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

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Form 836 (7/06)

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

Jian Wang, Steven M. Valone, Richard G. Hoagland, Timothy C. Germann

Problems in materials deformation processes are becoming approachable for the first time through the largest available computers that implement 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 are either transmitted through grain boundaries, cause plastic deformation in an adjoining grain, or cause the grain boundary to fail. Here dislocation pile-ups in an aluminum bicrystal with an asymmetric tilt grain boundary are simulated at several levels of resolution of the pile-up, gradually 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. Longer-time responses are examined more fully through accelerated molecular dynamics simulations.

Problems in materials deformation processes are becoming approachable for the first time through the combination of the largest available computers, such as LANL's Roadrunner, and several levels of atomistic modeling and simulation. Our goal is to understand processes that typically occur over microseconds to milliseconds of real time through ultrahigh resolution of atomistic simulations. By extending recently-developed accelerated molecular dynamics techniques to multiple "active regions" of a deformed material, modeled atom-by-atom on supercomputers, we can to reach the longer time-scales necessary to simulate events for their real duration. This project is designed to apply such algorithmic developments to understand how the several competing different mechanisms. We have targeted ductile spall failure in metals and dislocation pile-up at metal grain boundaries, as deformation processes of key, scientific interest. Under spall conditions generated by a shock wave, a greater understanding of the three central components of spall, nucleation, growth and coalescence of voids, is required. Competition among these three components takes place over elastically interconnected regions of plastically-deformed material. Simulations can supplement experiments through their ability to de-convolve the components of spall, elucidating kinetic rates from the simulations that are currently inaccessible by experiments. In the dislocation pile-up process, a greater understanding is required as to how dislocations are either transmitted through grain boundaries, cause plastic deformation in an adjoining grain, or cause the grain boundary to fail. Both algorithmic and physics modeling elements of the project are being pursued simultaneously.

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

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[1] MST-8: Structure/Property Relations

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

Los Alamos National Laboratory

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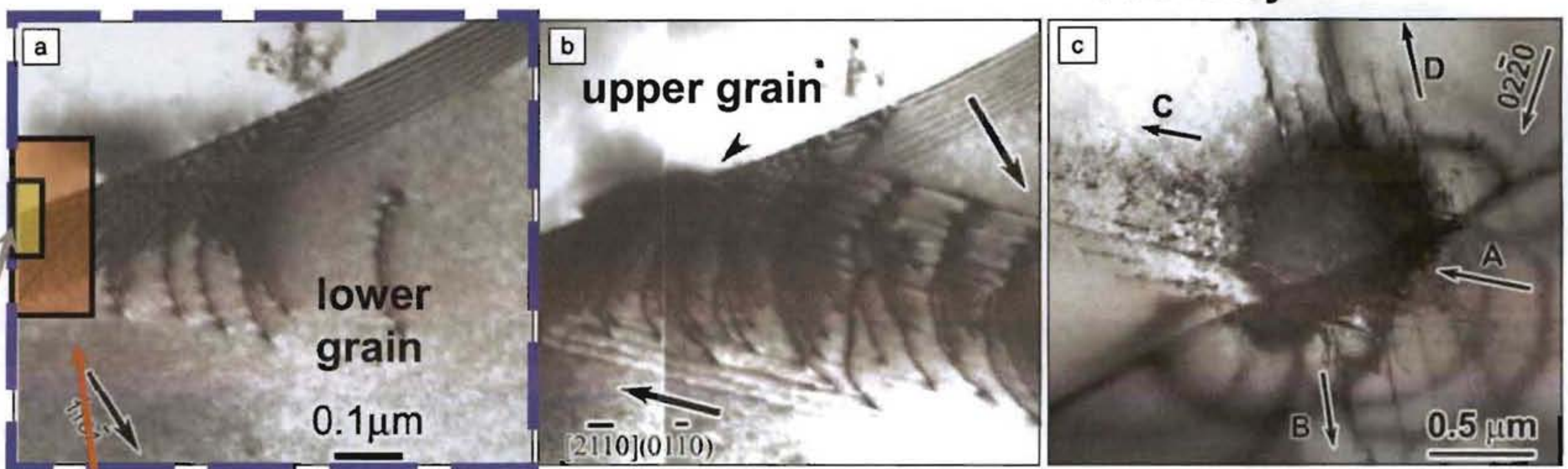
Project on Spatio-Temporal Frontiers of Atomistic Simulations in the Petaflop Computational World

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

Dislocation Pile-Up

Material under stress | **Dislocations moving** | **Penetration thru grain boundary**

Full capability



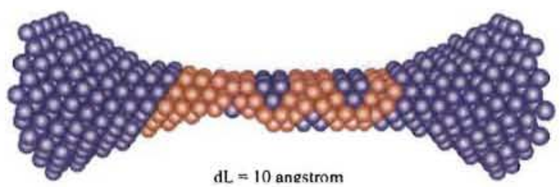
Present modeling capability

Early test runs on RR

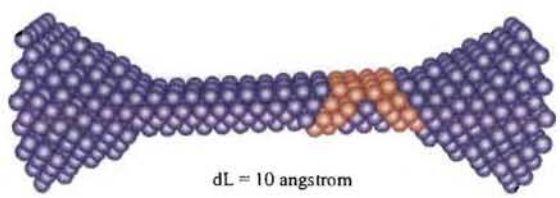
In-situ Transmission Electron Microscopy (TEM) image in α-Ti (hexagonal close-packed) of dislocations in lower grain interacting with upper grain, through grain boundary (I.M. Robertson *et al.*, MRS Bulletin, Feb 2008)

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

Atomic Structures of Grain Bdys

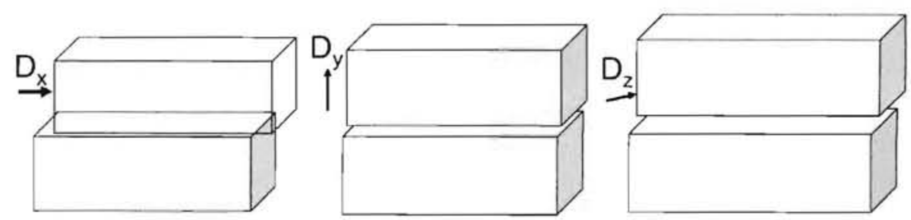
- GBs have multiple state structures: cf Local Minima Map

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

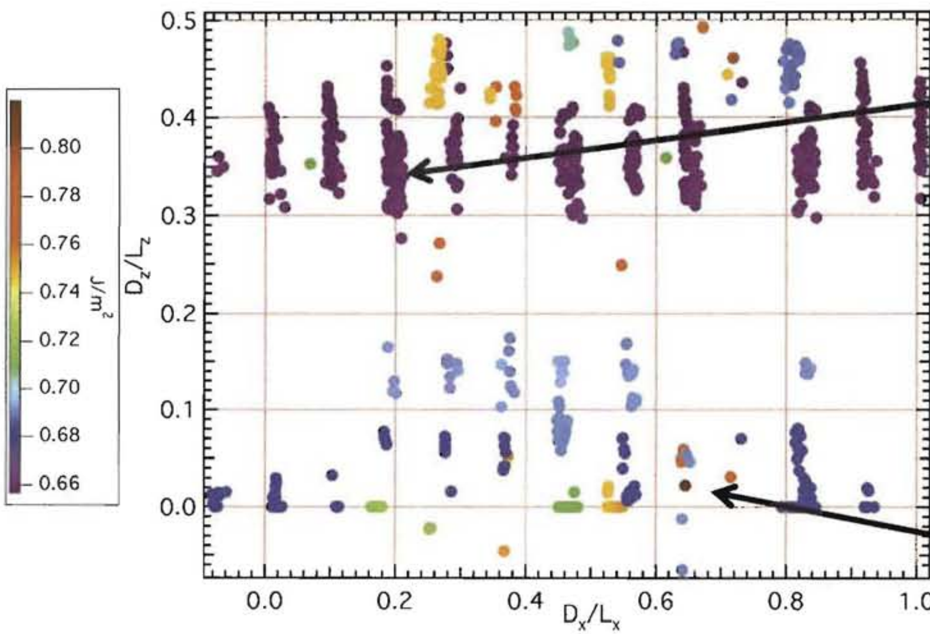
2. For each translation, relax all atom positions Both crystals allowed to translate in 3D, but not rotate

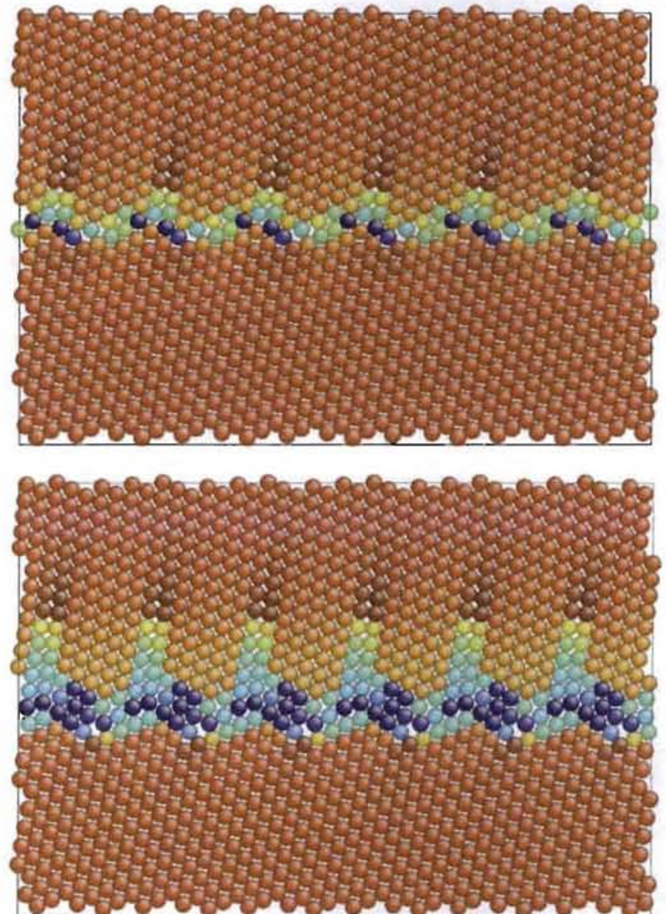
3. Check GB stability
   0 K and 300 K
   uniaxial stresses
   σ_{xx} = 1.5 GPa, σ_{yy} and σ_{zz} = 0 Gpa



Grain Boundary Structures

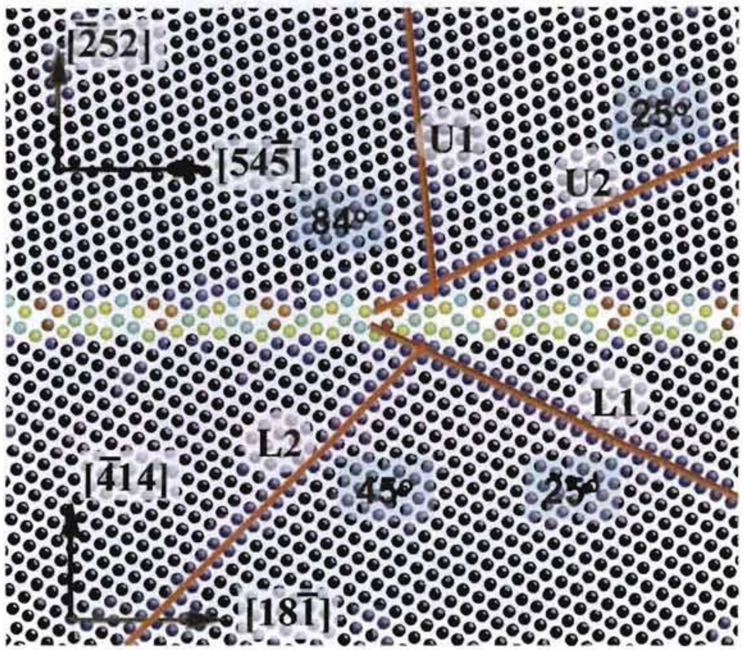
Local Minima Map



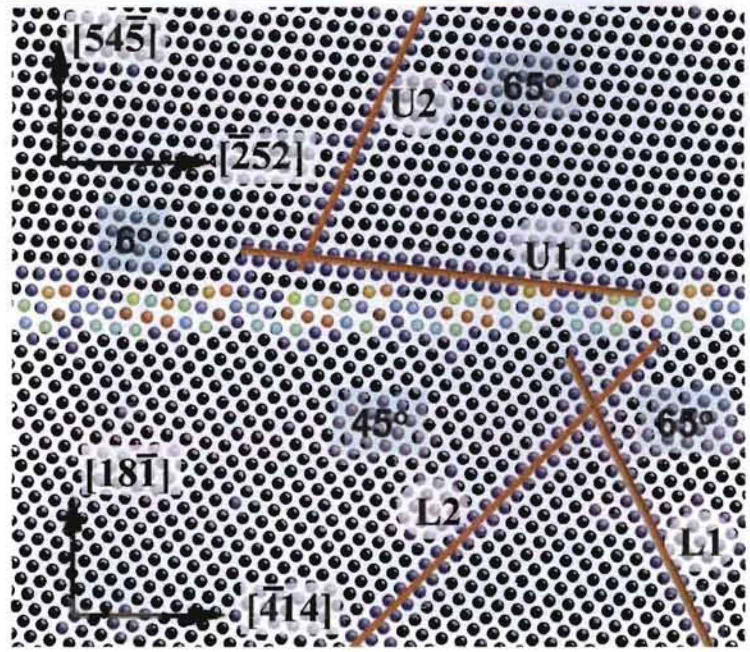


Jindal for Mishin Cu

Asymmetric Σ11 Grain Boundaries



GB-1

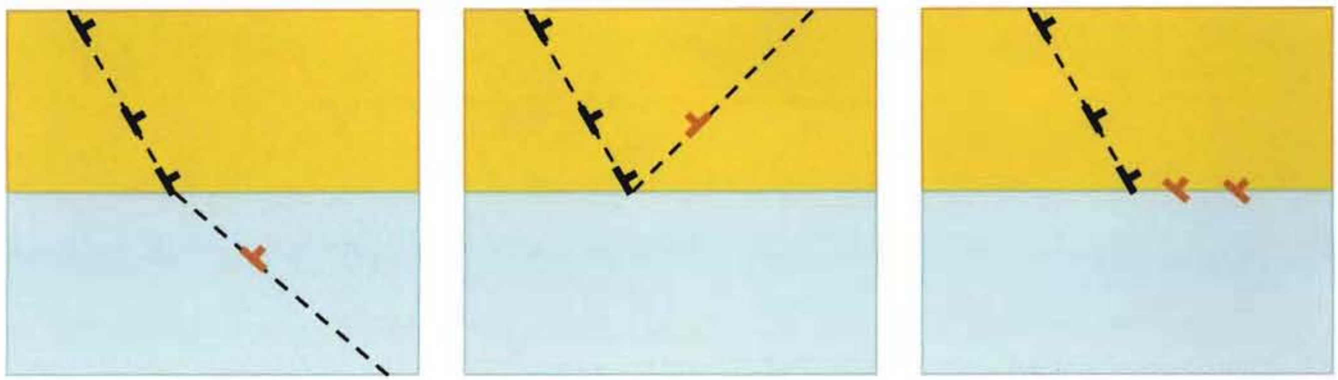


GB-2

Three slip systems are adopted 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



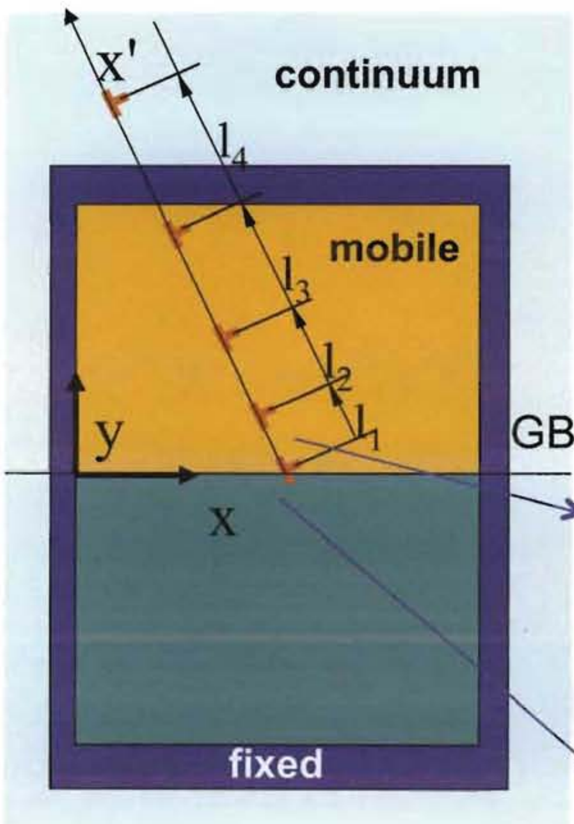
transmission　　reflection　　climb and/or glide

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

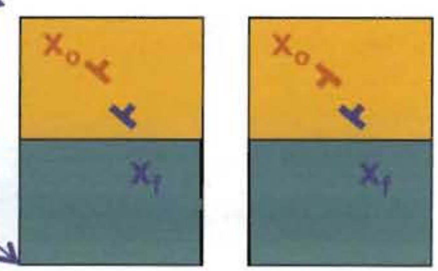
Issues

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

Introducing Dislocations



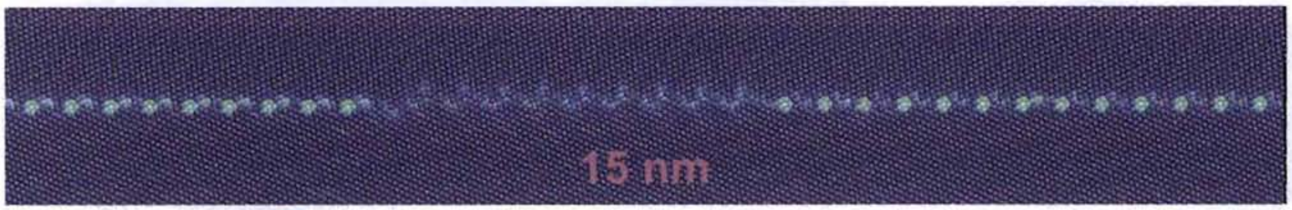
- Anisotropic, elastic solution for dislocation in bi-xtal
- Estimate dislocations positions: single stressed pileup model
- Three steps to eliminate shock effects
  - Relax cell at room temperature (RT) & under applied stress (σ^a) without dislocations
  - Apply displacement field of dislocation *b* at x_o in both mobile and fixed regions
    Relax at RT for 40 ps
    Quench – final position

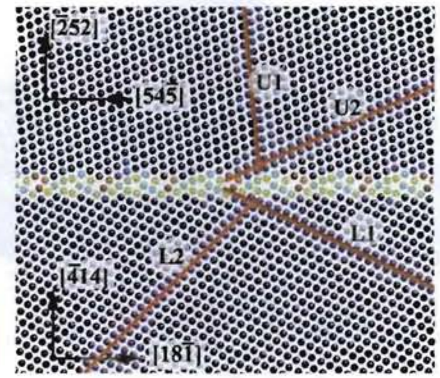


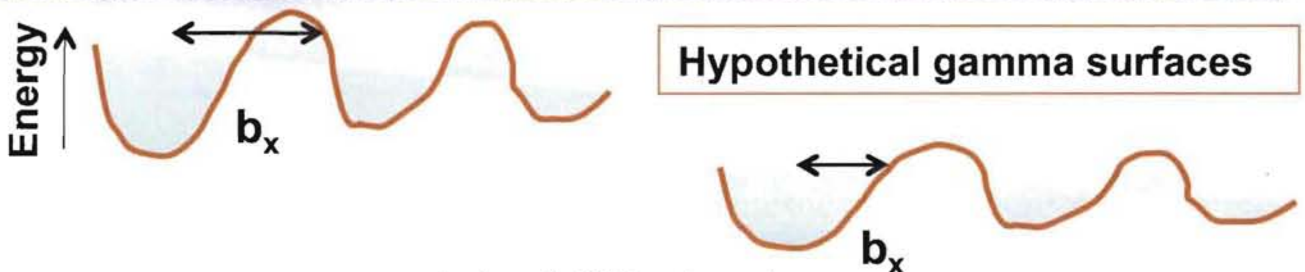
  - Correct displacements in fixed region
    Introduce dislocations *b* at x_f and -*b* at x_o
    Apply displacements in fixed region only
    Relax for 10 ps
  - Estimate position of next dislocation & repeat

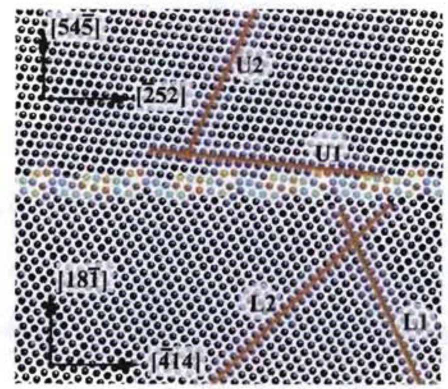
Single Dislocation Interacting with Grain Boundaries

Shear by glide

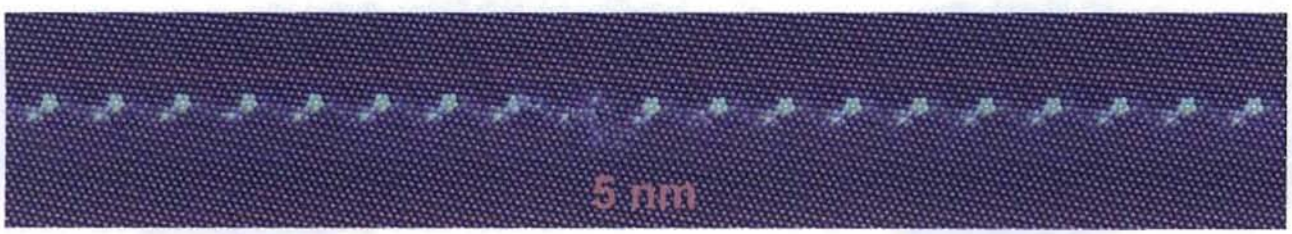








Intact GB structure



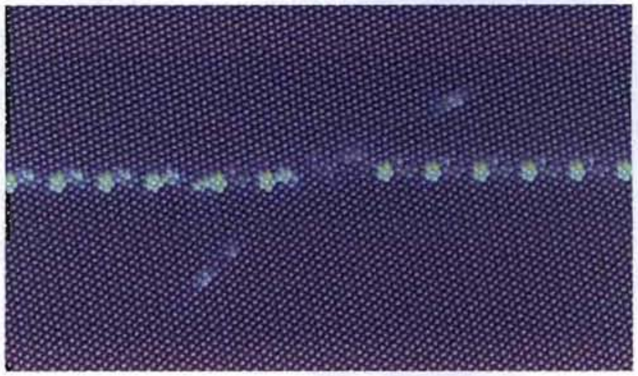
Ercolessi-Adams Embedded Atom Method Al

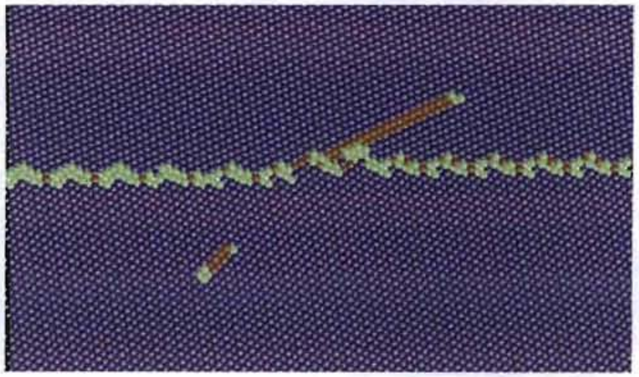
Grain Bdy 1: Transmission

Glide plane angles: 45.29° and 25.24°

$(-252)_{upper}$

$(-414)_{lower}$





6 mixed dislocations, resolved shear stress 150 MPa, 40 ps simulation
Two dislocations absorbed in GB
GB structures changes in 3-nm region

Transmission because of alignment of slip planes and repulsion from possible reflected dislocation

Grain Bdy-2: Reflection

$(54\text{-}5)_{upper}$

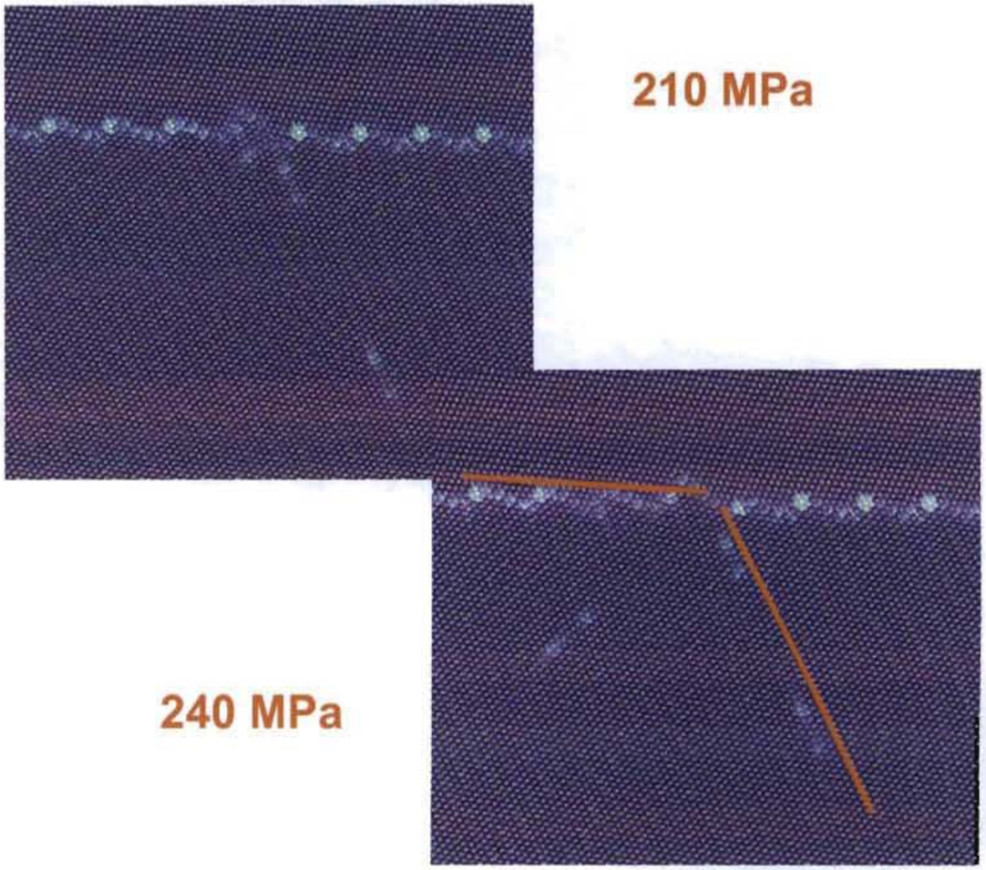
Glide plane angles:
64.76° and 5.77°

$(18\text{-}1)_{lower}$

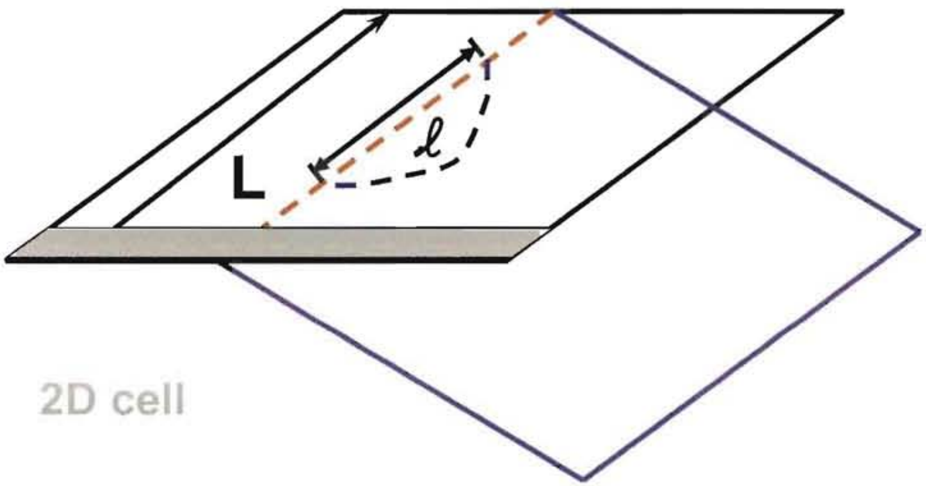
Same conditions

Get reflection because of the Schmid factor close to 0

Role of shear still under investigation



Determining dislocation loop size

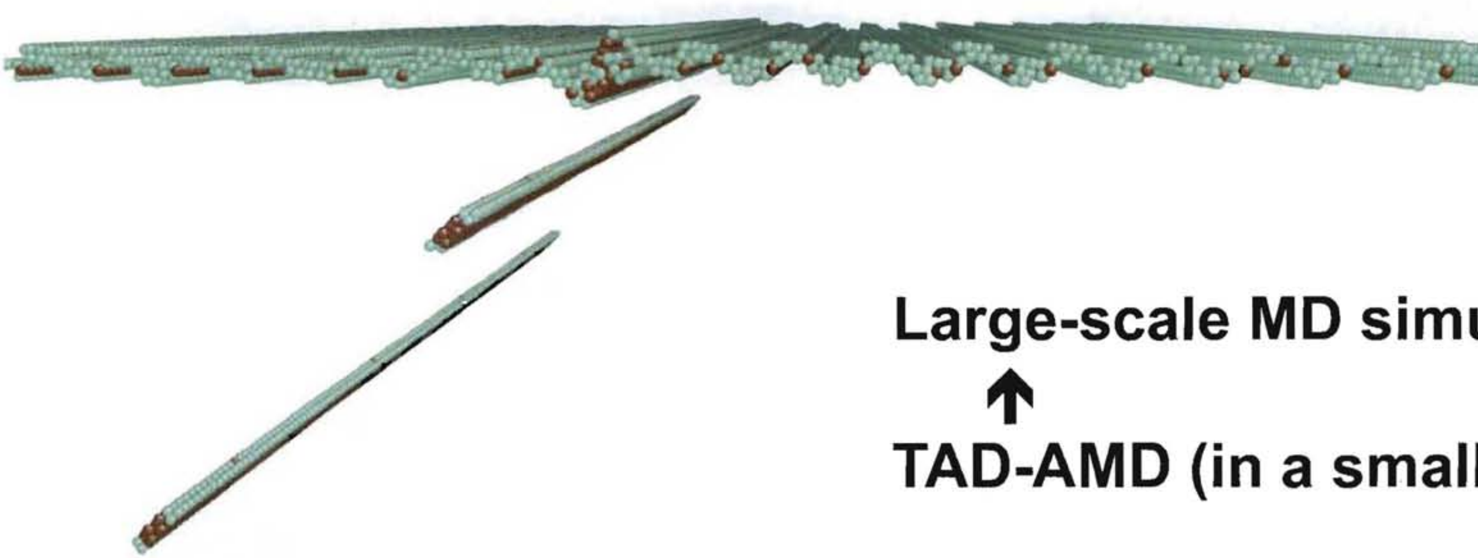


- In 3D transmission can occur in loop segments: Lower barriers
- Possible to investigate nucleation of transmission events
- Loop lengths and critical stresses depend on the loading conditions
  - Load directions
  - Far-field stress
  - Number of dislocations

3D Sample

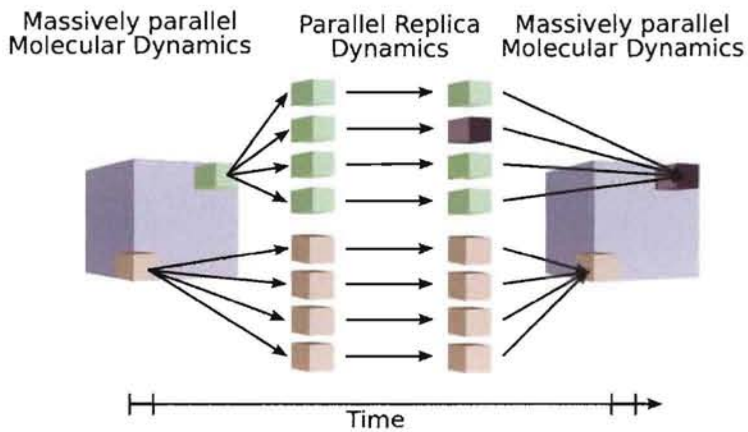
40 nm thick, GB-2 orientation
200 MPa, RT

Periodic loops form
Reduce stress levels needed to transmit dislocations



Large-scale MD simulation
↑ ↓
TAD-AMD (in a smaller block)

Accelerated MD – MD Coupling

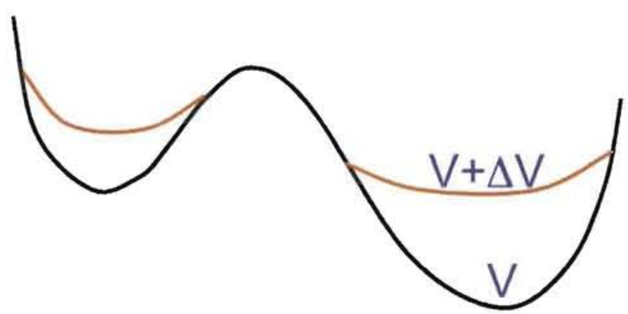


Concurrent SPaSM-AMD acceleration algorithm: **Alternate spatial and temporal parallelization**

Massively parallel local-bias hyperdynamics

Apply biases locally in space

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



Summary

- Grain orientations show strong preferences 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
- Future issues
  Multiple deformation modes
  Dislocations-velocity dependence
  Much lower strain rate, coupling to AMD
  Requires careful choices of GBs, orientations, conditions