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Title: Simulations of Dislocation Pile-ups at Asymmetric Tilt Boundaries in Aluminum

Author(s): Steven M. Valone, MST-8
Jian Wang, MST-8
Richard G. Hoagland, MST-8
Timothy C. Germann, T-1

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Simulations of Dislocation Pile-ups at Asymmetric Tilt Boundaries in Aluminum

Steven M. Valone, Jian Wang, Richard G. Hoagland, and Timothy C. Germann
Materials Science and Technology and Theoretical Divisions
Los Alamos National Laboratory
Los Alamos, NM 87545 USA

Materials deformation processes are increasingly approachable through the both conventional and accelerated molecular dynamics. In one deformation process, dislocation pile-up at a grain boundary, a greater understanding is required as to how dislocations transmit through grain boundaries, causing plastic deformation, or reflect and reconstruct the grain boundary, but with no macroscopic deformation. Here dislocation pile-ups in an aluminum bicrystal with an asymmetric tilt grain boundary are simulated atomistically, introducing effects of dislocation interactions beyond linear elastic ones. The observed responses as functions of the number of explicitly modeled dislocations and the magnitude of the applied stress are discussed.

Typical conditions for the simulations consist of thermal relaxation room temperature, five active dislocations inserted within a 6.5-million-atom cell, and an additional fourteen dislocations represented within the atomistic simulation by their elastic strain fields. The dislocations are initially distributed according to linear elastic estimates of their positions in a double-ended pile-up from a chosen far-field stress. The whole cell is allowed to relax according to a procedure to be described. In the ensuing simulations, the system is propagated for some substantial period of time (10s of ps), followed by small increments of strain. After a number of such increments, we observe all of the anticipated events. Usually several of the closest dislocations are absorbed into the grain boundary, resulting in varying amounts of reconstruction. Reflections from the boundary are common and show a strong dependence on sample thickness. Transmission events are seen on both slip systems in the other grain. The particulars of these events will be described as well.

Simulations of Dislocation Pile-ups at Asymmetric Tilt Boundaries in Aluminum

Steve Valone[1], Jian Wang[1], Dick Hoagland[1], Tim Germann[2]

[1] MST-8: Structure/Property Relations

[2] T-1: Physics and Chemistry of Materials

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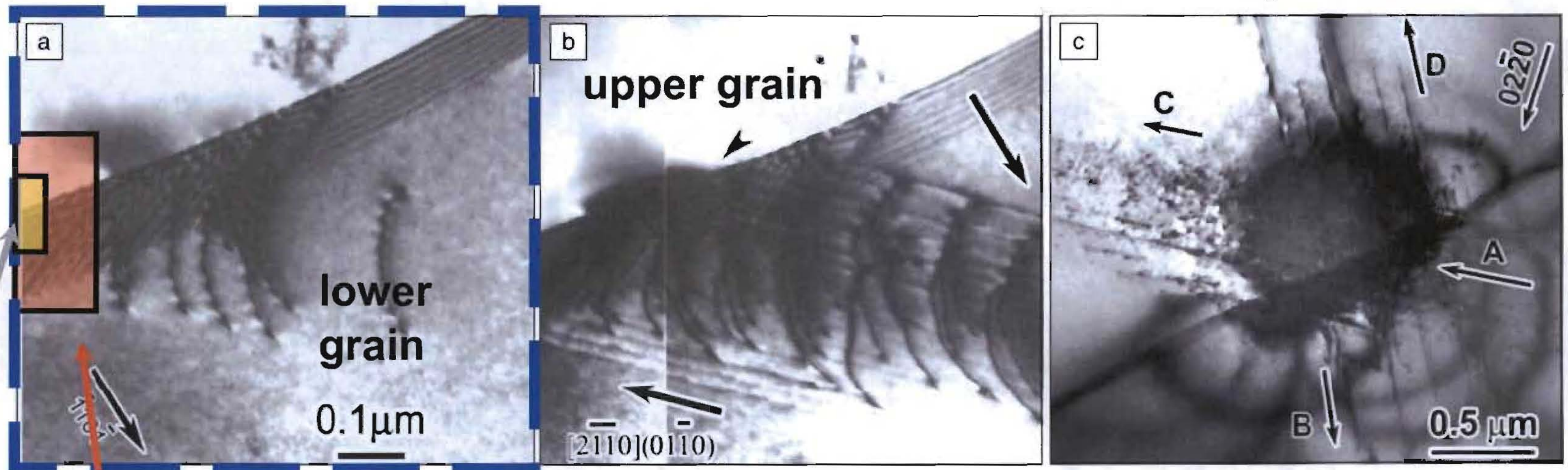
Project on Spatio-Temporal Frontiers of Atomistic Simulations in the Petaflop Computational World

Collaborators: Art Voter, Danny Perez, Jim Hammerberg, Davis Tonks, Joel Kress, Steve Sintay, Sriram Swaminarayan, Shengnian Luo, Saryu Fensin

Dislocation Pile-Up

Material under stress | Dislocations moving | Penetration thru grain boundary

Full capa bility



Present modeling capability

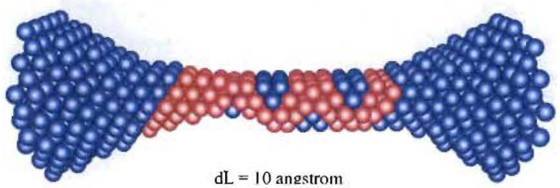
Early test runs on RR

In-situ Transmission Electron Microscopy (TEM) image in α-Ti (hexagonal close-packed) of dislocations in lower grain interacting with upper grain, through grain boundary
(I.M. Robertson *et al.*, MRS Bulletin, Feb 2008)

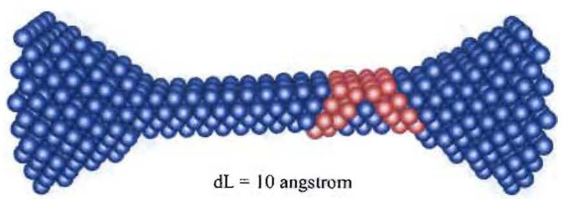
Dislocation pile-ups featured in Hall-Petch strength models

Rate Dependent Processes

Ag (EAM) nanowire in tension: *30 % strain*



Parallel-Replica Dynamics [Voter, 1998]: 10^4/s



Traditional MD: 10^8/s

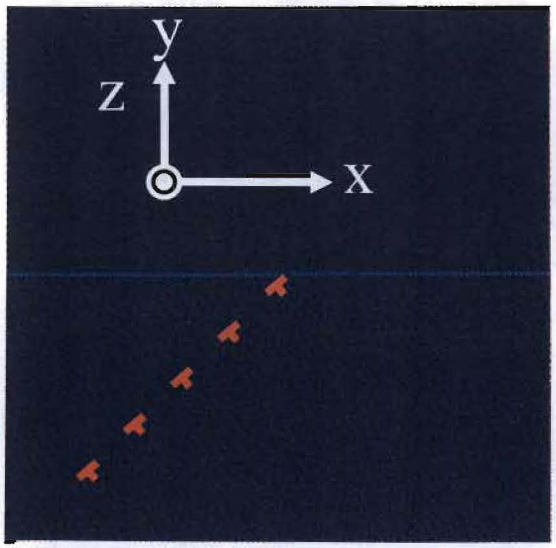
Strain rate effects widely recognized

Longer simulation times allow slower, more realistic strain rates

Alternate large-scale MD w/ AMD

Setup of MD Simulations

Grain Boundary Simulations



{111}top||{110}bottom
Σ_{11} tilt

Ercolessi-Adams Embedded Atom Method Al

Simulation cell

GBs : asymmetrical Σ_{11} in Al (x-z plane)
Boundary: periodic along z
Dimension: X = Y = 160 nm

z (nm):	3	10	20	30
atoms: (x 10^6)	4	12.5	25	37

Active and passive dislocations

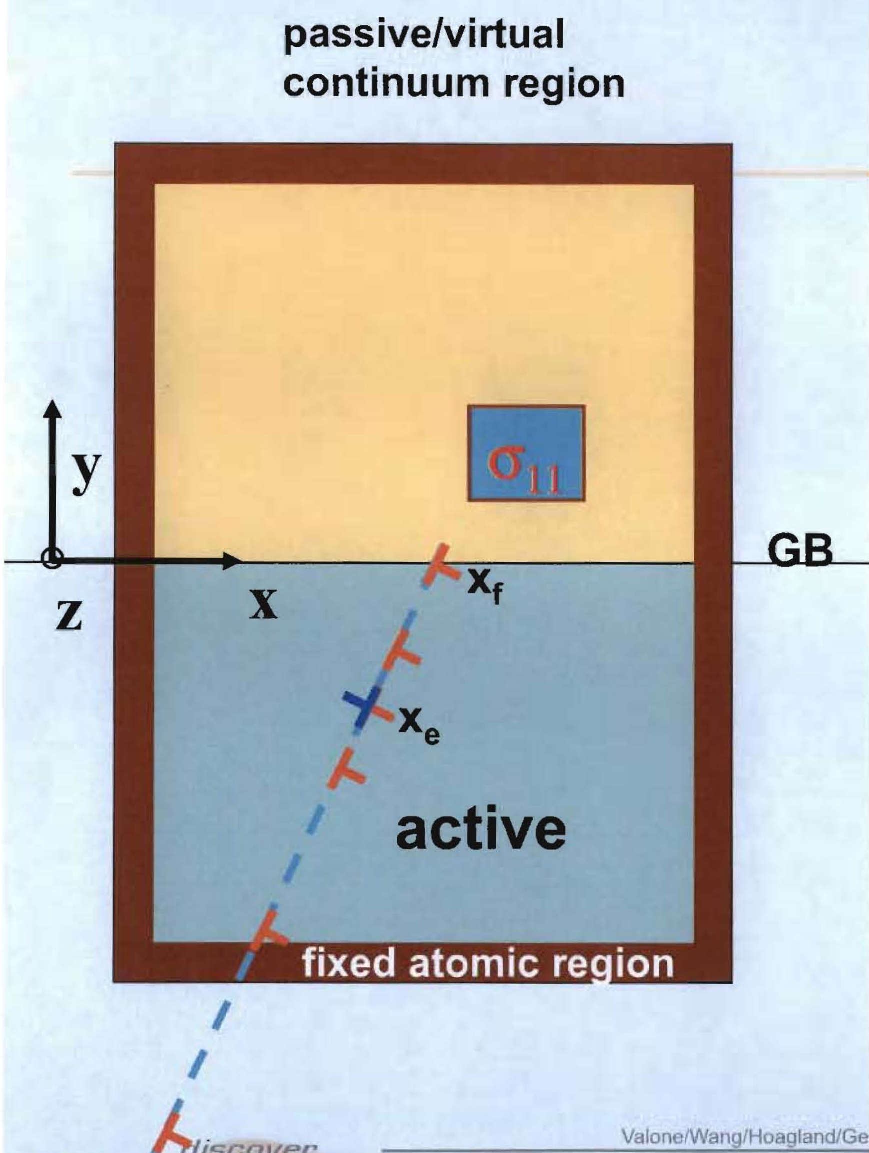
MD simulations

Loading: uniaxial tension along the x axis

- Start at RSS = 0.75 GPa at 1st dislocation
- For a given stress, run MD for 50 ps
- Increase applied stress in 0.03 GPa Repeat MD

Simulation cell

Method for Introducing dislocations



- 3 steps: **Estimate-Introduce-Correct**

  In order to minimize shock effects:
  - **Estimate**
    - Predict the position x_e for the next dislocation using elastic solution.
  - **Introduce**
    - A dislocation b at $x_{e.}$
    - Relax at room temperature for 40 ps followed by quenching.
    - Determine the final position (x_f).
  - **Correct**
    - Introducing a dislocation b at x_f and the other -b at x_e by applying their displacements in the **fixed region.**
    - Relax for 10 ps. The displacements in the boundary region is corrected.

Atomic Structures of Grain Boundaries

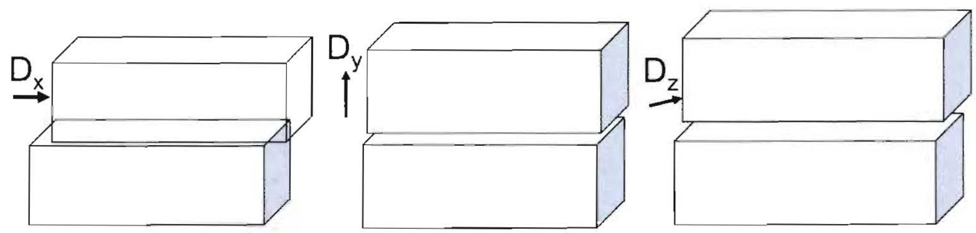
- **GBs have multiple state structures: cf Local Minima Map**

Choosing initial GBs structures

1. **Translated top grain in interface plane relative to the lower grain with a mesh 20×2 in x-z plane within Boundary Unit Cell**

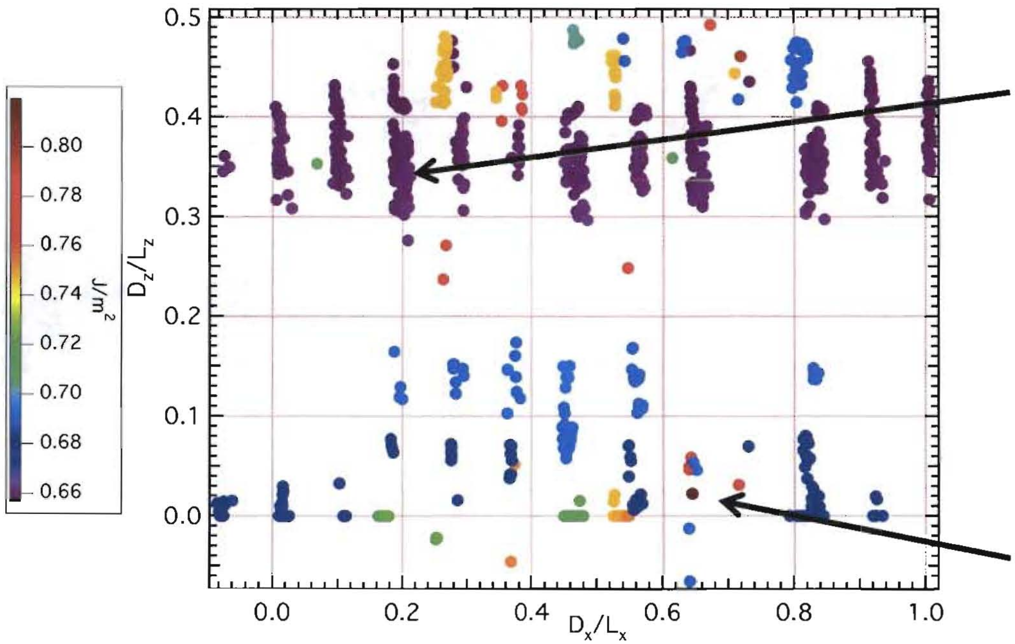
2. **For each translation, relax all atom positions Both crystals allowed to translate in 3D, but not rotate**

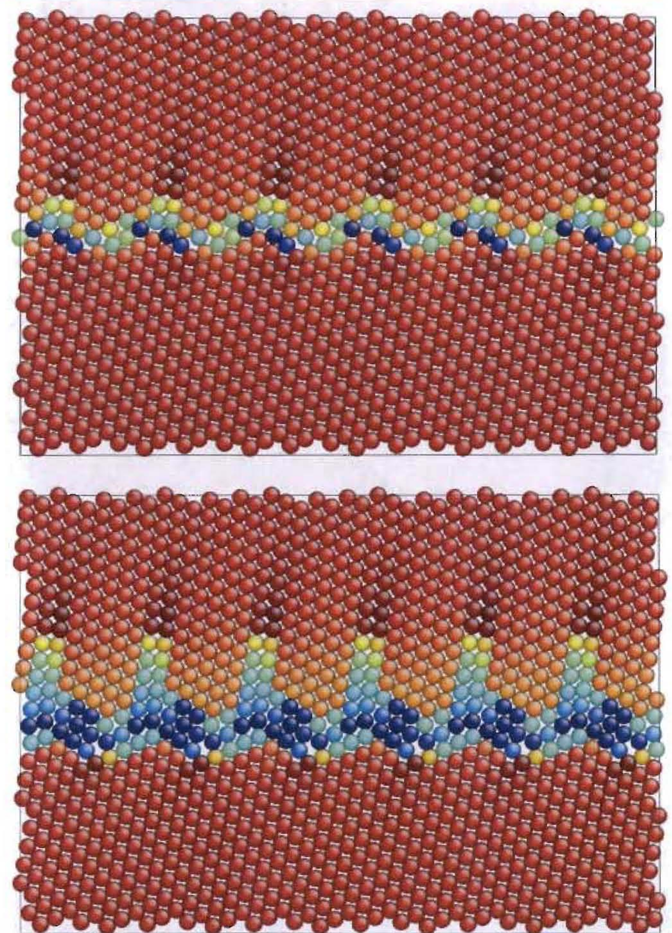
3. **Check GB stability**
   0 K and 300 K
   uniaxial stresses
   $\sigma_{xx} = 1.5$ **GPa,** σ_{yy} **and** $\sigma_{zz} = 0$ **GPa**



Asymmetric Σ_{11} Grain Boundary Energetics and Structures

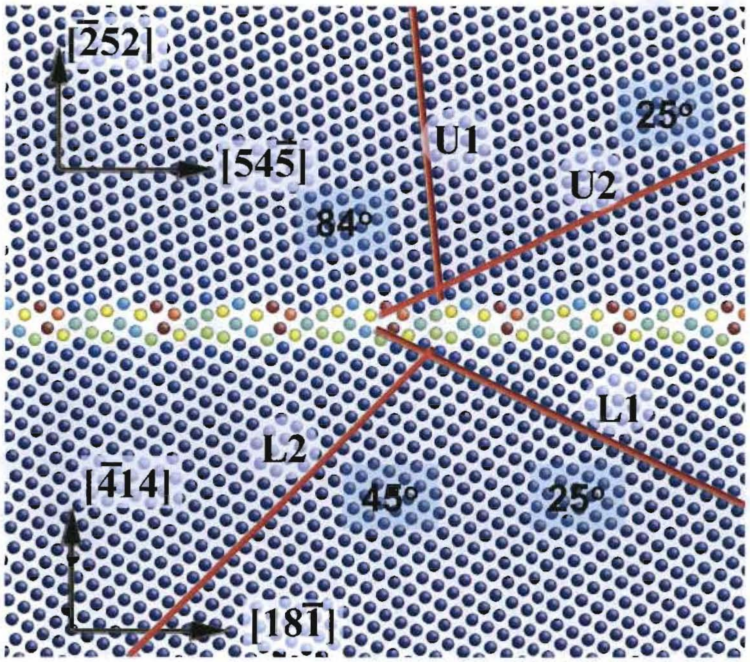
Local Minima Map



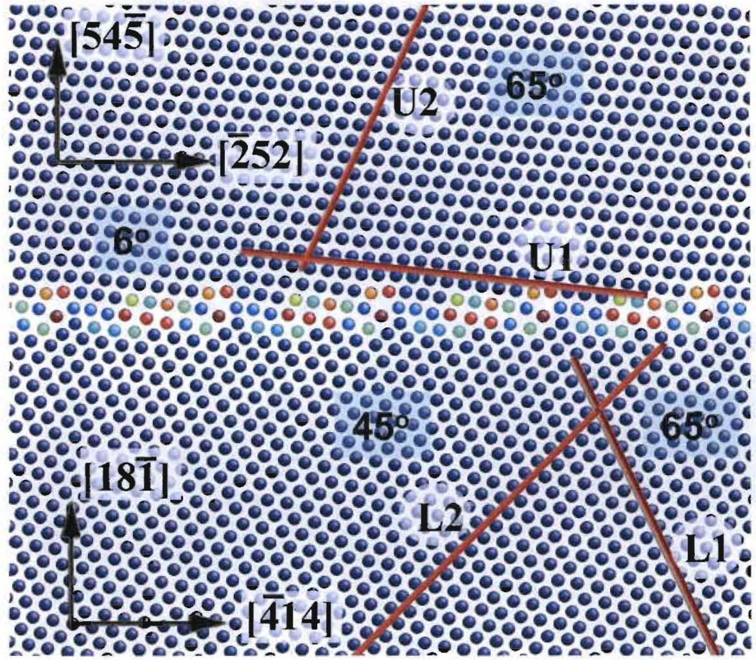


Fensin for Mishin Cu

Asymmetric Σ_{11} Grain Boundaries with Slip Planes



GB-1

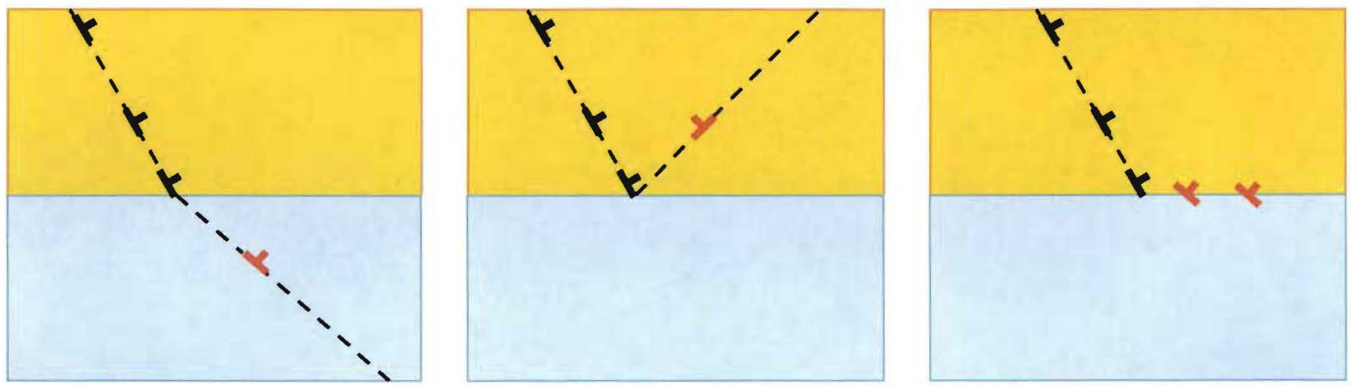


GB-2

Three slip systems are evident in this study

1. **Dislocations pile up on L2 in GB-1** (transmission and reflection)
2. **Dislocations pile up on L1 in GB-2** (reflection and climb)
3. **Dislocations pile up on L2 in GB-2** (transmission)

Grain Bdy-Dislocations Interactions



transmission | reflection | climb and/or glide

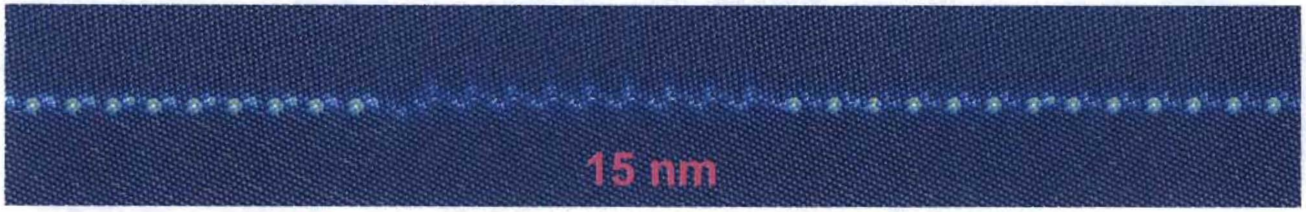
Common deformation modes:
Instability in GB structures
Deformation twinning, shear band formation
Intergranular fracture
Individually or coupled

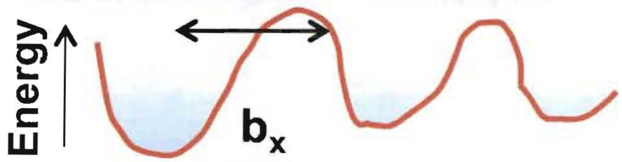
Issues

1. Kinetics of each unit event (no strain rate)
2. Influence of strain rate on each unit event
3. Multiple deformation modes

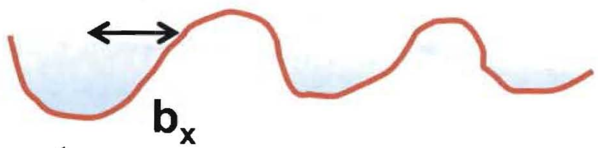
Single Dislocation Interacting with Grain Boundaries

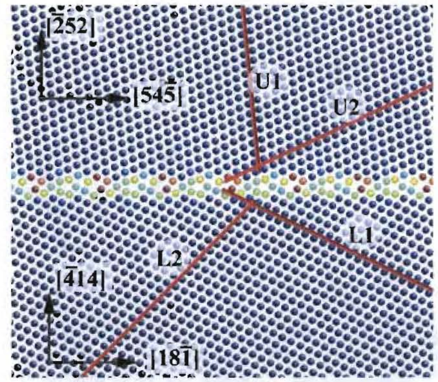
Shear by glide

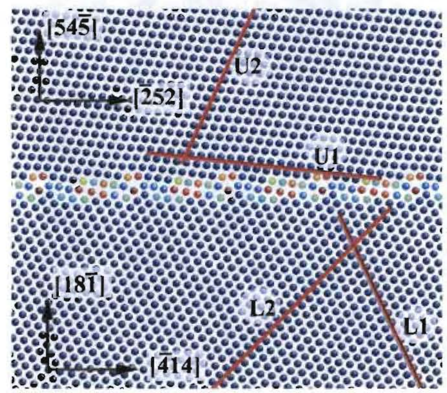




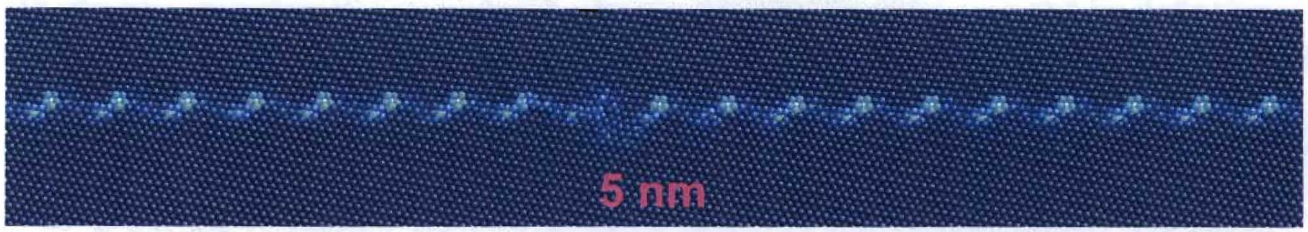
Hypothetical gamma surfaces





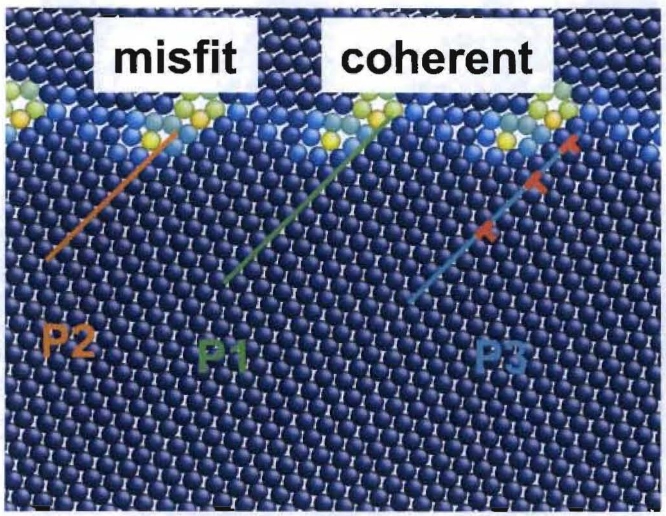


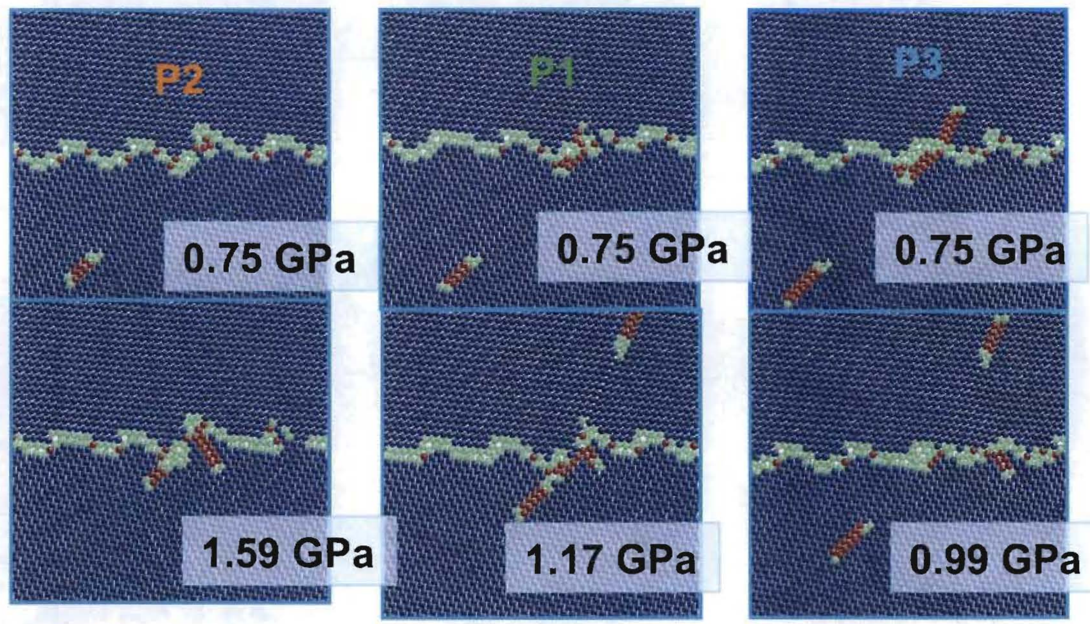
Intact GB structure



Slip-Plane/GB Intersection Alters Local Atomic Structures

Same dislocation pile-up on three adjacent slip planes



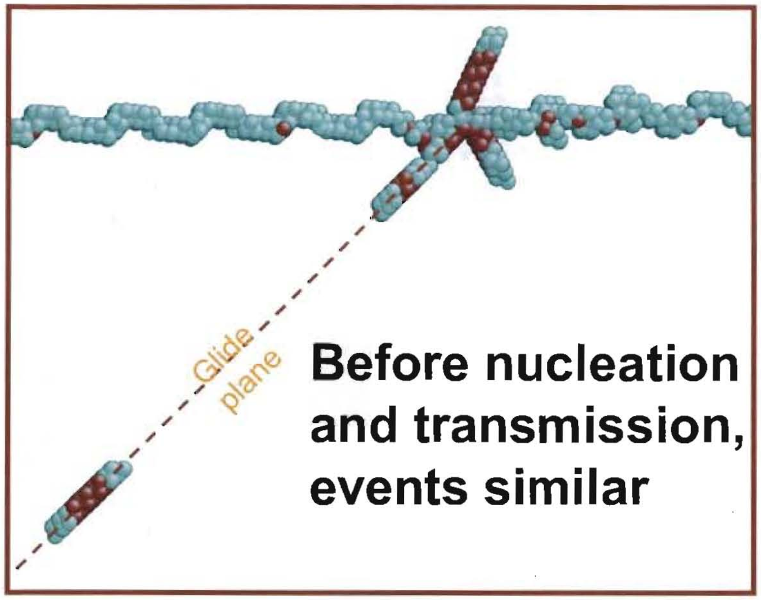


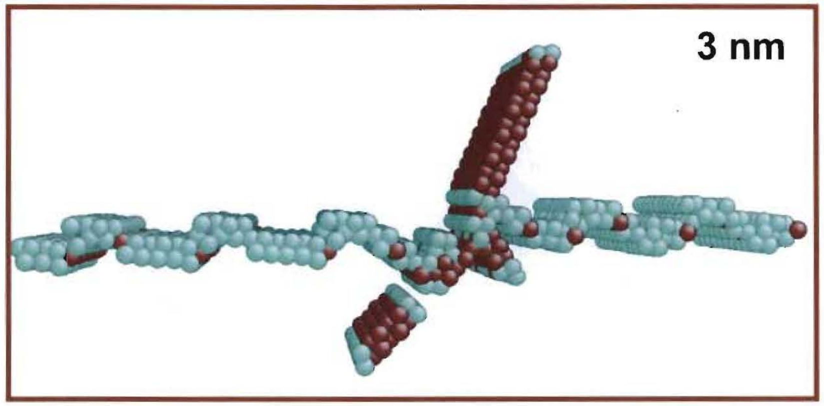
Detach

Detach

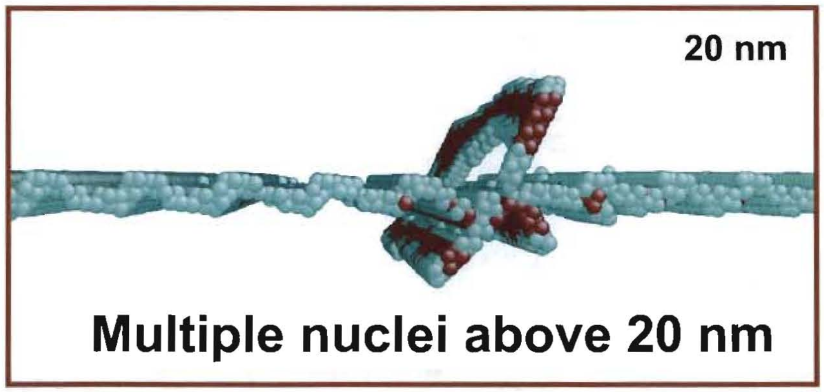
Transmission easier thru coherent zone
Change of mechanism unknown

Slip transmission with thickness

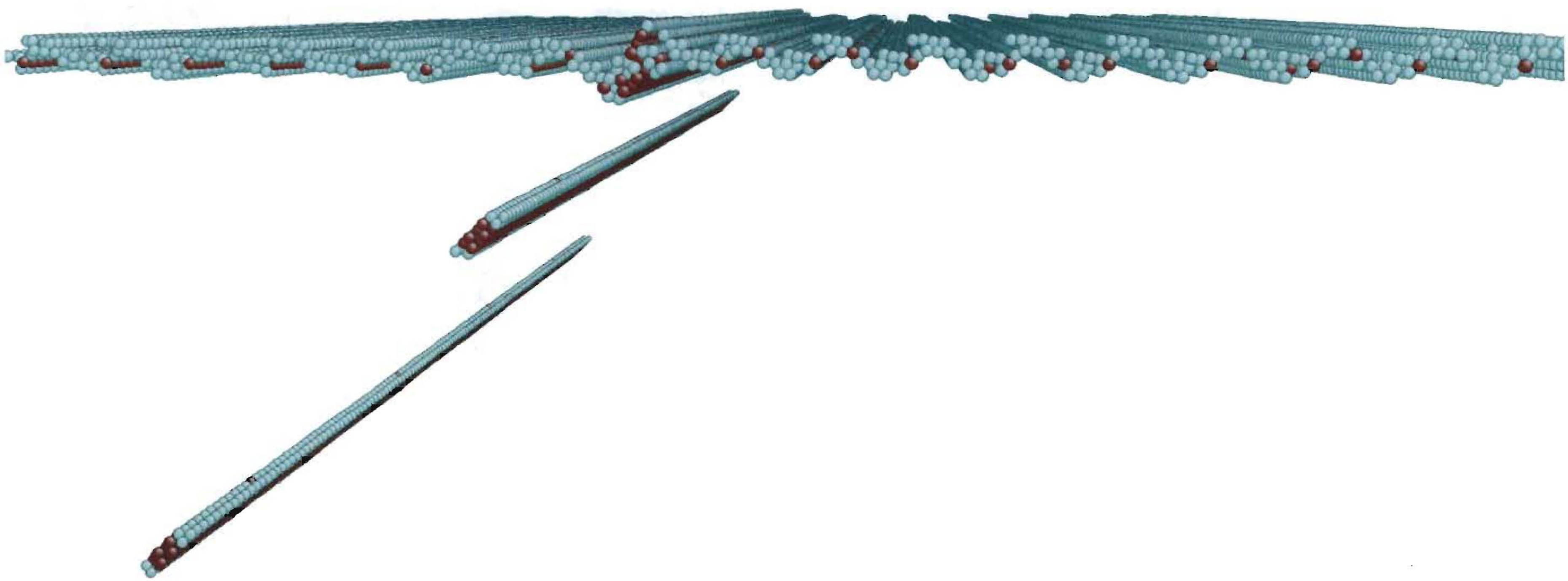




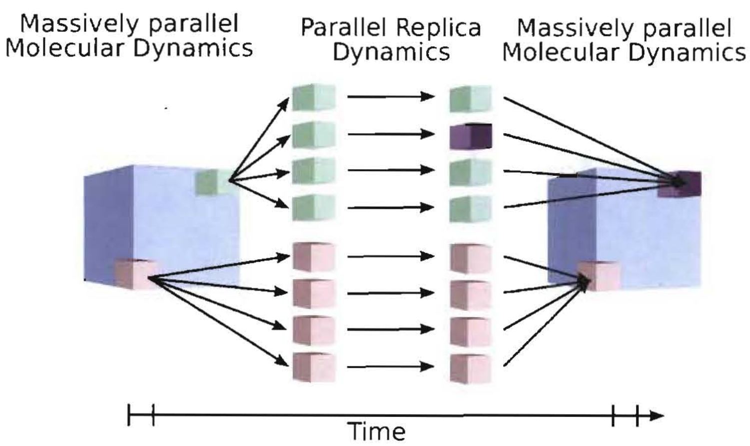
Single nucleus below 10 nm

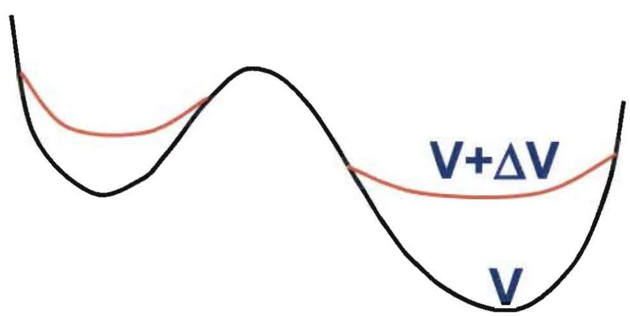


Nucleation can be blocked



Accelerated MD – MD Coupling





Concurrent SPaSM-AMD acceleration algorithm:
Alternate spatial and temporal parallelization

Massively parallel local-bias hyperdynamics

Apply biases <u>locally</u> in space

Maintain acceleration (10-10000x) while simulating larger domains

Summary

- Grain orientations differ in preference for transmission or reflection
- Low-energy does not directly control grain boundary shear from interaction with dislocations
- Three dimensional dynamics crucial for estimating critical stresses for transmission even at high strain rate and nucleation of transmission events
- Slip-plane/GB intersection point added to list of controls
- Future issues
  Multiple deformation modes
  Much lower strain rates, coupling to AMD
  Refine choices of GBs, orientations, conditions in search of mechanisms