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Title: Atomistic Modeling of Dislocation-Interface Interaction

Author(s): J. Wang, I.J. Beyerlein, A. Misra, S. Valone, T.C. Germann

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Atomistic modeling of dislocation-interface interaction

J. Wang, I. J. beyerlein, A. Misra, S.M. Valone, T.C. Germann
Materials Science and Technology Division,
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Interfaces are a common planar defect in materials, and can act as *Sources*, *Sinks* and *Barriers* for point defects and line defects. Interfaces may block slip even when dislocations move easily in both of the bounding crystals, enhancing materials strength. Grain boundaries, interfaces in polycrystalline single-phase, single-component materials, are quintessential examples of effective barriers to slip. Interfaces possess many metastable states for a given set of macroscopic degrees-of-freedom. These various states may differ in energy, but by relatively small amounts, and may be separated by small energy barriers. Consequently, they may easily change state and configuration, in response to changes in stress, temperature, and composition. These easy configurational changes enable such multi-state interfaces to actively participate in and influence a broad array of reactions and processes.

Using atomic scale models, interface structures and properties, and the interaction of interface with dislocations are studied. The model system is Cu-Nb multilayers. The results show that interfaces play a crucial role in determining material strength due to the dislocations-interfaces interactions and in nucleating lattice dislocations in associated with the reconstruction of interface structures.

Atomistic Modeling of Dislocation-Interface Interaction

Jian Wang

Collaborators: A.Misra, I.J. Beyerlein, S.M. Valone, T.C. Germann
R. G. Hoagland, J. P. Hirth, N. Mara

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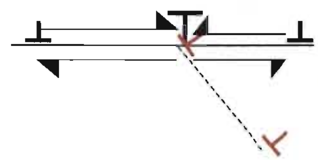
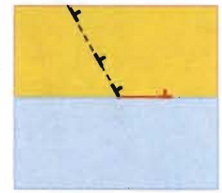
Motivation

Weak interface strengthening mechanisms

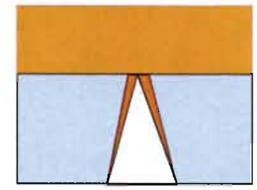
- "Weak" interfaces act as the strong barriers for glide dislocations crossing interfaces, strengthening materials.
- This is ascribed to the interface shear which generates the attraction force on the lattice dislocation and the core spreading of lattice dislocation within the interfaces which traps lattice dislocation at the interfaces.



Interface shear is accomplished via the creation and glide of interfacial dislocations. (RG Hoagland et al, Philos. Mag. 2006)



The sliding and migration of GBs via the glide of grain boundary dislocation with response to GB shear due to dislocation pile up.



Crack-tip blunting due to the presence of interfaces (CT Liu, Compos Struct, 1997)

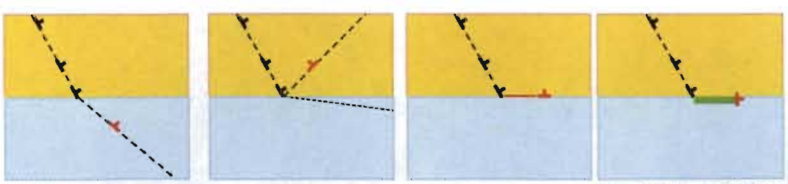
Motivation

Grain-boundary strengthening (or Hall-Petch strengthening):

(1) Grain boundaries impede dislocation movement.

(2) The number of dislocations (dislocation pile up) have an effect on how easily dislocations can traverse grain boundaries.

GB-Dislocations Interactions



Transmission | Reflection | Glide | Climb/Disconnection

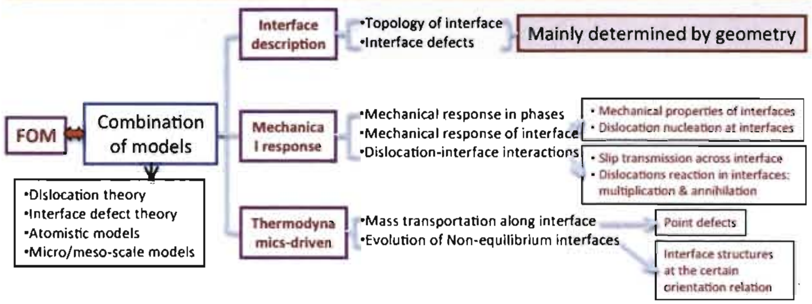
When these processes occurs at GBs, either individual or couple, many deformation modes can be activated. Such as instability of GB structures, migration of GBs, sliding of GBs, deformation twinning, shear band formation, intergranular fracture etc.

Outline

- Atomistic simulations
  - Geometric-based classification scheme for interfaces
  - Interface shear: strength and mechanisms
    - Atomic structures of interfaces
    - The bond strength
  - Interaction of lattice dislocations with interfaces
  - Slip transmission
- Summary

Strategy corresponding to theoretical effort

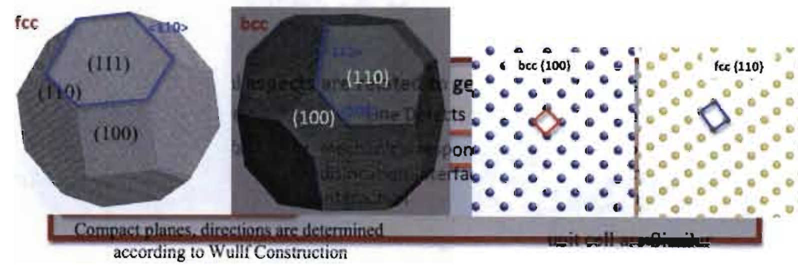
Predict mechanical stable interfaces by using models that couple interface physics: interface description, defect-interface interactions, and evolution of interface characteristics



Is it possible to correlate interface structures and properties through geometry consideration?

Geometrical Factors for classifying interface structures

1. **Habit planes are compact plane.**
2. **Habit planes contain compact direction.**
3. **Atomic structures of habit planes, unit cell are Similar.**
4. **Other factors….**



Six interfaces of Cu/Nb composites

Orientation Relationship		Interface Plane	Compact Plane	Compact direction	Similarity of unit cell
K-S	TYPE-5	y-z	(No, No)	(No, No)	(No, No)
	TYPE-2	z-x	(No, No)	(Yes,Yes)	(No, No)
	TYPE-1	x-y	(Yes,Yes)	(Yes,Yes)	(No, No)
N-W	TYPE-3	y-z	(No, Yes)	(No, No)	(Yes,Yes)
	TYPE-4	z-x	(No,Yes)	(Yes, Yes)	(No, No)
	TYPE-1	x-y	(Yes,Yes)	(Yes, Yes)	(No, No)

Kurdjumov-Sachs (K-S) Orientation

Fcc: $x_A = [\bar{1}10]$ $y_A = [\bar{1}\bar{1}2]$ $z_A = [111]$

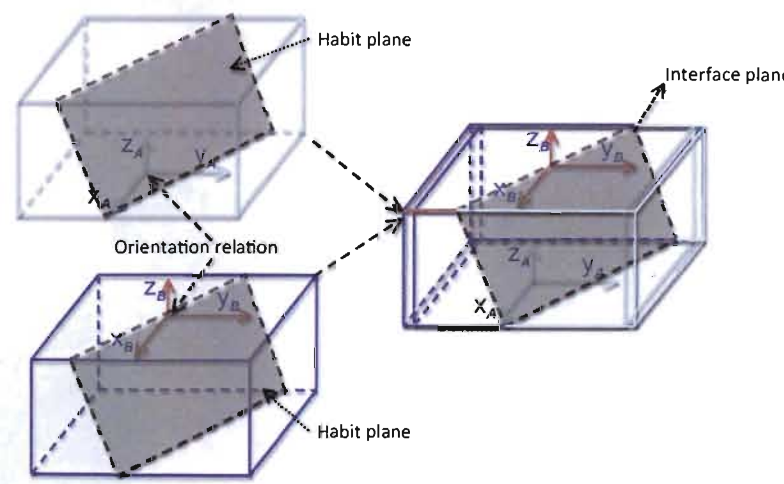
Bcc: $x_B = [\bar{1}11]$ $y_B = [1\bar{1}2]$ $z_B = [110]$

Nishiyama-Wassermann (N-W) Orientation

Fcc: $x_A = [10\bar{1}]$ $y_A = [\bar{1}2\bar{1}]$ $z_A = [111]$

Bcc: $x_B = [00\bar{1}]$ $y_B = [\bar{1}10]$ $z_B = [110]$

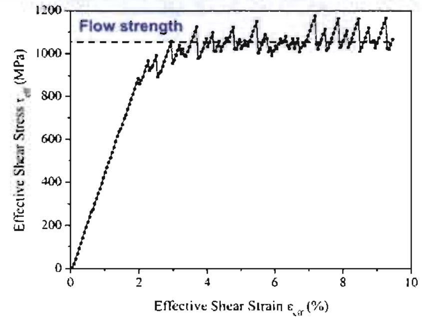
Orientation, Habit plane and Interface plane



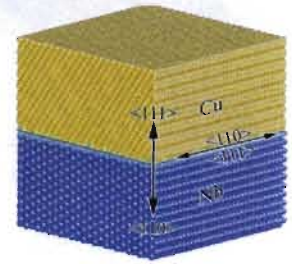
The dependence of interface shear strength on atomic structures of interfaces & on the dilute heats of mixing

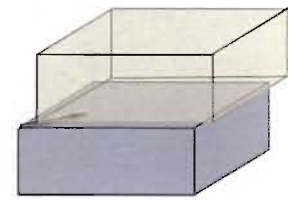
Potentials	*dH*(Nb in Cu) (eV)	*dH*(Cu in Nb) (eV)	a_{CsCl}(Å)	B_{CsCl}(GPa)
Expt./VASP	1.02 [16]	0.48 [16]	3.22 (VASP)	168 (VASP)
EAM-dH1	1.40	0.800	3.19	188
EAM-dH2 (Cu-Nb)	1.03	0.436	3.19	188
EAM-dH3	0.76	0.351	3.17	188
EAM-dH4	0.26	-0.004	3.16	188
EAM-dH5	-0.39	-0.61	3.16	188

Interface shear strength is determined by using atomistic simulations



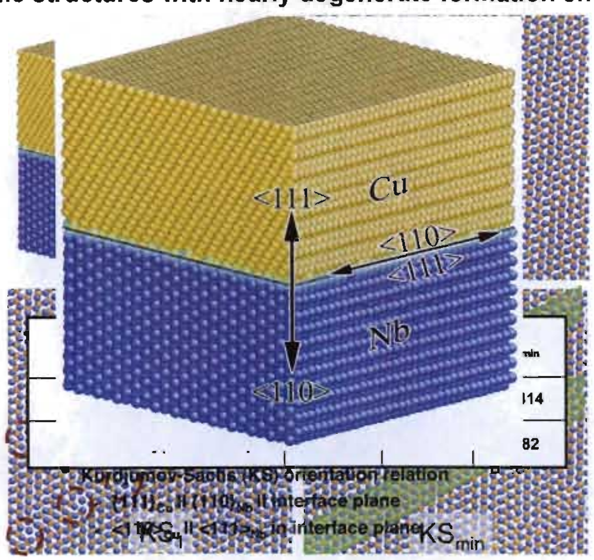
Effective stress-strain behavior



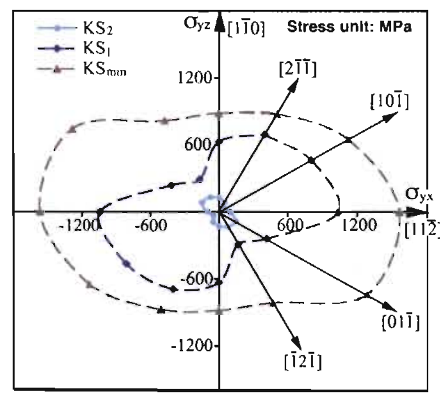


- Gradually increase shear strains while maintain the equilibrium of the bicrystal.
- Periodic boundaries are adopted in the both in-plane directions

Atomistic modeling of fcc/bcc interfaces reveals multiple states of atomic structures with nearly degenerate formation energy



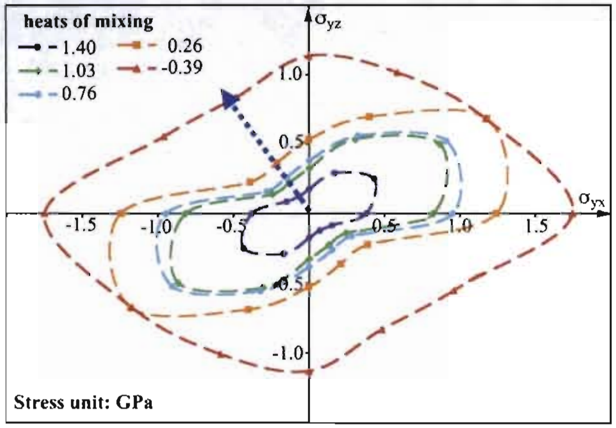
Shear strength of interfaces depends on their atomic structures and is anisotropic.



Two-dimensional flow strength of Cu/Nb interfaces

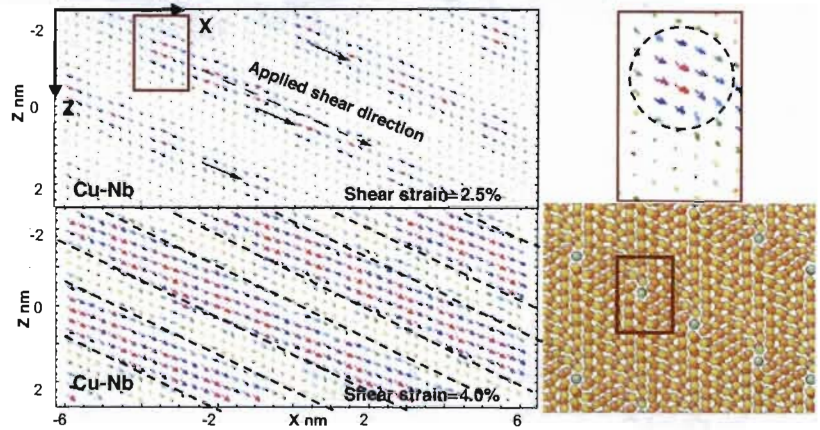
Shear strength is lower than the theoretical shear strength in Cu and Nb.

Shear strength of interfaces increases with the decrease of the dilute heats of mixing and is anisotropic.



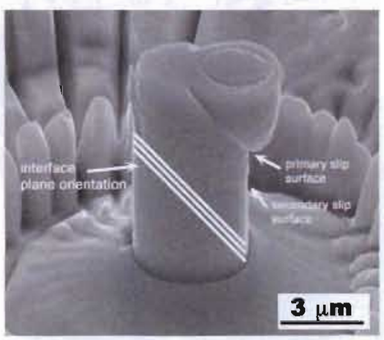
Shear strength is lower than the theoretical shear strength in Cu and Nb.

Low shear resistance results from the ease of creation and glide of interface dislocations

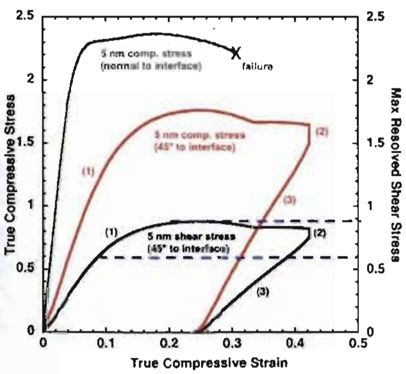


Vector plot of disregistry across the Cu-Nb interface plane

Micropillar compression tests validate "weak" interface in Cu/Nb layered composites.



5 nm CuNb multilayers: layer interface oriented 45° relative to compression axis

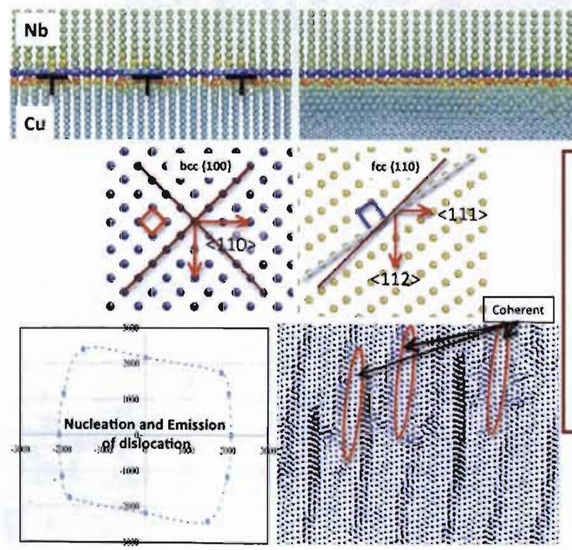


- Deformation is limited to the interface in Cu/Nb multilayers due to "weak" interfaces.
- Experiment results agree with MD simulation.

Type 3: similarity of unit cell

NW fcc{101}||bcc{001}

(No Yes) (No, No) (Yes, Yes)



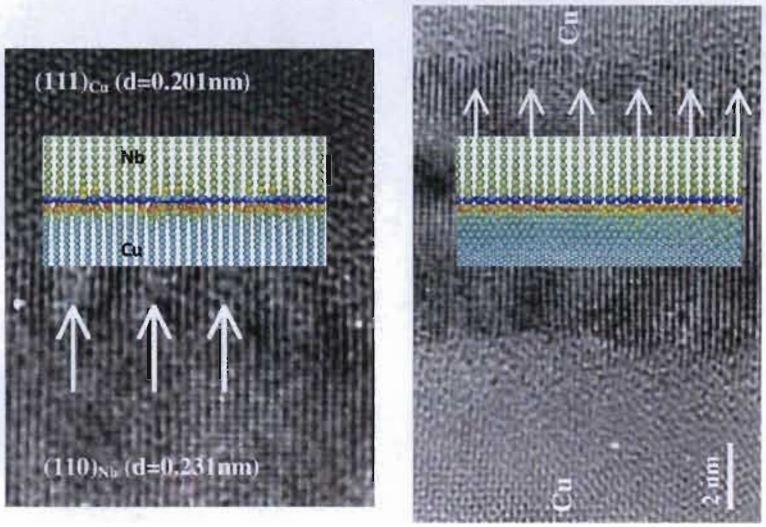
Similarity of unit cell:
1. Contain same numbers of atoms
2. Shape of unit cell

Several features

1. Interface plane is flat.
2. Interface plane is composed of "coherent" and "in-coherent" regions.
3. The boundary between "coherent" and "in-coherent" planes could act as sources of lattice dislocation.

Interface shear response: dislocation nucleation from interface and propagation into phases

HRTEM of NW fcc{101}||bcc{001} interface

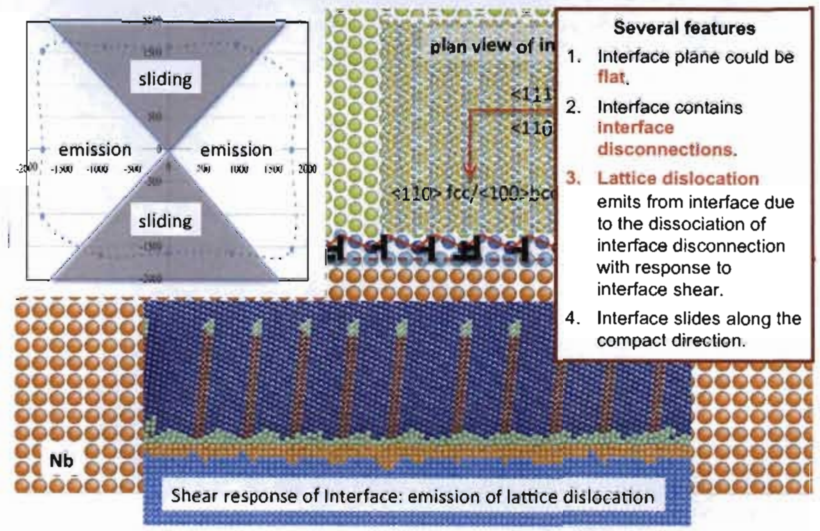


X. SAUVAGE et al, Acta Mater 49, 2001, 389

Type 4: combination

(No, Yes) (Yes, Yes) (No, No)

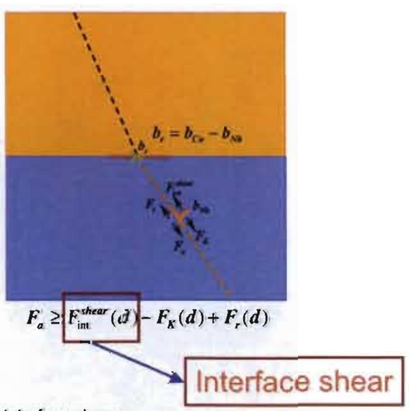
NW fcc{121}||bcc{110}



Several features

1. Interface plane could be flat.
2. Interface contains interface disconnections.
3. Lattice dislocation emits from interface due to the dissociation of interface disconnection with response to interface shear.
4. Interface slides along the compact direction.

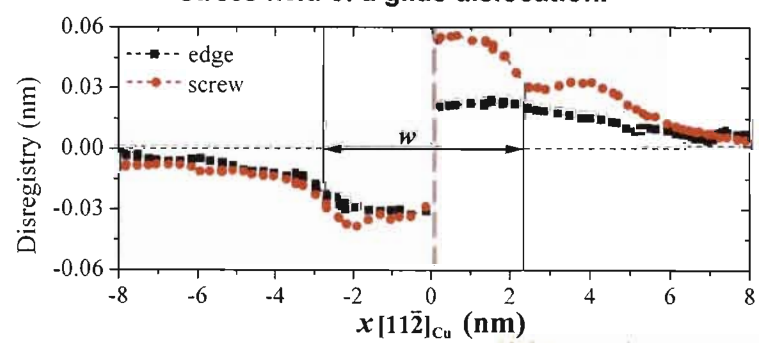
Slip transmission across interfaces



$$F_a \geq F_{int}^{shear}(d) - F_K(d) + F_r(d)$$

- F_K Koehler force
- F_a Applied stress
- F_{int}^{shear} Attraction due to interface shear
- F_r Interaction force between residual dislocation at interfaces and lattice dislocation

"Weak" interfaces are readily sheared under the stress field of a glide dislocation.

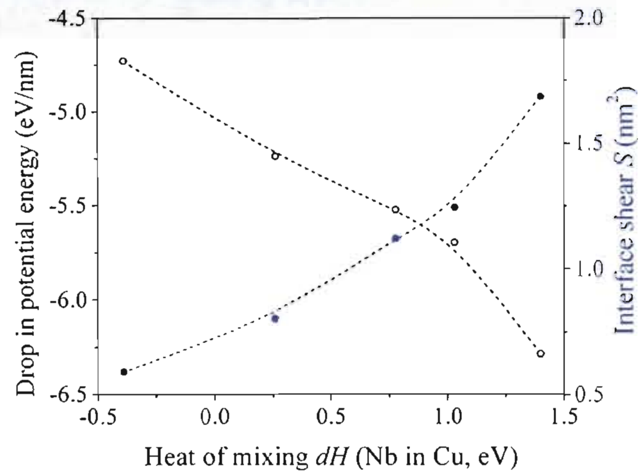


- The spreading width of the dislocation core within the interface plane can be determined according to the disregistry.
- The shear extent of interface can be calculated according to the shear displacement of the interface.

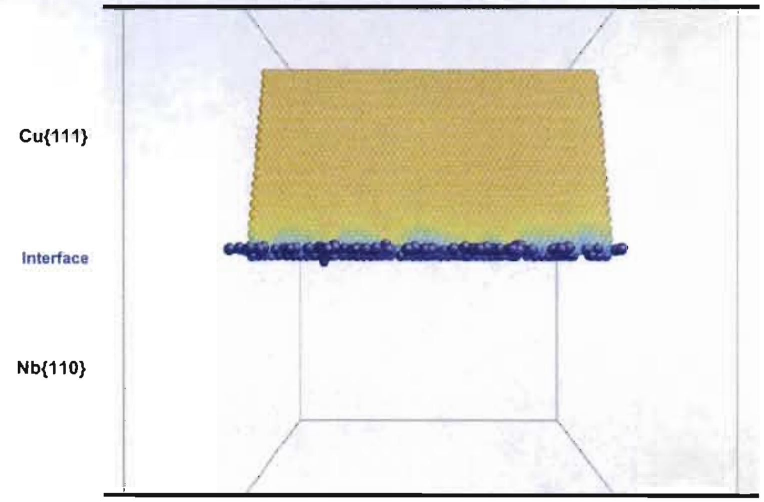
Extent of interface shear

$$S = \frac{1}{L}\int_{-L/2}^{L/2}\int_{-\infty}^{\infty}\left|d_{(x,z)}\right| dx\,dz$$

The extent of interface shear is greater for weaker interfaces



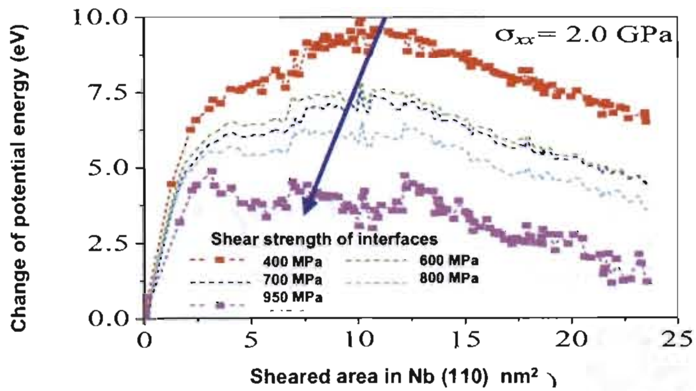
Slip transmission via the nucleation and propagation is determined by using the chain of state method.



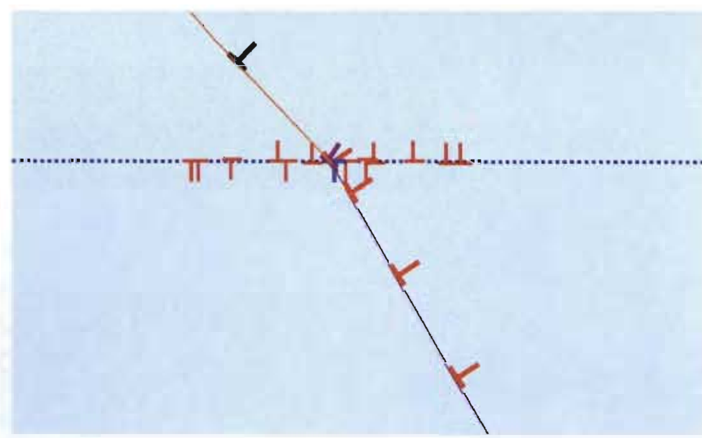
Resolved shear stress on the slip system {110}<111> in Nb is 0.48 GPa.

Work to be done for creating a dislocation loop strongly depends on the interface shear strength.

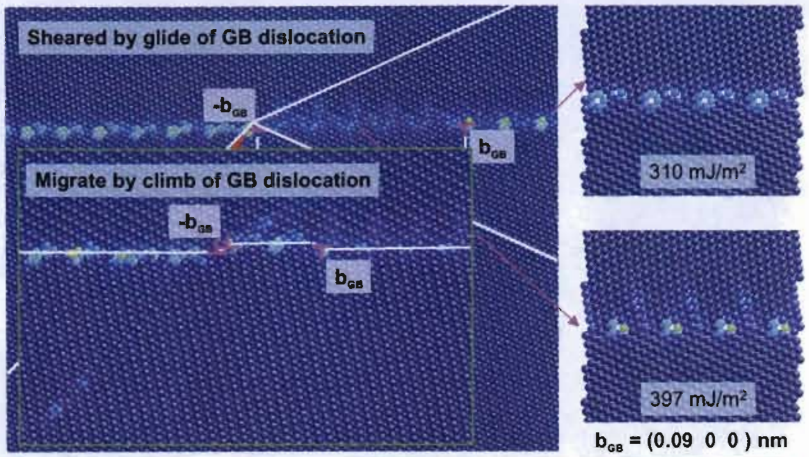
Results shown for transmission from Cu to Nb



Weak interface strengthening mechanisms



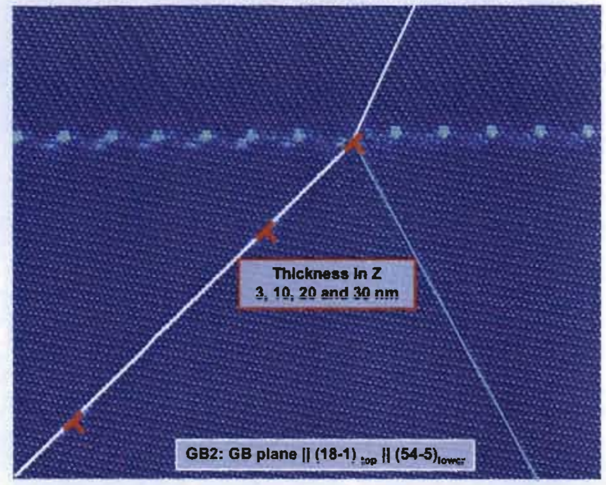
GBs are sheared and can locally migrate.



b_{GB} = (0.09 0 0) nm

- The GB dislocation can be identified using γ surface. [R. G. Hoagland, Philo. Mag. 2002]
- Detach of a dislocation from GB is at RSS = 1.36 GPa, MD running at 300 K for 620 ps.

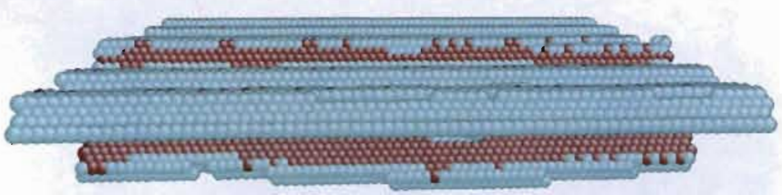
Slip transmission with thickness



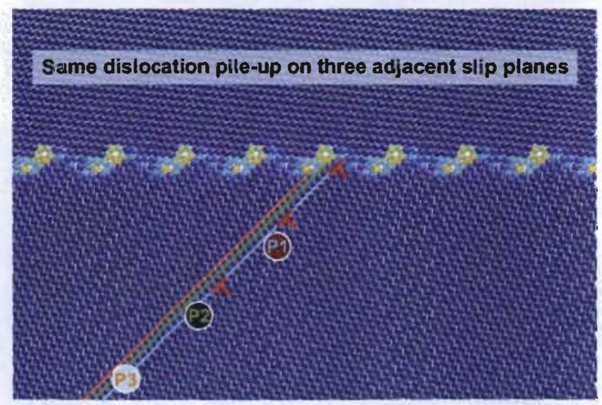
Similar processes are identified in all simulations (details in the following slides and poster).

Large-scale simulations of transmission mechanisms reveal the critical length (5 nm) for the nucleation of a dislocation loop

20 nm example

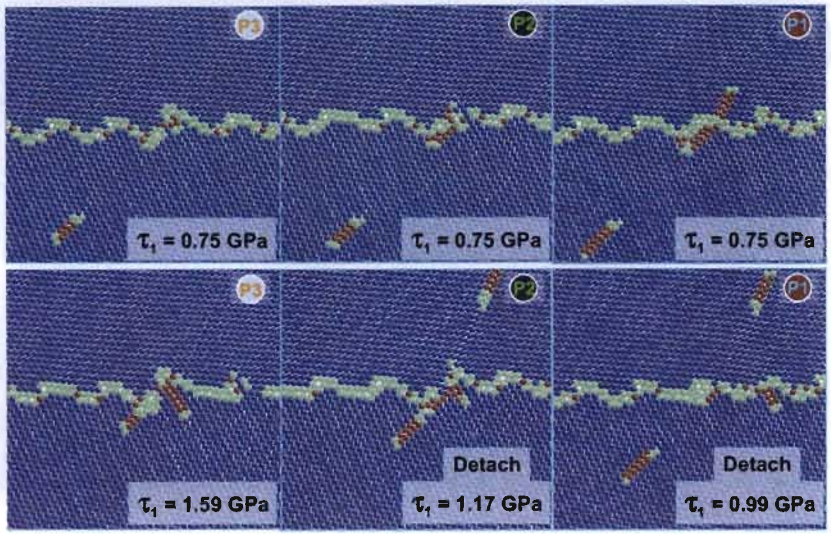


Local atomic structures of GBs change transmission kinetics.

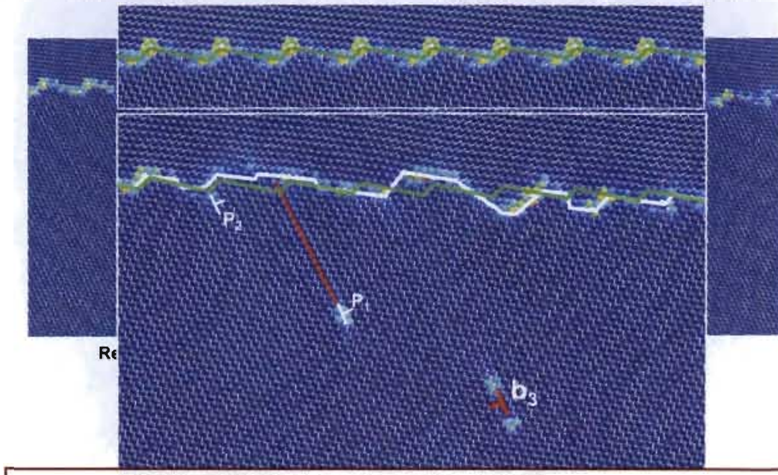


- 5 of N (5, 10, 20, 30) dislocations in MD region.
- Transmission becomes more difficult from P1 to P3.

Response of GBs with respect to interaction position

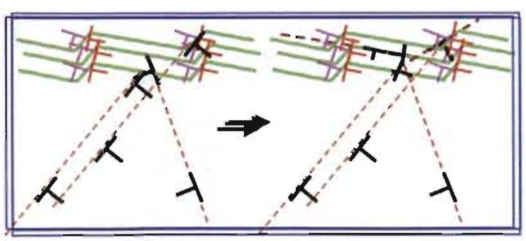


Two dislocations are smeared in GBs in association with the migration of GB, destroying dislocation pile-up.



1. When the discontinuity of slip systems become bigger, dislocations entering into GB result in the migration of GB through the move and reaction of GB dislocations (climb and/or gliding, reassemble and emission). 2. Blunting the stress concentration at the intersection of dislocations with GB.

Dislocation Model



Climb
Reassembly
Dissociation
&
Transmission
Glide

Summary

Weak interface Strengthening Mechanisms

- Interfaces have low shear strength due to the ease of nucleation and glide of interfacial dislocations enabled by the atomic structure.
- The stress field of a glide dislocation easily shears the "weak" interface, resulting in attraction and trapping via core spreading of glide dislocation in the interface.
- The attraction force on a glide dislocation from a "weak" interface scales inversely with the shear strength of the interface.
- Work to slip transmission scales inversely with the shear strength of the interface.