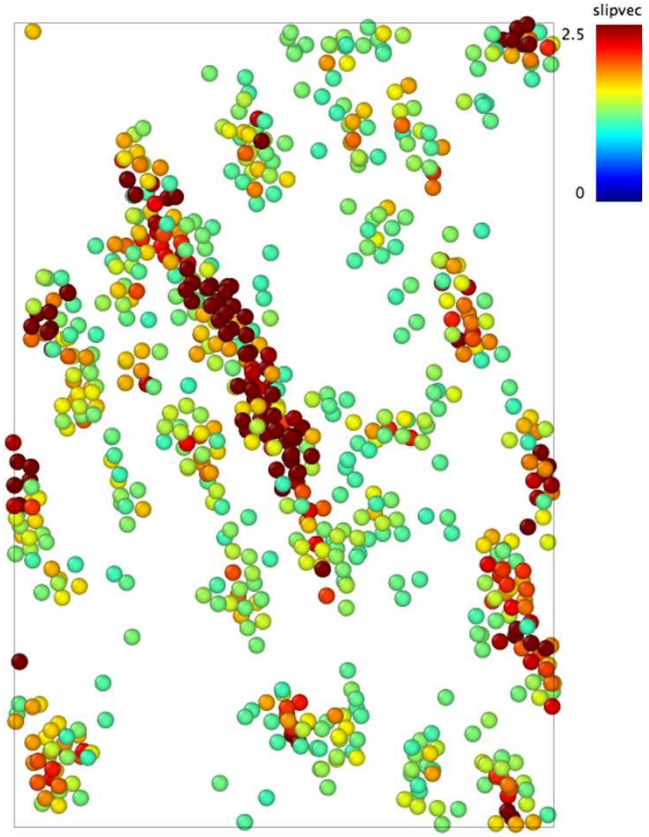
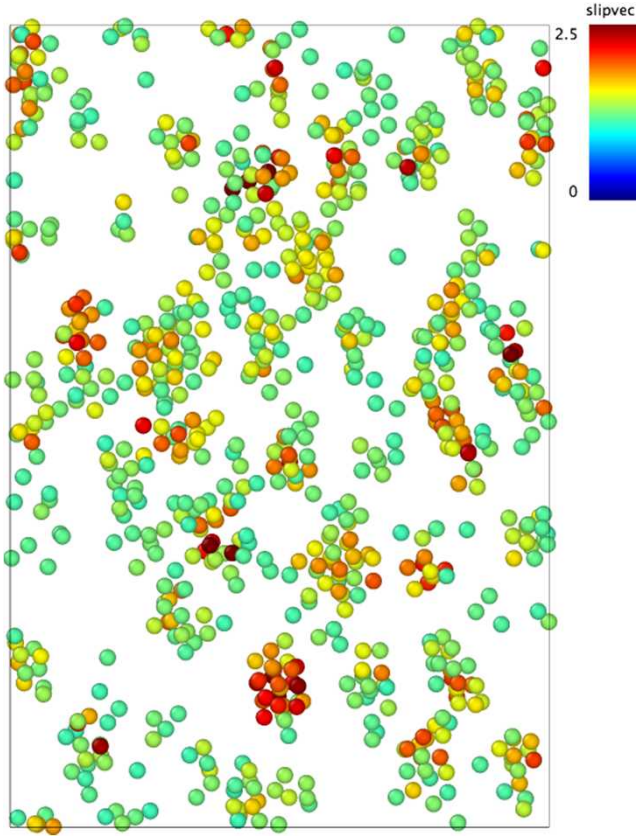
u_0 = 0.005 eV/at.



u_0 = 0.025 eV/at.



Nucleation of *highly localized* and *highly slipped* regions gives way to the formation of *numerous distributed* island nuclei at higher driving forces

Contrast between roughening and non-roughening behaviors

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Static and Dynamic Roughening boundaries propagate by the nucleation and growth of islands

- Boundary position moves non-uniformly
- Low temperature (static) or low force (dynamic)
  - Few nuclei consisting of highly slipped atoms
  - Strong crystallographic alignment
- High temperature (static) or high force (dynamic)
  - Many nuclei of consisting of slightly slipped atoms

Thermally activated and antithermal boundaries migrate by dislocation mediated mechanisms

- Boundary position moves uniformly
- Mechanism can be cooperative or local

Grain Boundary Mobility: *More than the slope of a line*

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- Mobility is a complicated phenomenon not easily classified by a unique activation energy
  - Characterization of motion mechanism by features of mobility plot is insufficient to determine *atomistic* mechanism of motion
- Tracking motion of individual atoms to determine mechanism is difficult and to easily misses important collective motion
- Recommended characterization approach
  - Utilize metrics (e.g. slip-vector)
  - Focus on collective behavior of atoms
    - In lieu of trying to match the motion of atoms to explain an 'activation energy'

Can a metric-based characterization of atomistic motion mechanisms inform our understanding of what crystallographic parameters govern mobility?