Exploration of the Radiation Resistance of Near-Theoretical Strength Nanolayered Composites

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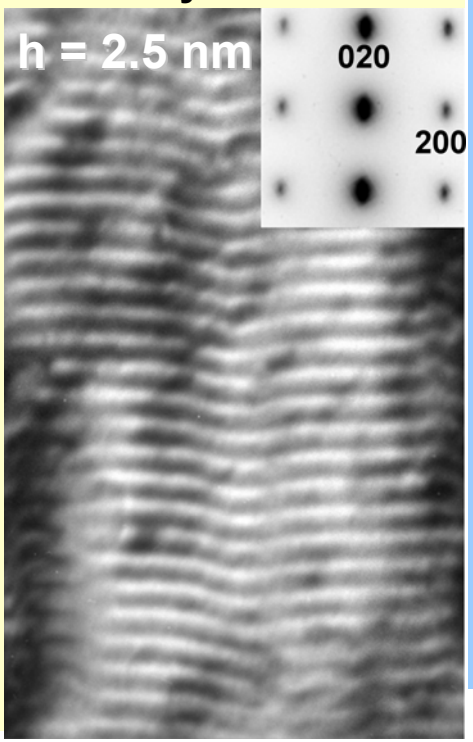
Why Nanolayered Materials?

- Recent findings of a joint PNNL-LANL project (BES funded) reveal that multi-layered composites consisting of many alternating, dissimilar metal layers, each only a few nanometers thick, possess enormous strength, approaching theoretical limits, due to their large internal interfacial areas and stresses. A typical 25 mm x 25 mm x 5 mm composite has ~125 m^2 of interface area
- These materials also unexpectedly display great thermal and mechanical stability
- Their properties derive from operation of deformation mechanisms that do not occur in conventional metallic materials. Property tailoring can be achieved through control of the layer thickness and the lattice mismatch by careful selection of composite constituents

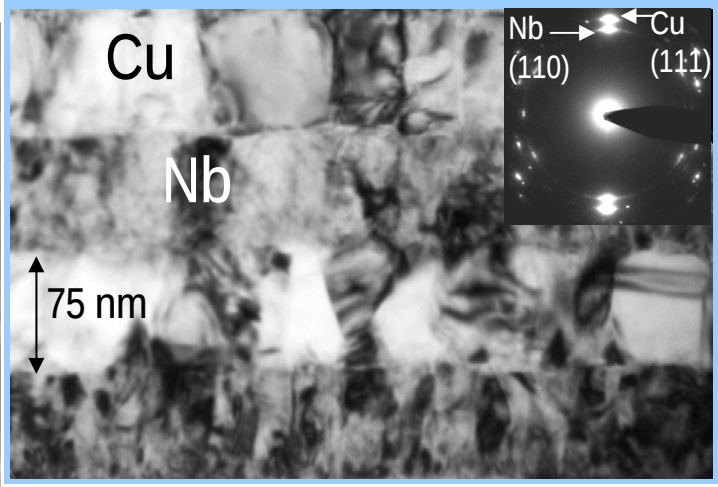
Synthesis by Physical Vapor Deposition

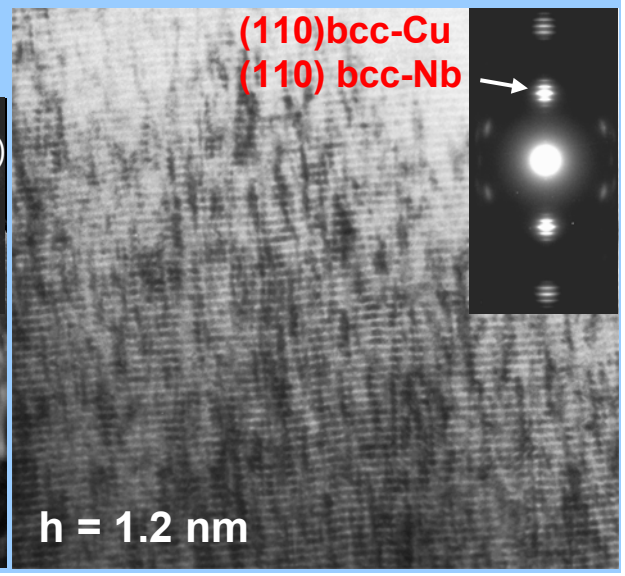
- Magnetron sputtering and e-beam evaporation
- Deposition rates ≈ 0.5 - 1 nm/s
- Layer thickness varied from 4 mm to 1 nm
- Total sample thickness up to 20 mm

Single Crystalline Evaporated Cu-Ni Multilayers

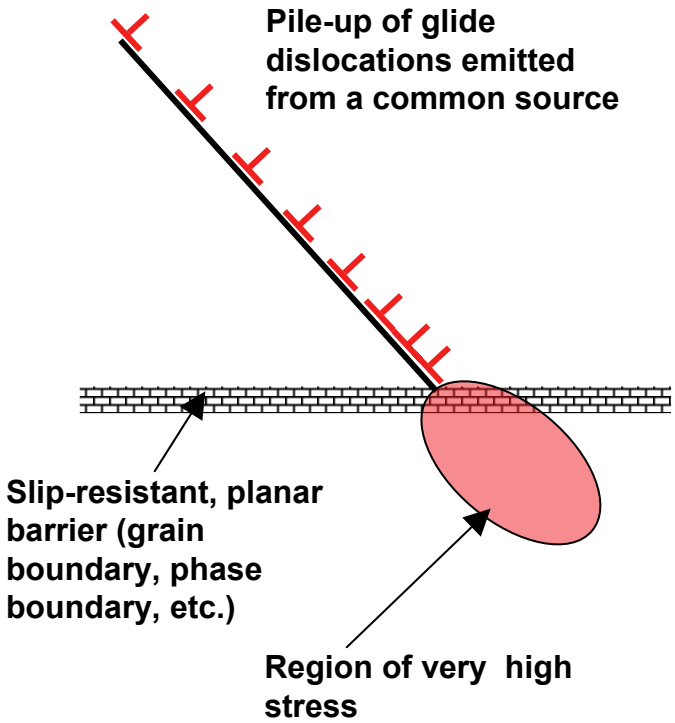


Textured Polycrystalline Sputtered Multilayers





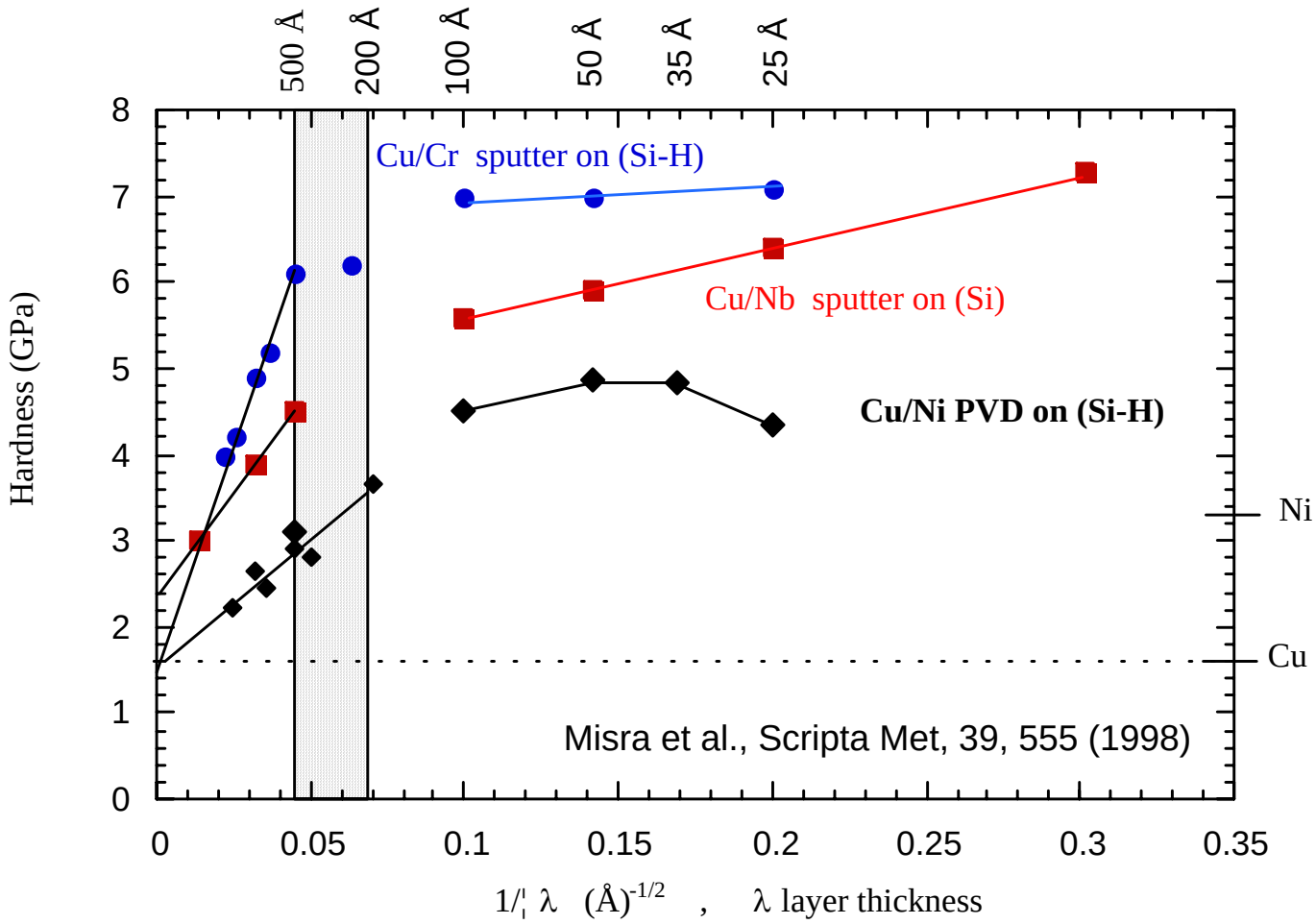
The Dislocation Pile-Up - An Important Slip Mechanism Common to Conventional Materials



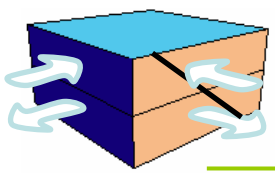
- The stresses near the tip of the pile-up are amplified by the number of dislocations in the pileup and can easily become very large even when applied stresses are low .
- The stresses are proportional to the square root of the length of the pile-up. This is the origin of Hall-Petch (inverse root grain size) behavior.
- Stresses at pile-up tip can easily exceed theoretical shear strength triggering slip on the opposite side of the barrier. Deformation tends to remain localized.
- Stresses can also exceed theoretical tensile strength triggering void nucleation (leading to ductile fracture) or cleavage (brittle fracture).

The spacing between barriers must be relatively large for this to happen

Length-scale Effect on Hardness in Multilayers



A Short List of Critical Issues



Coherency stresses due to lattice mismatch - σ_{coh}

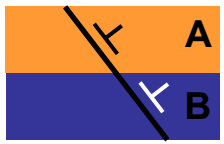
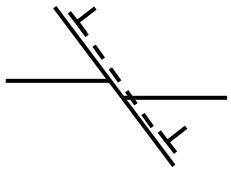
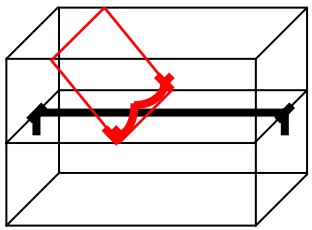


Image (Koehler) stresses due to elastic modulus mismatch - σ_K



Crossing involves creation of a step (possibly faulted) on the interface and a change in stacking fault energy - σ_S and σ_{sf}

Misfit dislocation core structure

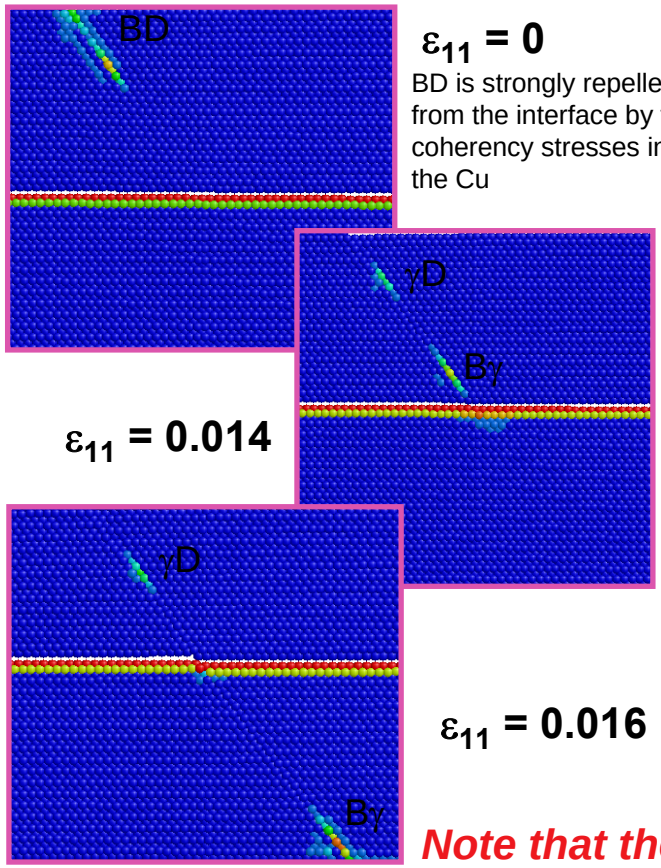


Glide dislocations crossing a semicoherent interface must cut/interact with misfit dislocations

Highlights - Coherency Stresses

In a coherent Cu / Ni bilayer, an edge partial crosses the interface when the stress in the Cu changes sign during uniaxial tensile loading

Strength is largely determined by coherency stresses

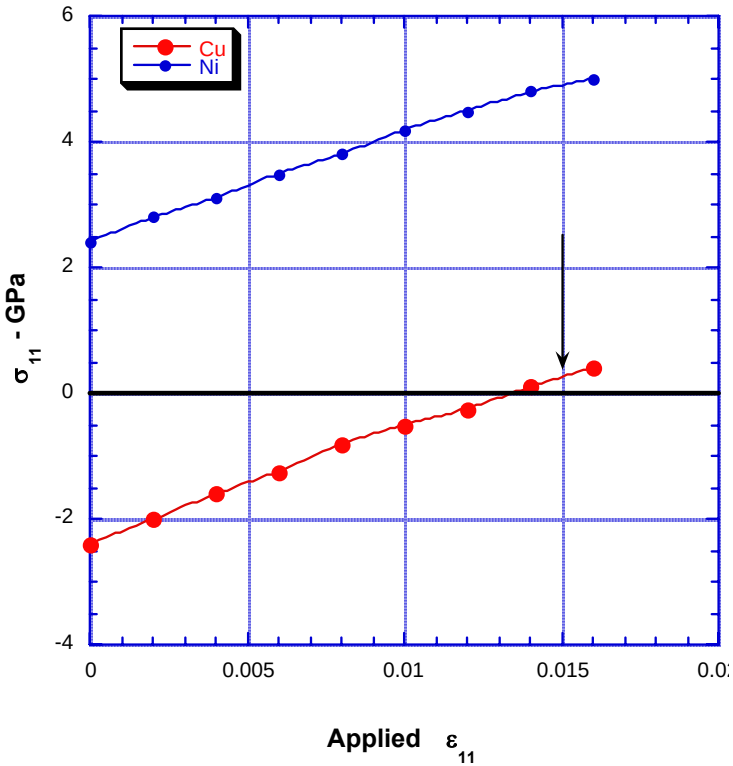


$\varepsilon_{11} = 0$

BD is strongly repelled from the interface by the coherency stresses in the Cu

$\varepsilon_{11} = 0.014$

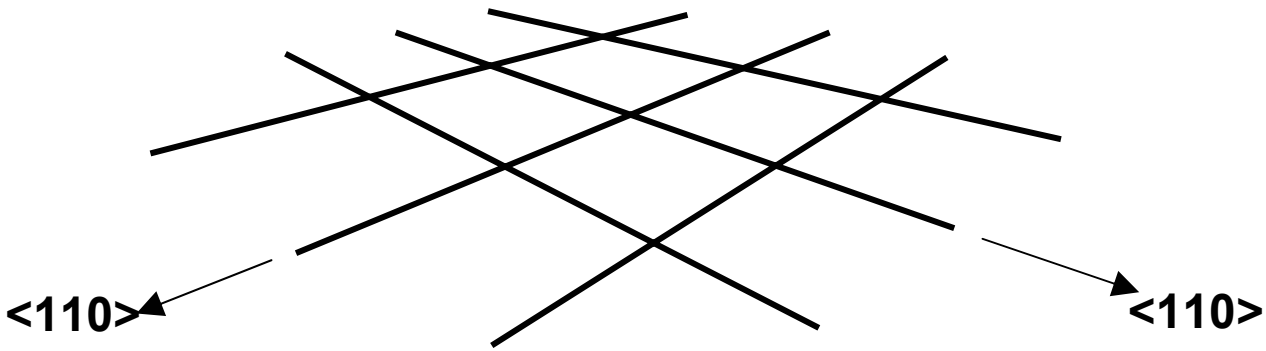
$\varepsilon_{11} = 0.016$



Note that the tensile stress in the Ni layer becomes very large

Highlights - The Role(s) of Misfit Dislocations

Above a critical layer thickness it becomes energetically favorable for a coherent interface to acquire a network of misfit dislocations thereby becoming semicoherent



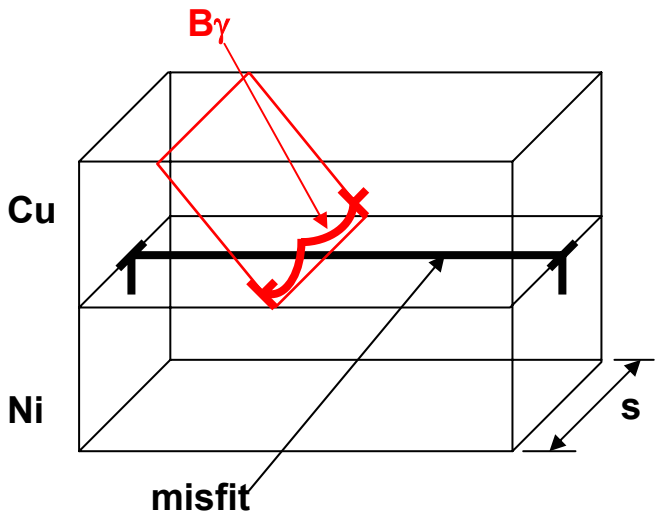
Misfit dislocation network in FCC / FCC composites

Misfit dislocations:

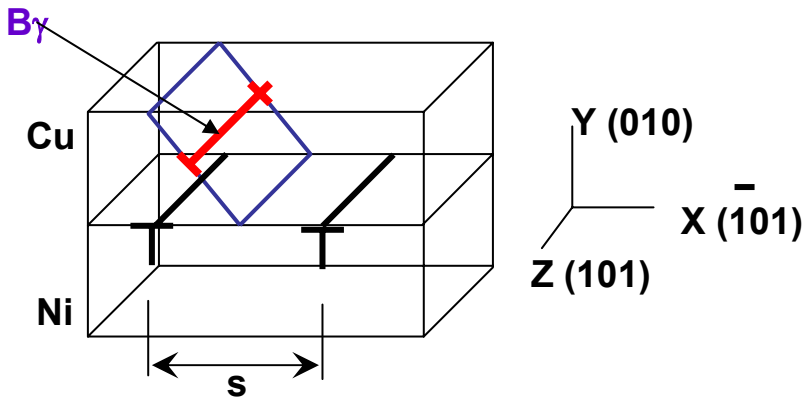
- **Decrease or eliminate the coherency stresses away from the interface (but not at the interface)**
- **Interact with glide dislocations in several ways**

Highlights - The Role(s) of Misfit Dislocations

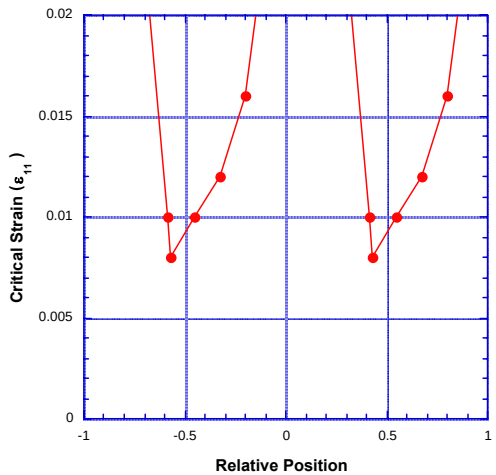
Barrier Strength



Misfit dislocations *perpendicular* to incoming glide dislocations are easily cut - resolved shear stress required is ~ 120 MPa.



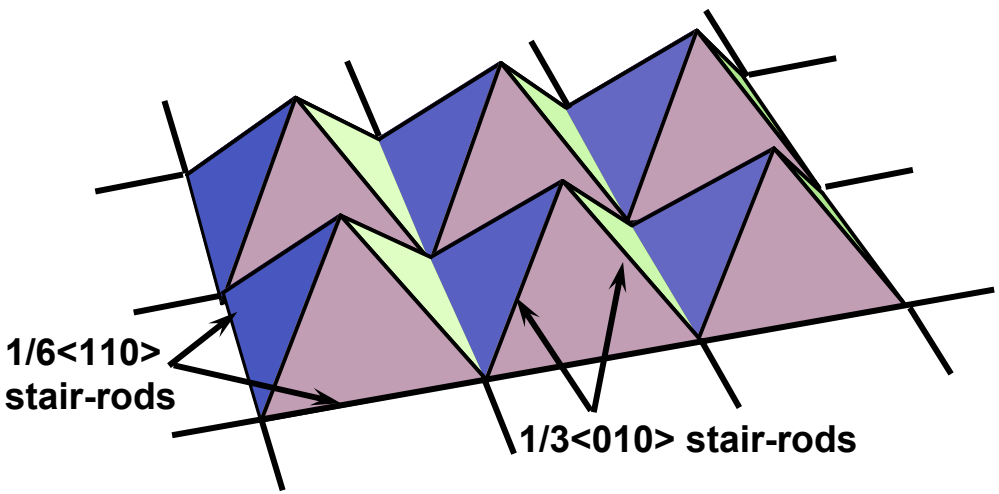
Misfit dislocations *parallel* to incoming glide dislocations effectively block about one half of the interface



Highlights - The Role(s) of Misfit Dislocations

Core Structure

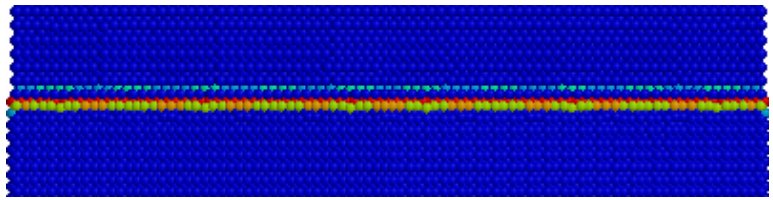
The dissociation of the misfit dislocation array produces a 3D array of stacking fault pyramids that is not only resistant to slip but also may be more stable than the square array.



Cu / Ni

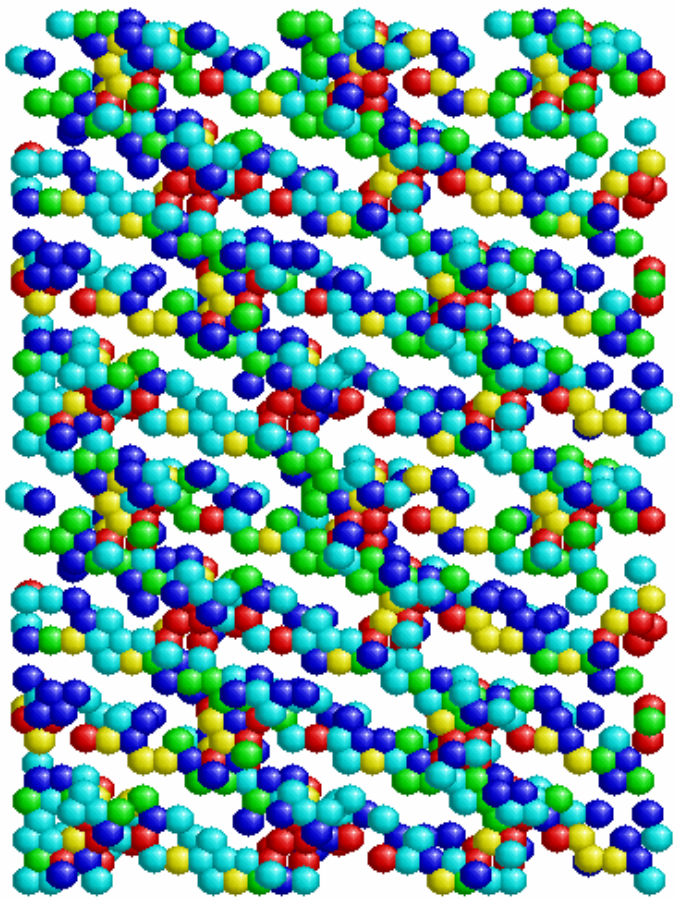
In contrast, the cores of misfit dislocations in Cu / Ag are wide. As a result:

- Misfits are confined to the interface (unable to dissociate)
- Misfits are very mobile
- Misfits react readily with incoming glide dislocations
- Misfits eliminate or reduce coherency stresses almost everywhere



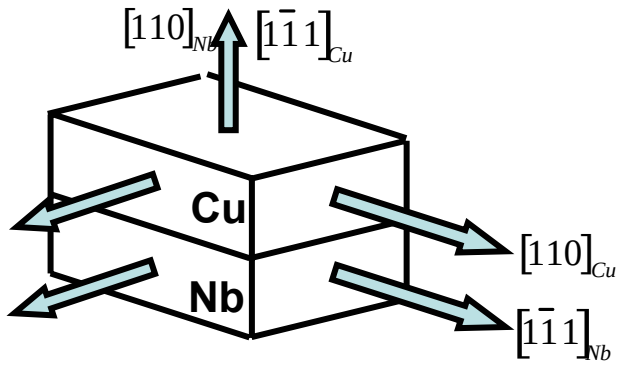
Cu / Ag

Cu / Nb



Atoms associated with dislocations at the interface

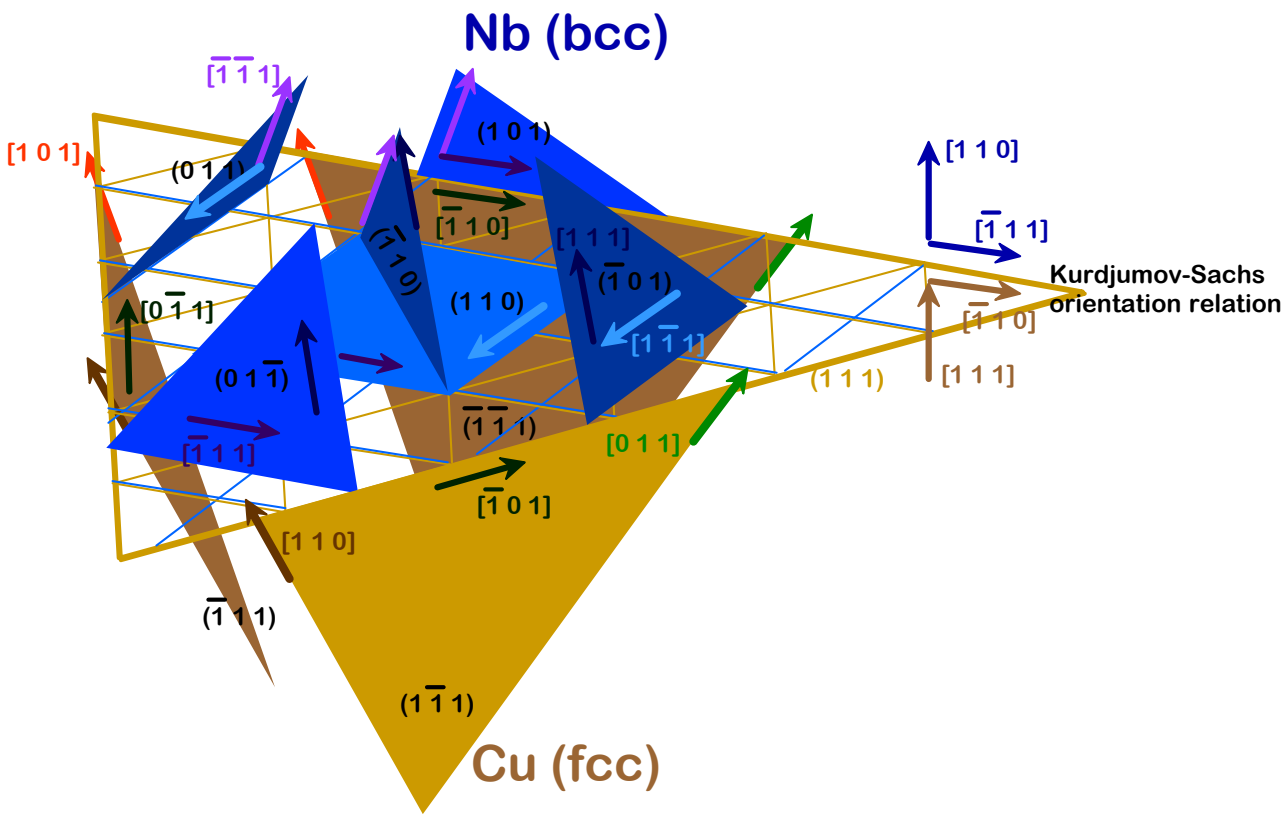
A Kurdjumov-Sachs orientation relation



The interfacial structure in the epitaxially-oriented Cu(fcc) / Nb(bcc) system is more complex than in the fcc / fcc systems. Misfit dislocations are formed but they consist of different types - both mixed and screw. ***This suggests a far richer spectrum of mechanisms than in fcc / fcc.***

Cu / Nb

The relative orientation of slip planes at the interface in KS-oriented Cu / Nb composites

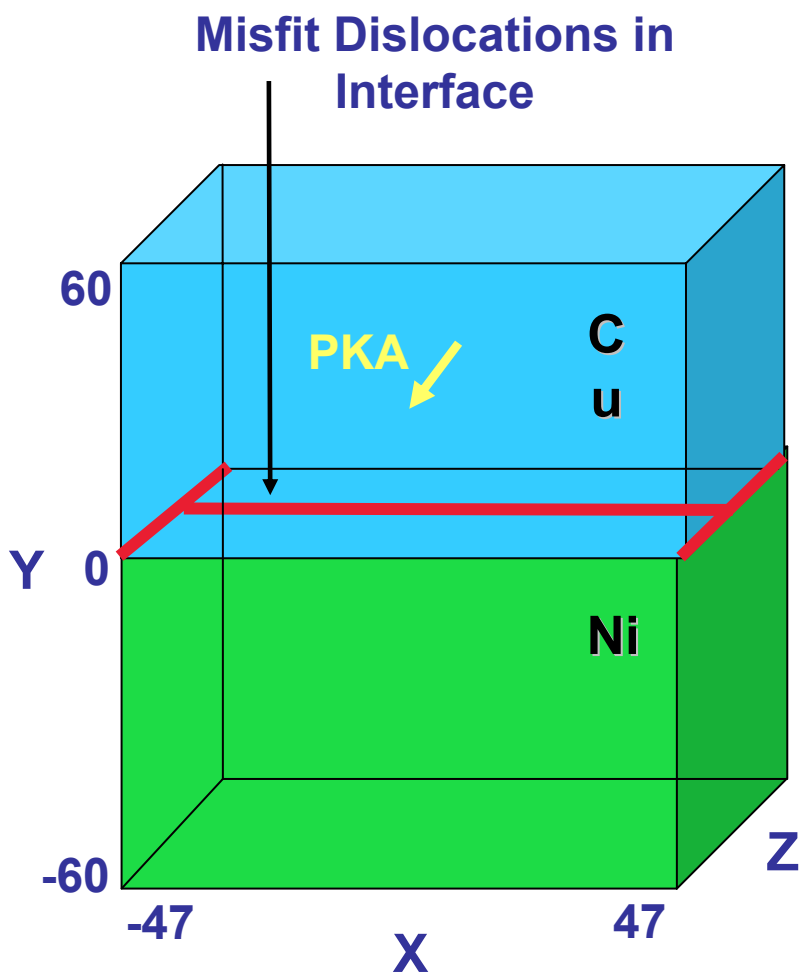


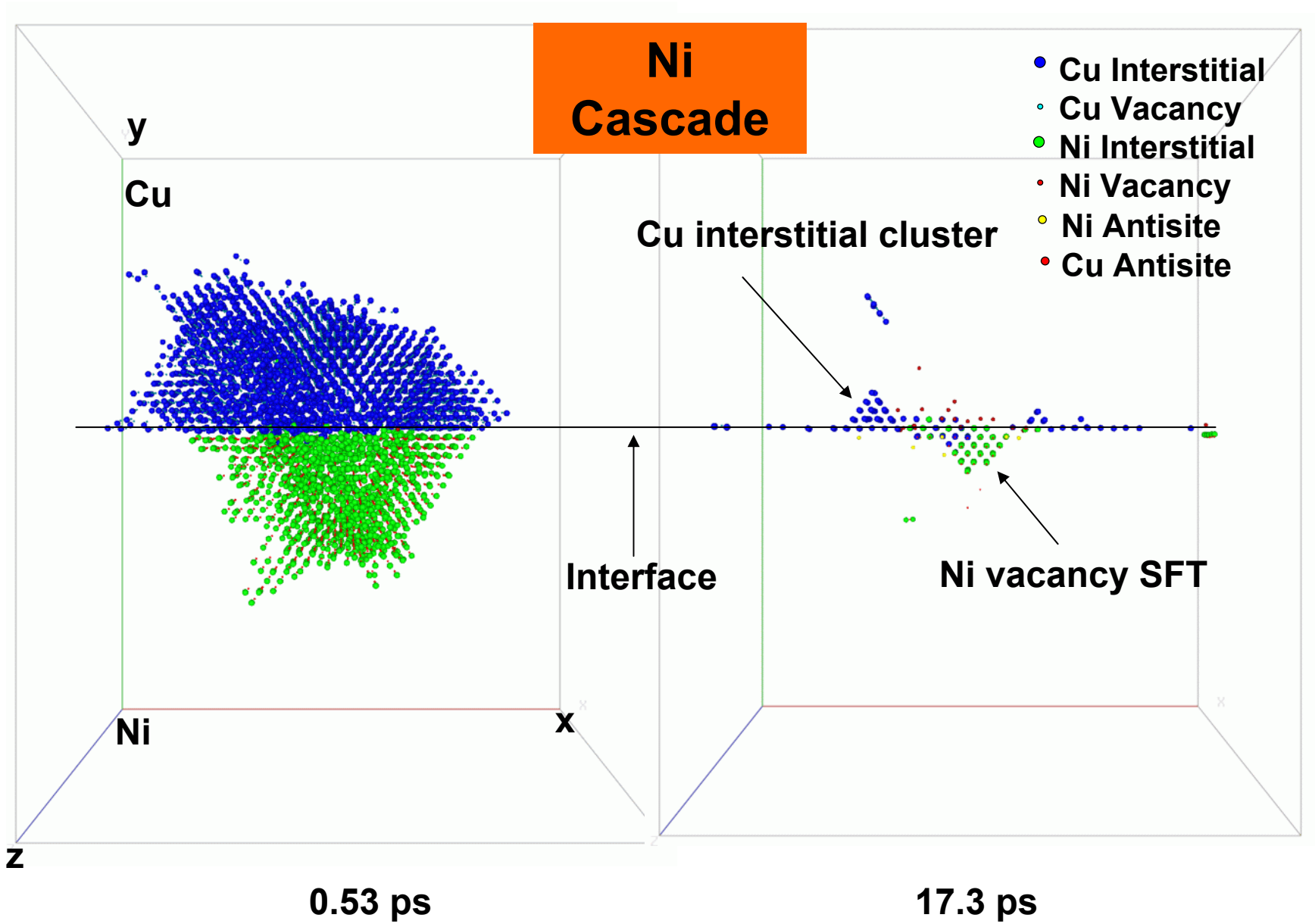
Exploratory Research Program

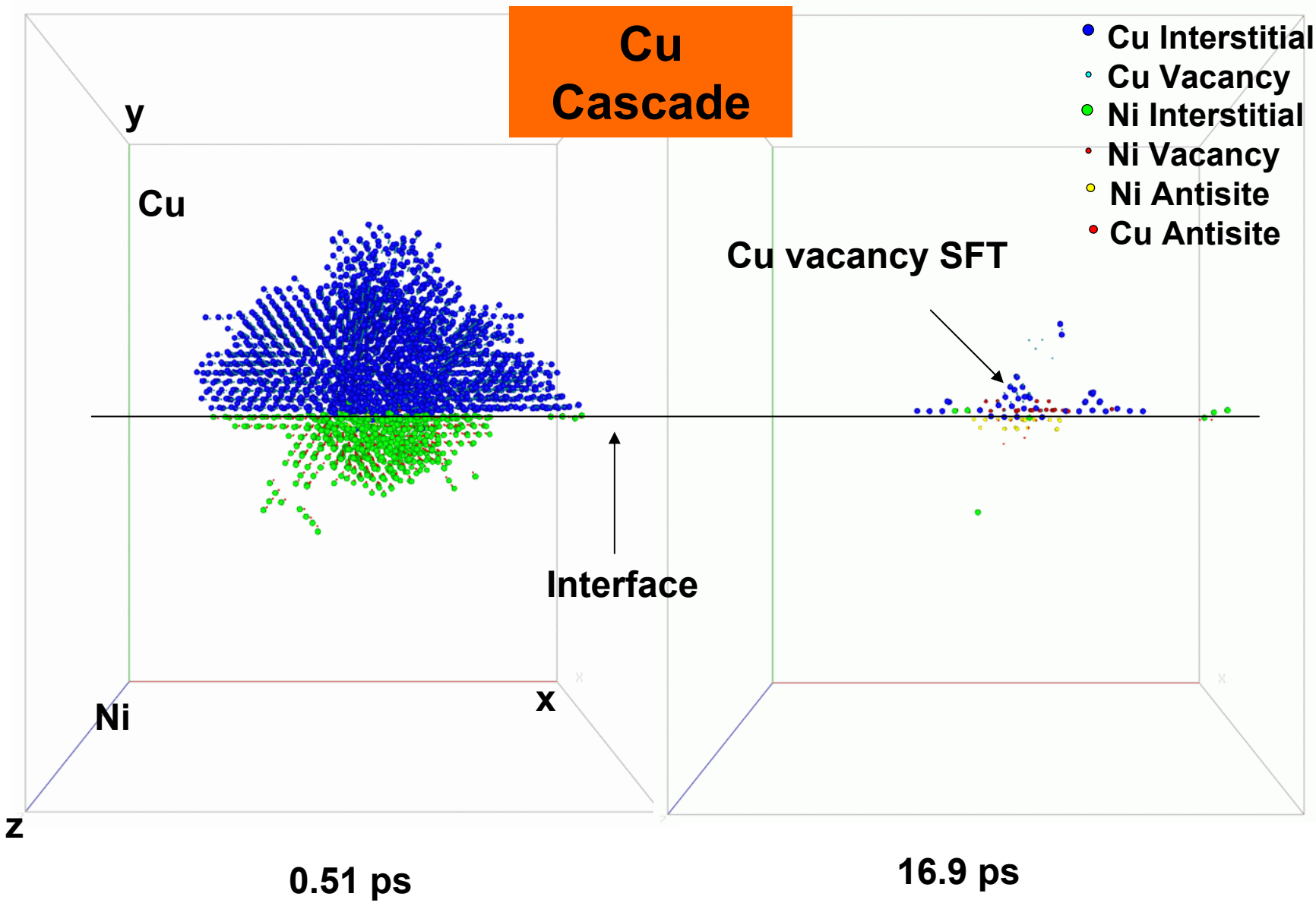
- The project will use an array of computational and experimental techniques to explore the effects of radiation on interface stability
- Cu / Ni, Cu / Ag, and Cu / Nb composites will be studied initially since they are readily available from LANL and represent a range of solid solubility and interface epitaxy
- MD techniques will be used initially to study:
  - The effects of displacement cascades on interfaces
  - The effects of interfaces on cascade damage
  - The role of cascade mixing in interface integrity
  - The role of defects in interface integrity
- Experimental studies will be conducted with heavy ions, protons and neutrons for comparison with computational predictions
- Analytical electron microscopy and nanoindentation techniques will be used to study the microstructures produced under irradiation

Cascades in Cu / Ni Nanolayers

- Computational Cell: ~96k total movable atoms, 95 x 120 x 93 Å
- Fixed boundaries in x and y directions, periodic in z
- Misfit dislocation in the interface along the x-axis (z = 0, y = 0) and transverse misfits at (x = 47.3, y = 0) and (x=-47.3, y=0)
- EAM potentials for Cu, Ni and Cu/Ni cross pair, with repulsive potential fitted at small separations
- The atoms in the cell were relaxed, then equilibrated at 100 K
- Two Cascades were run:
  - 5 keV PKA started in Ni layer at (-14,-5,-24), directed along [513]
  - 5 keV PKA started in Cu layer at (18,32,6), directed along [-3-5-1]




Ni
Cascade
Cu Interstitial
Cu Vacancy
Ni Interstitial
Ni Vacancy
Ni Antisite
Cu Antisite
y
Cu
Cu interstitial cluster
Interface
Ni vacancy SFT
Ni
x
z
0.53 ps
17.3 ps


Cu
Cascade
Cu Interstitial
Cu Vacancy
Ni Interstitial
Ni Vacancy
Ni Antisite
Cu Antisite
y
Cu
Cu vacancy SFT
Interface
Ni
x
z
0.51 ps
16.9 ps

Very Preliminary Observations

- Cascades are attracted toward the interface
- Large vacancy and interstitial clusters are formed near the interface
- Cu and Ni vacancy SFTs are formed near interface in both layers
- Interstitial SFTs (?) are observed only in the Cu layer
- Atomic mixing is small and appears only at or near the interface