LA-UR-11- 11-01569

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Title: Shear-Rate Dependence in Dislocation Pile-ups at Asymmetric Tilt Boundaries in Aluminum

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Intended for: Invited presentation at 2011 TMS Meeting
San Diego, CA
27 Feb - 03 Mar 2011

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Shear-Rate Dependence in Dislocation Pile-up Simulations at Asymmetric Tilt Boundaries in Aluminum

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Materials deformation processes are increasingly approachable through atomistic methods. In one deformation process, dislocation pile-up at a grain boundary, how dislocations transmit through grain boundaries is of intense interest. Here dislocation pile-ups in an aluminum bicrystal with an asymmetric sigma-11 tilt grain boundary are simulated. Dislocations are initially distributed according to linear elastic estimates from a far-field stress of 40 MPa. The system is propagated for different periods of time, representing different shear rates. Incremental loading occurs every 40 ps or every 80 ps. In spite of the factor of two difference in shear rate, differences in the events are quite marked. At the higher rate, dislocations are transmitted on both available slip systems. The entities transmitted are perfect dislocations. At the slower rate, transmission and reflection events consist of multiple Shockley partial dislocations, parallel to each other, on one of the slip planes.

Shear-Rate Dependence in Dislocation Pile-ups at Asymmetric Tilt Boundaries in Aluminum

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Supported by Laboratory Directed Research and Development Program
Project on Spatio-Temporal Frontiers of Atomistic Simulations in the Petaflop Computational World

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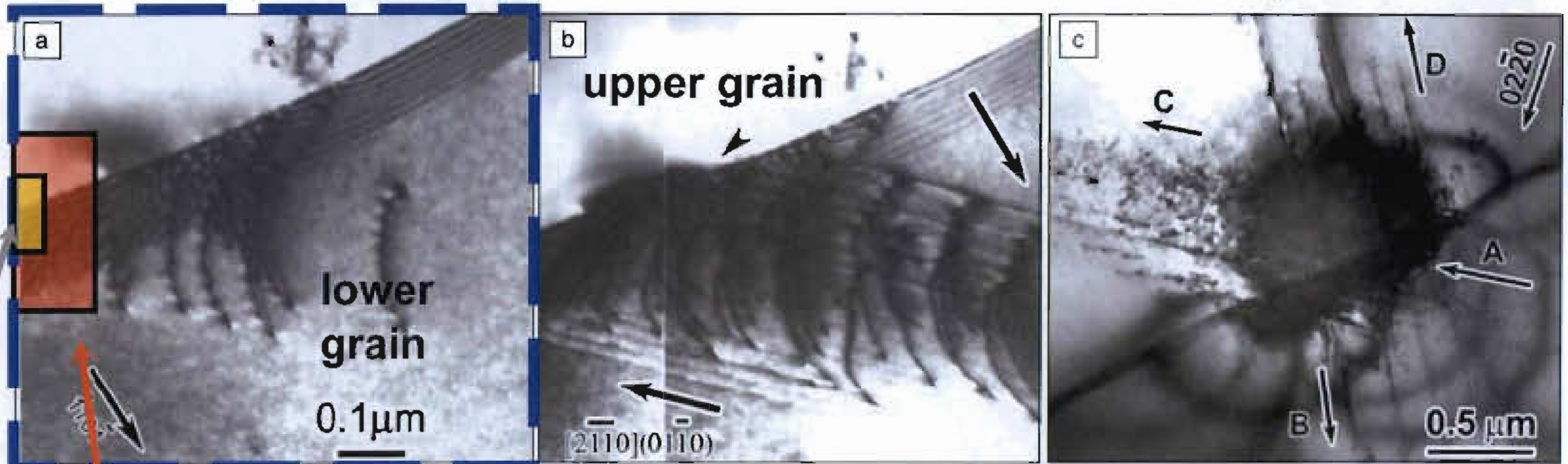
Dislocation Pile-Up

Material under stress | Dislocations moving | Penetration thru grain boundary

Full capability



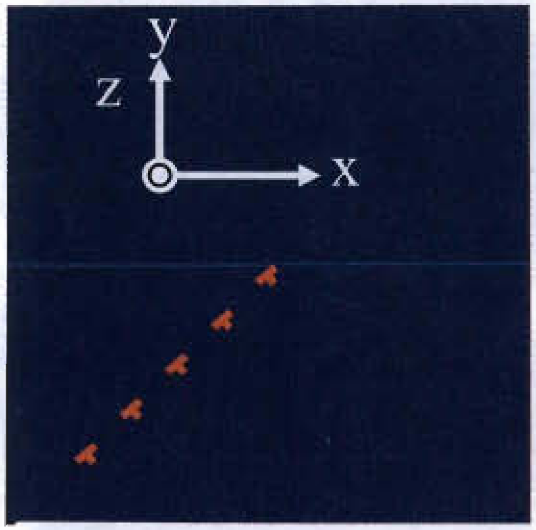
Prior modeling capability

Present runs on hybrid

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

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

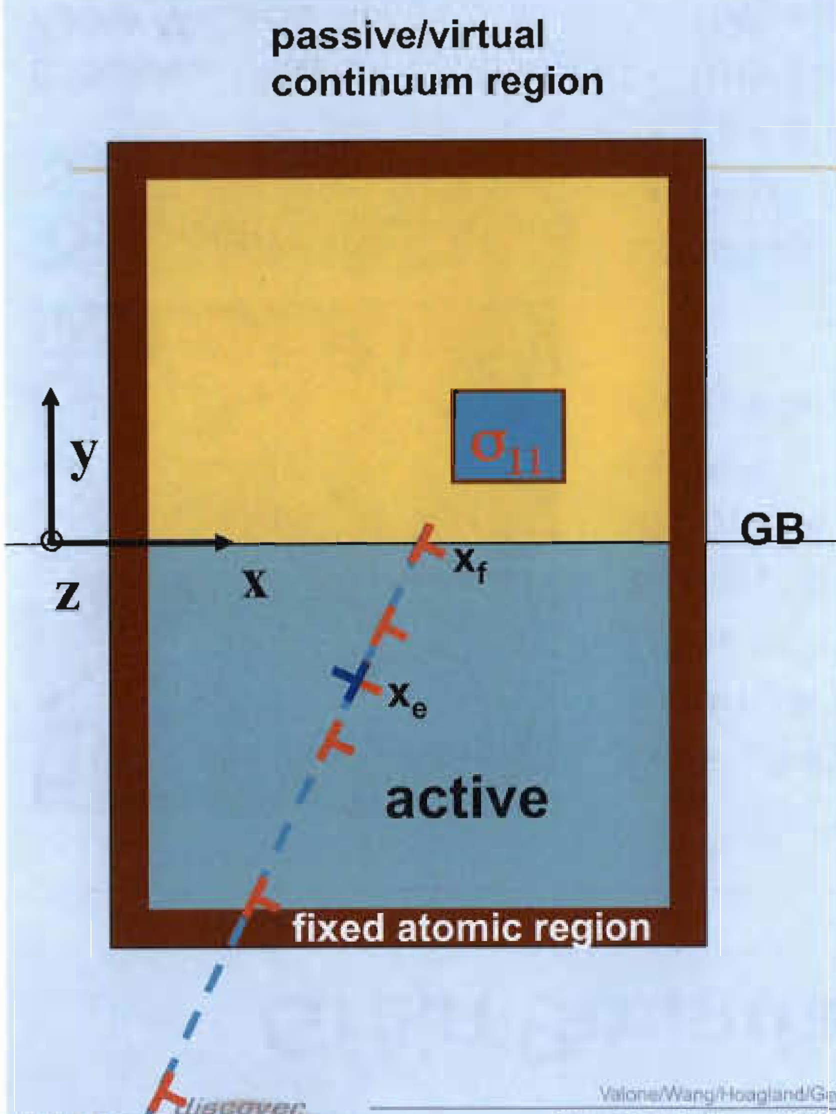
MD simulations

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

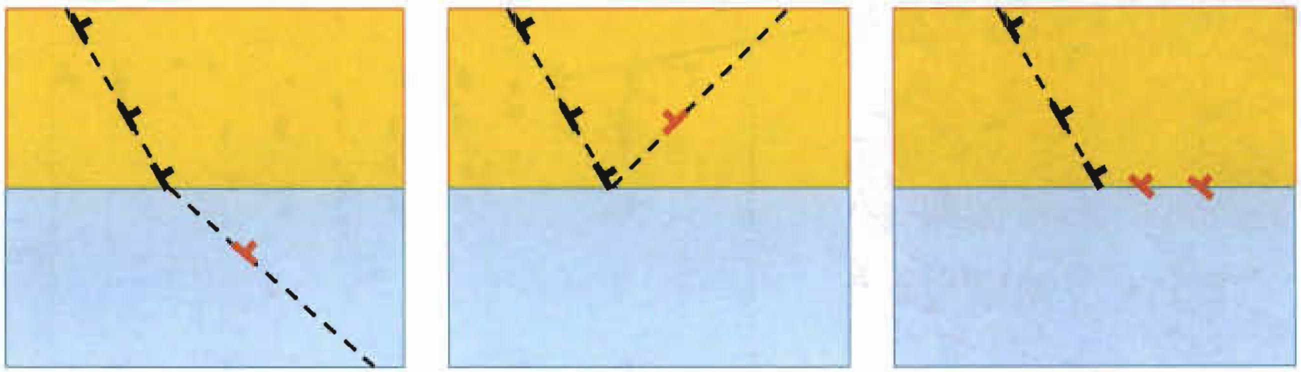
Method for Introducing dislocations



- 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.

Grain Bdy-Dislocations Interactions



transmission reflection climb and/or glide

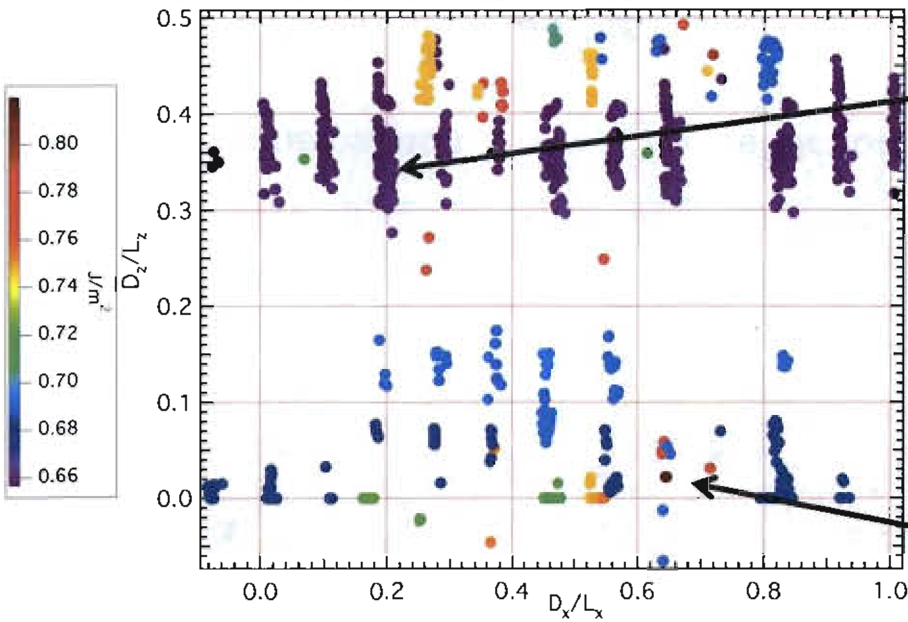
Common deformation modes:
Instability in GB structures
Deformation twinning, shear band formation
Intergranular fracture
Individually or coupled

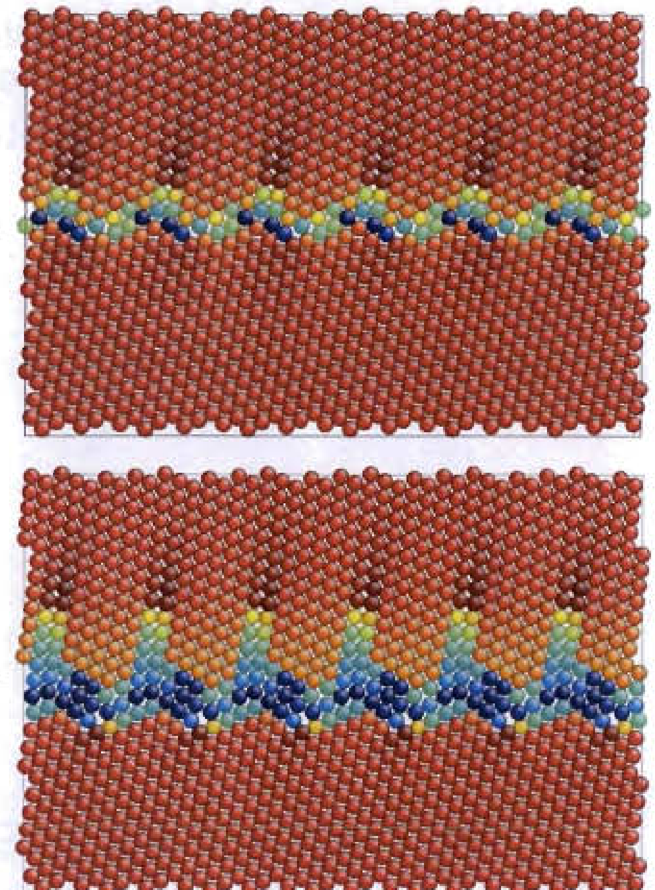
Issues

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

Asymmetric Σ_{11} Grain Boundary Energetics and Structures

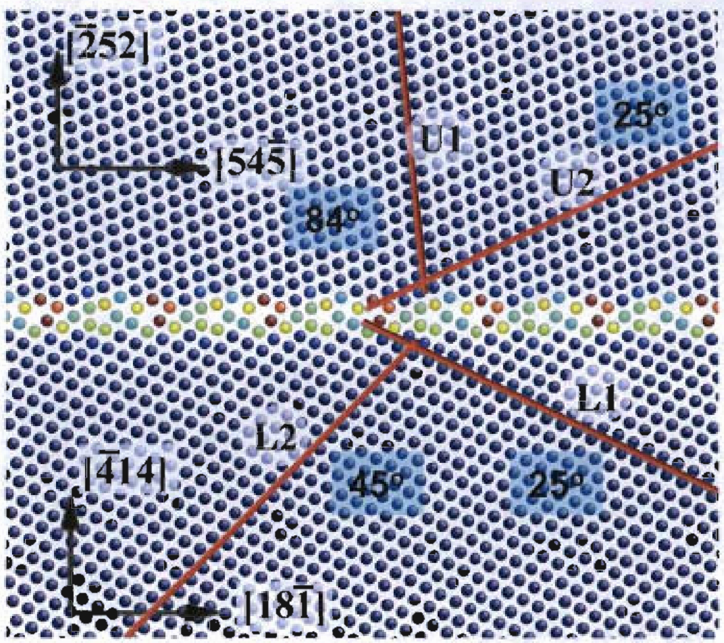
Local Minima Map



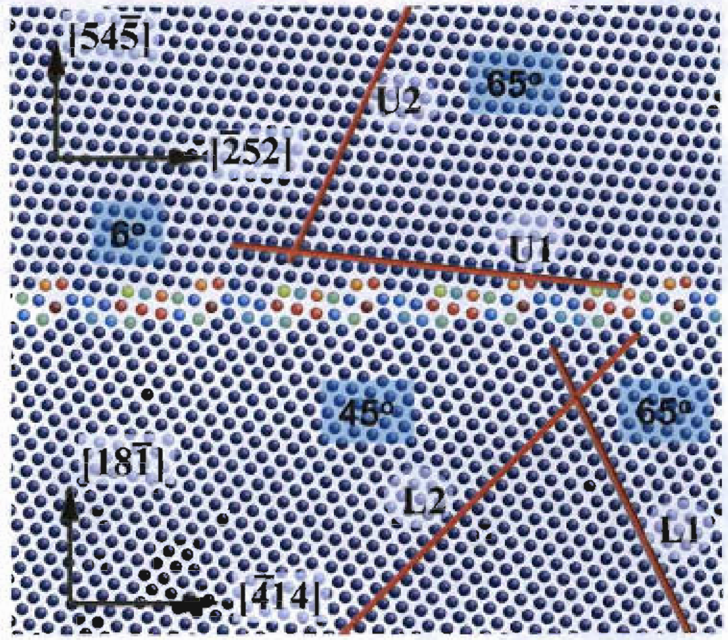


Fensin for Mishin Cu

Asymmetric Σ_{11} Grain Boundaries with Slip Planes



GB-1



GB-2

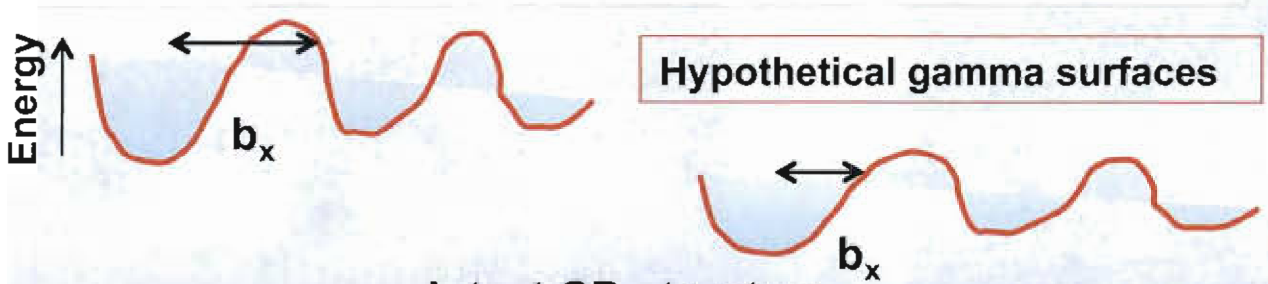
Three slip systems are evident in this study

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)

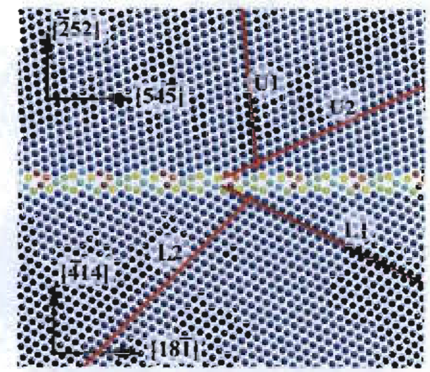
Single Dislocation Interacting with Grain Boundaries

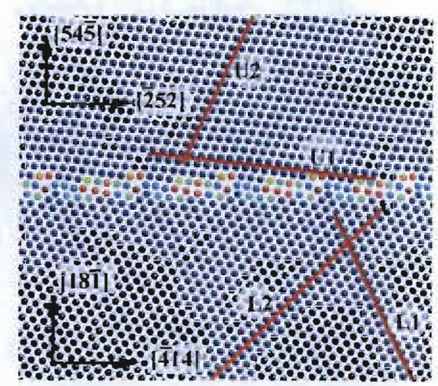
Shear by glide

15 nm



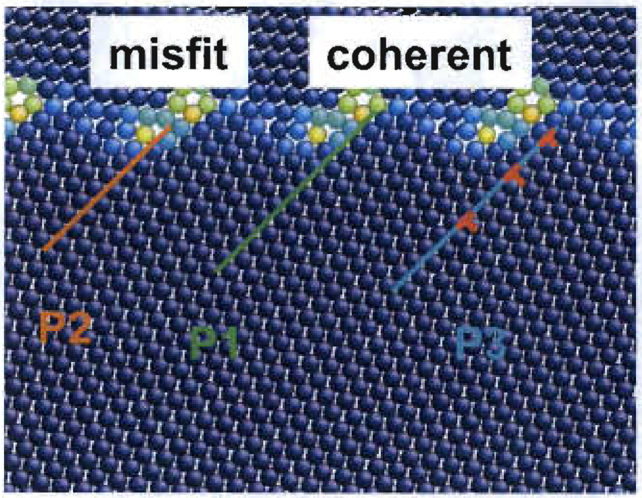
Intact GB structure

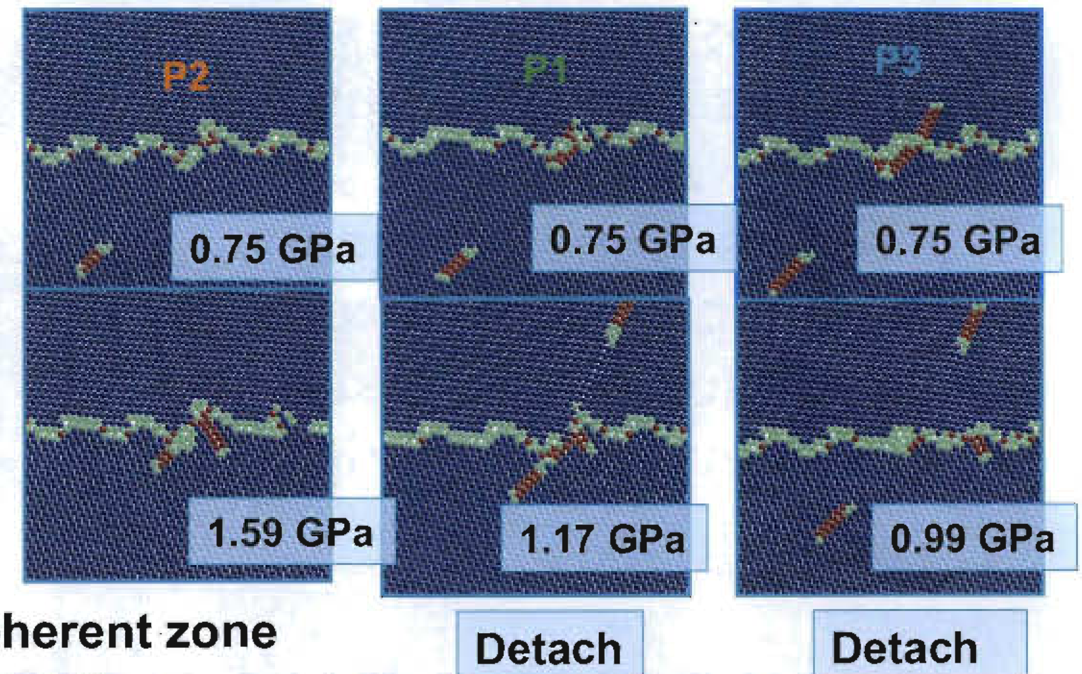




Slip-Plane/GB Intersection Alters Local Atomic Structures

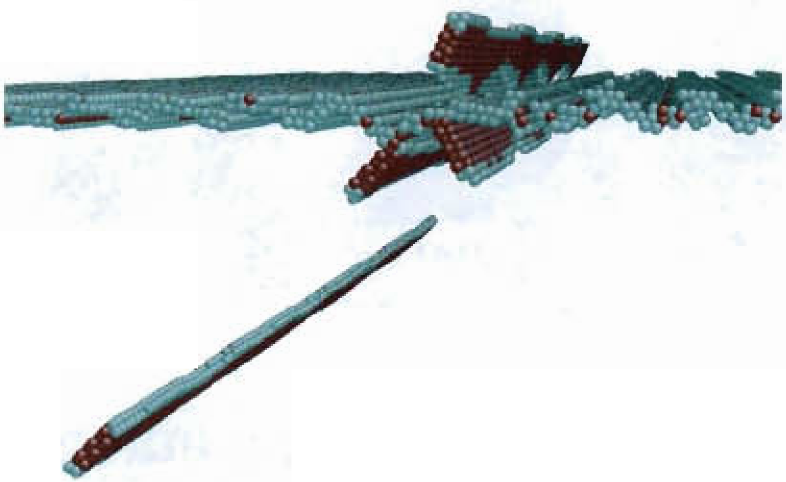
Same dislocation pile-up on three adjacent slip planes





Transmission easier thru coherent zone
Change of mechanism unknown

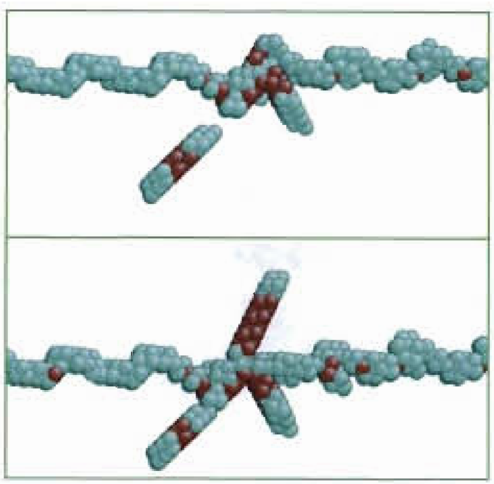
Transmission and Reflection

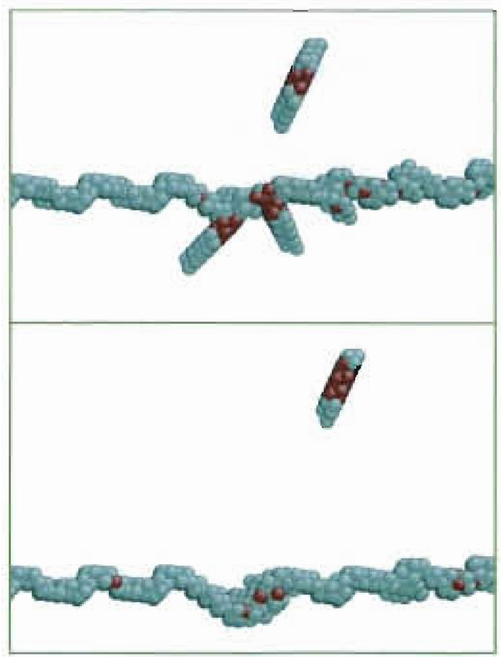


1. Slip-plane normals and directions in both grains
2. Maximize directions and resolved shear stress in 2nd grain better
3. With minimal residual dislocation in GB better
4. Direct transmission rare
5. No shear-rate dependence

Lee et al. 1990

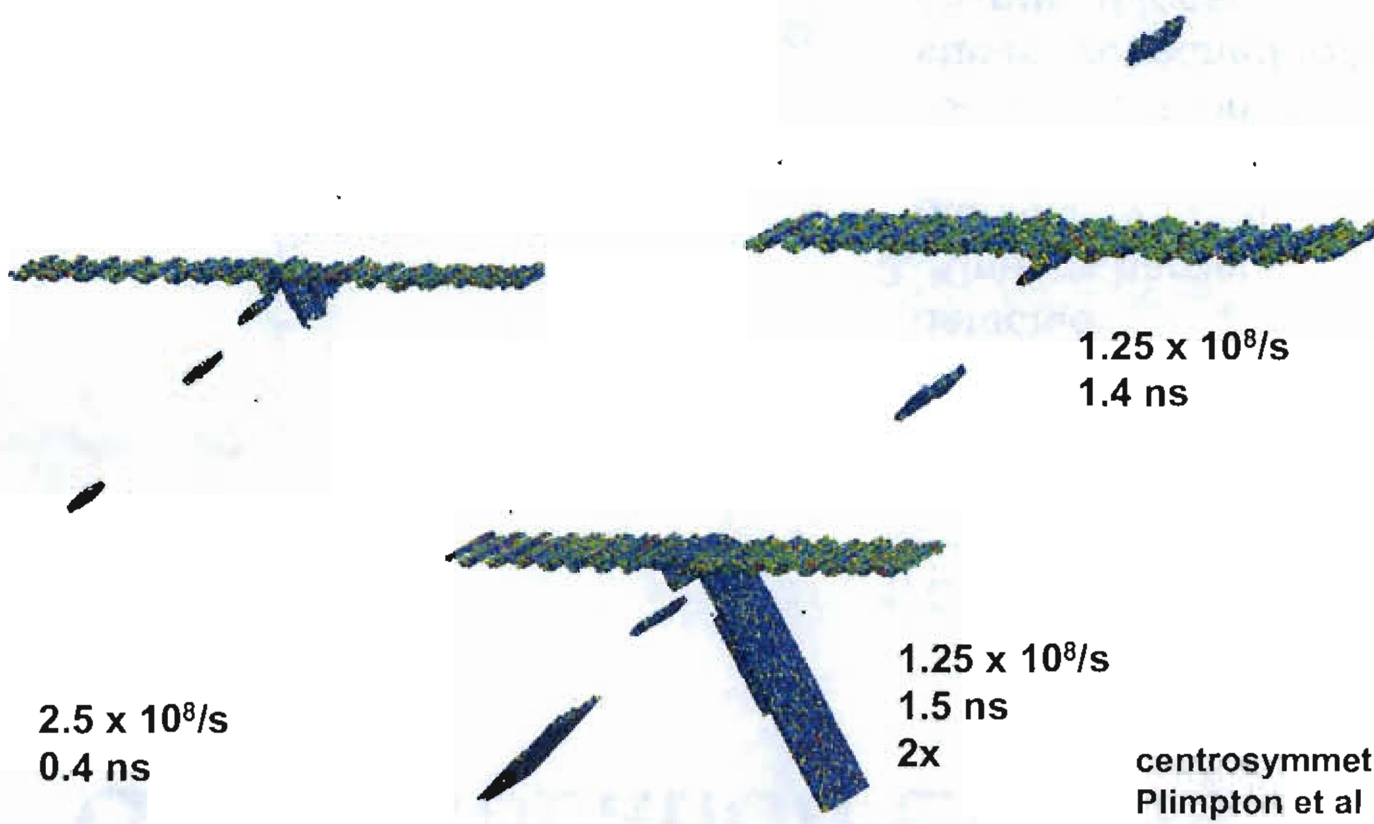
GB-Dislocation Events





1. Dislocation detaches from GB at 1.17 GPa and 720 ps
2. Multiple local stable configurations are detected
3. Kinetics barriers are less than 0.5 eV for all transitions.
4. Before detachment, most states are related to the change of local structures near GB-slip plane intersection

Transmission Events at Different Rates



centrosymmetry:
Plimpton et al

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 orientations, loading conditions in search of mechanisms