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Title:	Understanding of interface structures, defects, and mechanical properties at general fcc-bcc interfaces using "tunable" potentials
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3rd International Conference on Heterogeneous Material Mechanics (ICHMM-2011)
(Invited talk)

Understanding of interface structures, defects, and mechanical properties at general fcc-bcc interfaces using "tunable" potentials

X.-Y. Liu, R.G. Hoagland, J. Wang, B.P. Uberuaga, M. Nastasi, A. Misra, J.P. Hirth, M.J. Demkowicz*,

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Abstract:
Nanolayered Cu-Nb composites exhibit high strength and enhanced radiation damage tolerance. To understand the relevance of interface structures to interface properties in general fcc-bcc systems, "tunable" potentials offer a fairly simple way to selectively vary parameters independently. In this work, the parameterization of the EAM interatomic potentials in fcc-bcc system is modified to understand the interface structures, defects, and mechanical properties. We first change the dilute heats of mixing between Cu and Nb and investigate the effect on interface structures. We also demonstrate that the variation in heats of mixing has a strong influence on both the interfacial shear strength and the active shear plane at the interface. To understand the interface behavior in different lattice misfit geometries, the relative lattice constants ratio between Cu and the bcc crystal is varied. Interface dislocation analysis based on Frank-Bilby formulation is to be presented, together with atomistic simulation results. Finally, the effect of the interface dislocation contents on defect-interface interaction is discussed, in the context of effort to construct the figure-of-merit of radiation damage tolerance at interfaces.

Key Words:
Multilayer interfaces; misfit dislocations; defects; interface shear; interatomic potentials

Understanding of Interface Structures, Defects, and Mechanical Properties at *General* FCC-BCC Interfaces Using Tunable Potentials

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Collaborators: Richard G. Hoagland, Jian Wang, Blas P. Uberuaga, Michael Nastasi, Amit Misra, John P. Hirth (LANL), Michael J. Demkowicz (MIT)

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DOE, Office of Science, Office of Basic Energy Sciences, EFRC

Interface Structure

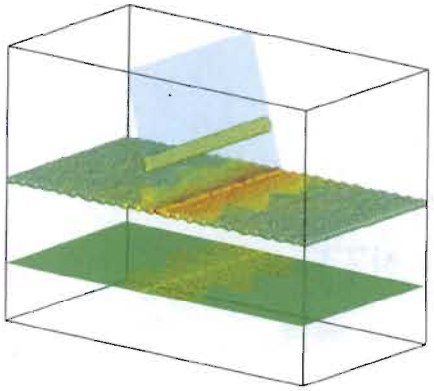
Relevance to

Deformation

•Control deformation by interacting with dislocations

Unit processes
- nucleate dislocations - block dislocations
- store dislocations - annihilate dislocations

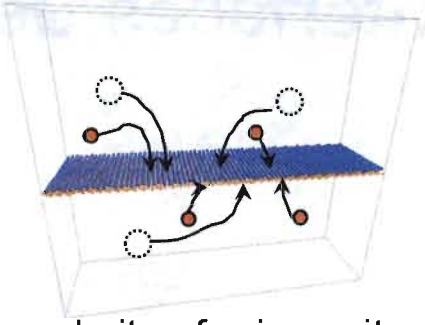
Important for understanding
- yield strength - work hardening
- recovery - fracture



Radiation damage

• Catalyst for point defect annihilation.

CuNb interfaces attract, absorb and annihilate radiation-induced point defects



• Preferred sites for impurity adsorption.

CuNb interfaces absorb noble gasses and delay bubble nucleation in He-implanted Cu-Nb nanolayers

X.-Y. Liu, R.G. Hoagland, J. Wang, T.C. Germann, A. Misra, Acta Mater. **58**, 4549 (2010).
M.J. Demkowicz, R.G. Hoagland, J.P. Hirth, Phys. Rev. Lett. **100**, 136102 (2008).
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Goals

- Based on our knowledge learned from Cu-Nb interface, investigate general fcc/bcc material systems.
- Predictive atomic-scale designs for mitigating radiation damage and high strength in nanolayered composites.

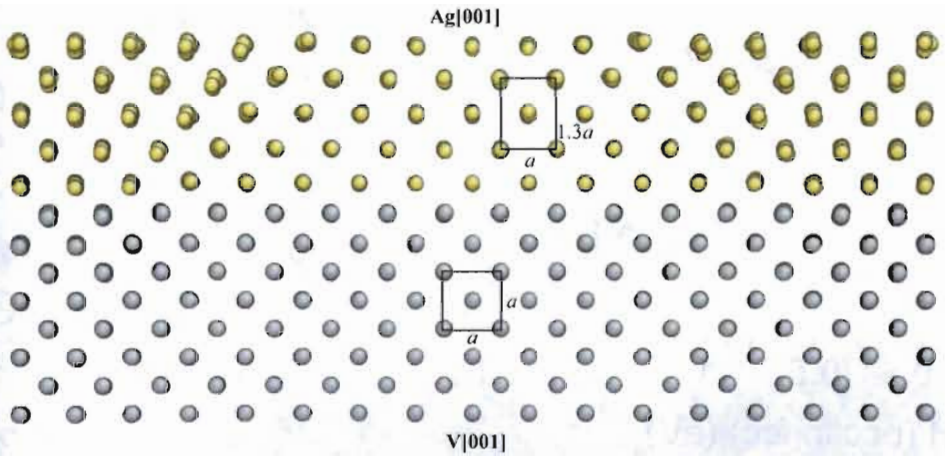
How to represent heterophase interface?

Geometry

- Crystallography (orientation relationships)
- Lattice mismatch: coherent, semi-coherent, incoherent, interface misfit dislocations
- Phase transformations due to interface

Thermodynamic energetics

- Heats of mixing and stability of interface
- Interface energy / enthalpy
- Defect formation energies at interface



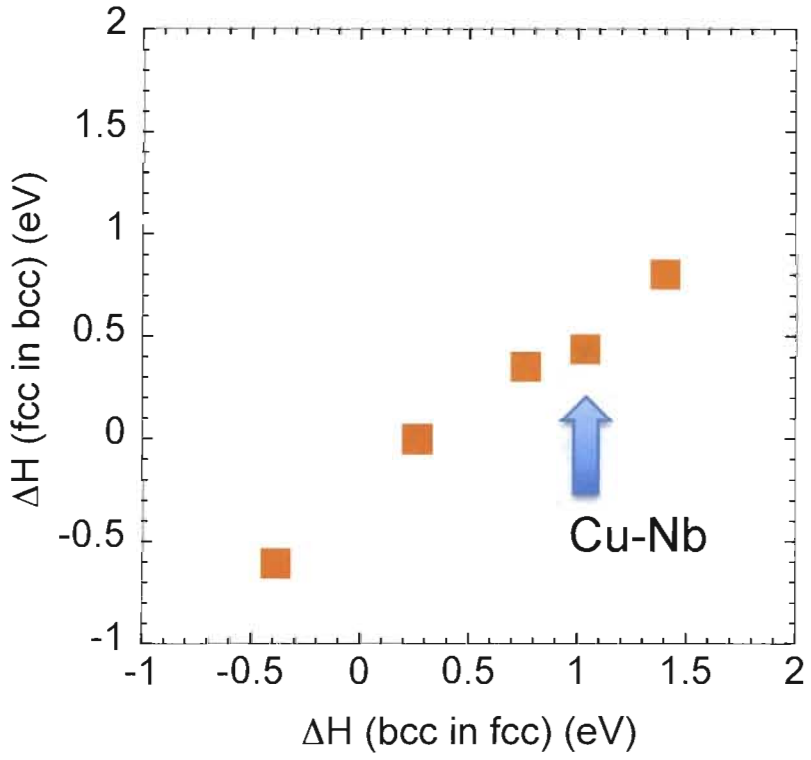
Q.M. Wei, X.-Y. Liu, A. Misra, Appl. Phys. Lett. **98**, 111907 (2011).

Manipulating Interface Properties via Tunable Potentials

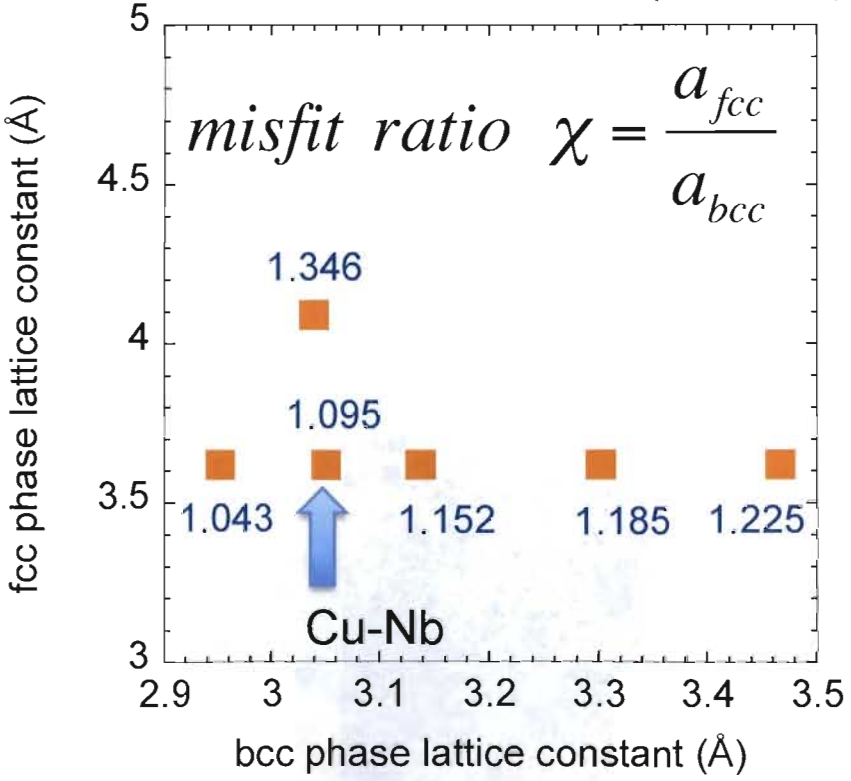
- Keep geometry constant, systematically vary heats of mixing
- Or keep heats of mixing constant, systematically vary geometry

➡ **Tune the parameterizations of the interatomic potential fcc-bcc**

- Interface energetics (heats of mixing)



- Variation of lattice mismatch (or misfit)

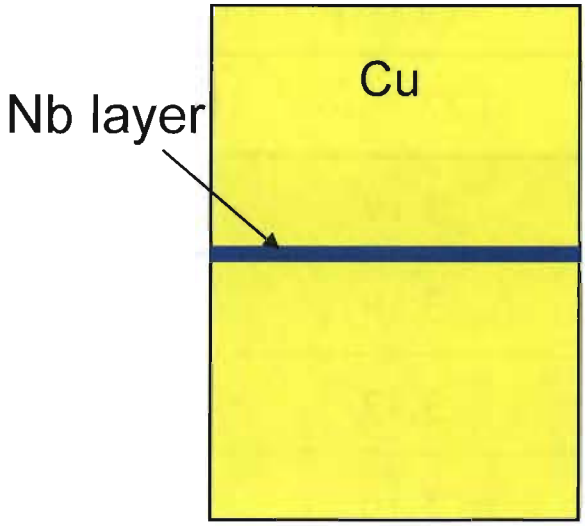


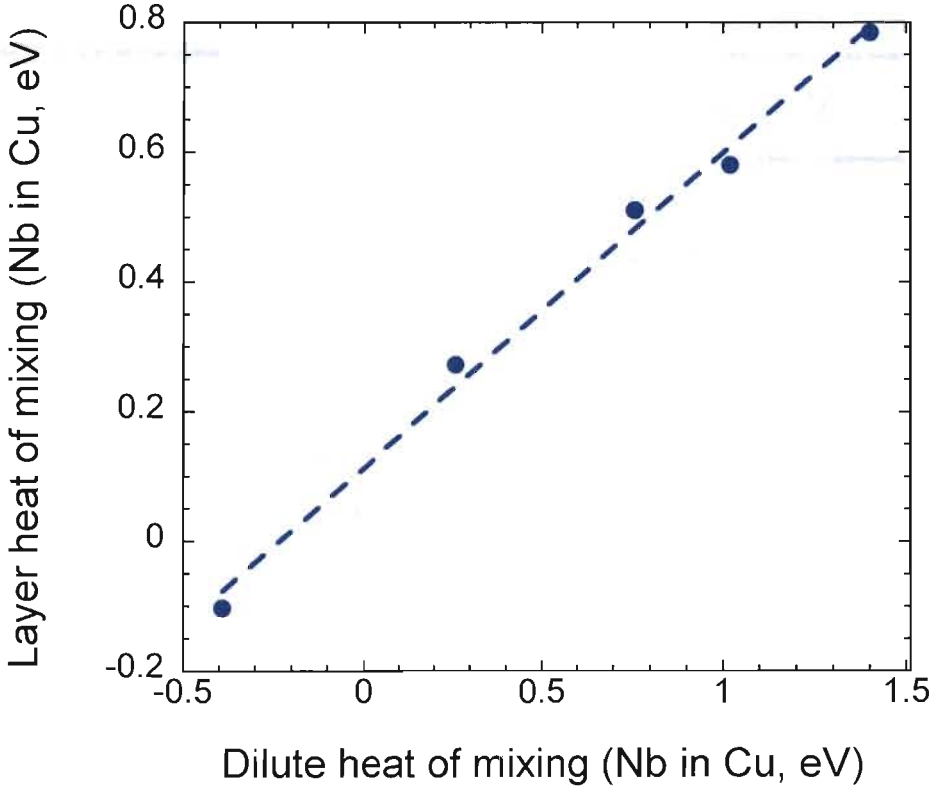
The dependence of interface shear strength on the dilute heats of mixing

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

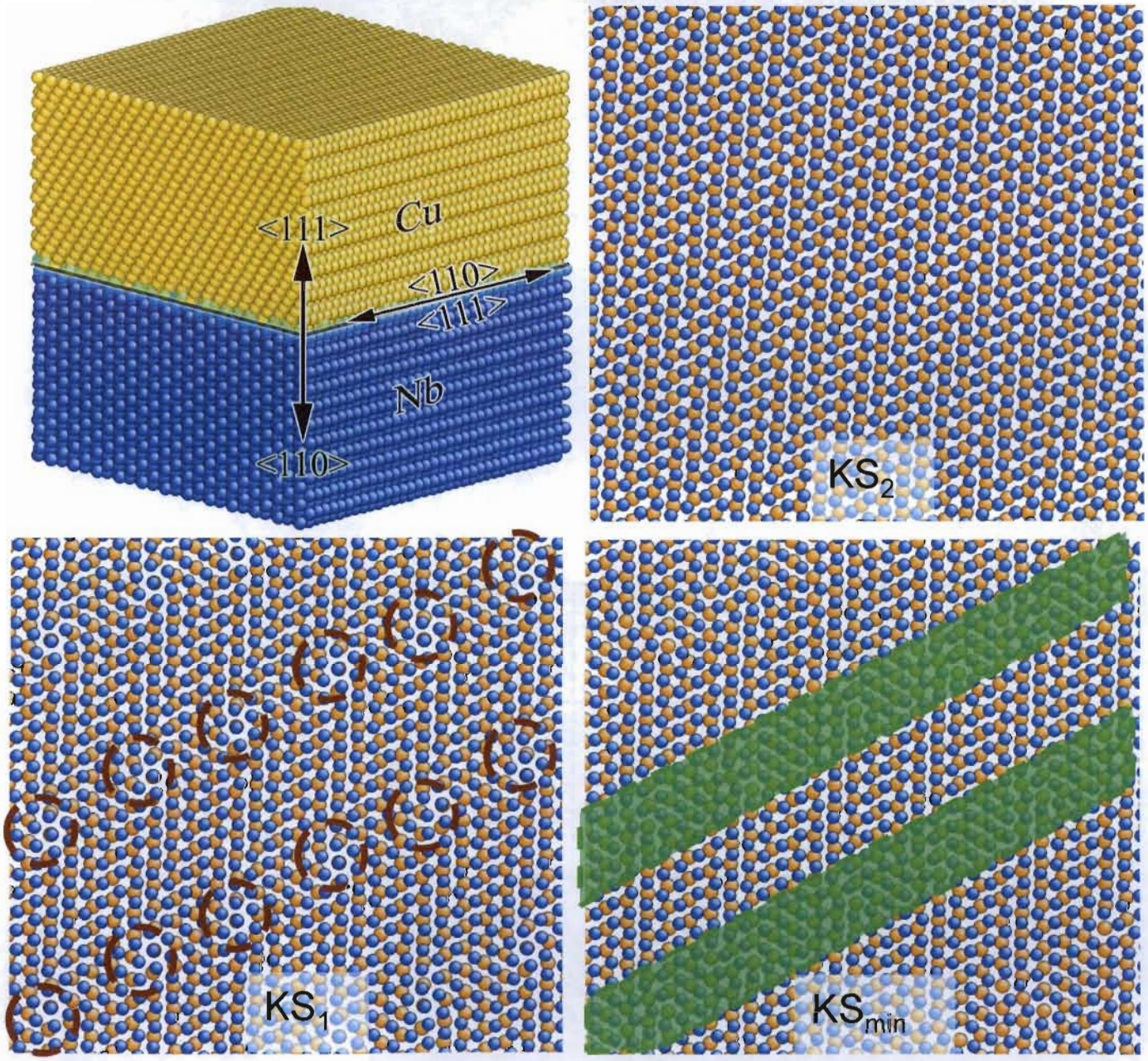
Heats of mixing (HOM): dilute HOM and layer HOM

How good is dilute HOM (single impurity atom in host matrix) in defining the interface bond change? Check with layer HOM calcs.





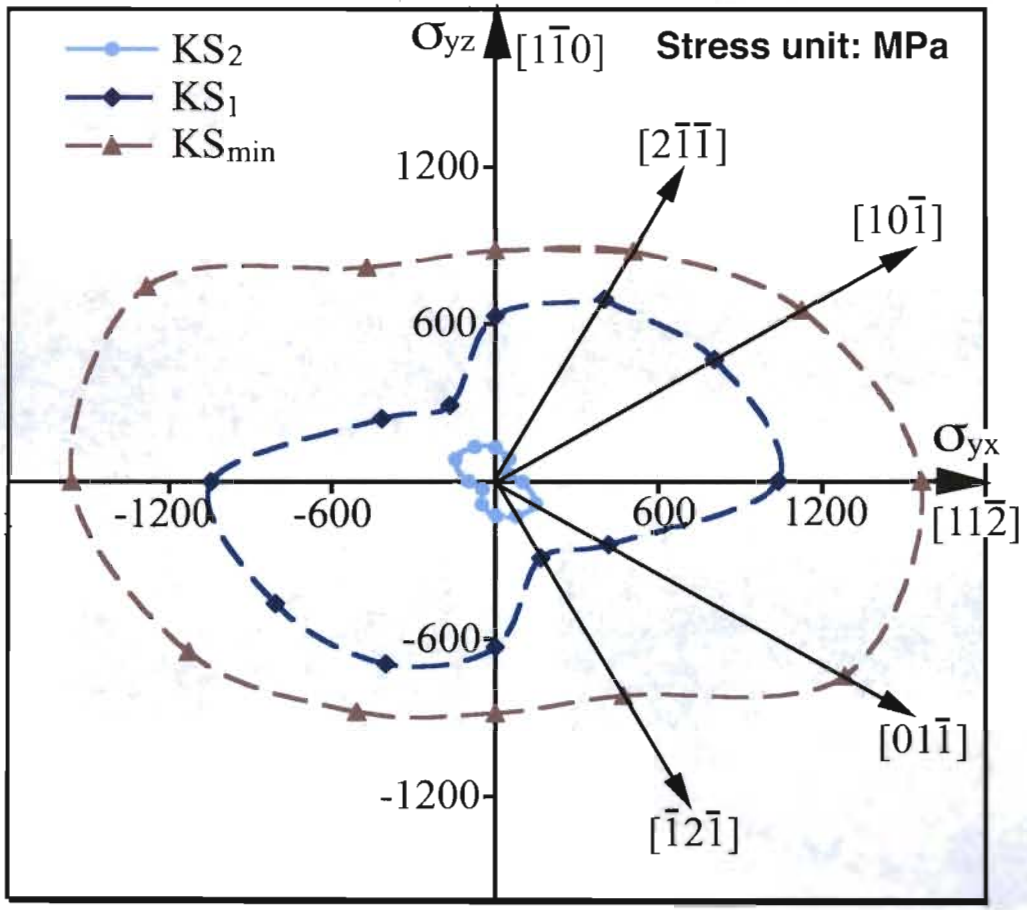
Atomistic modeling of fcc/bcc interfaces reveals multiple states of atomic structures with nearly degenerate formation energy



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

Configuration	KS_1	KS_2	KS_{min}
Interface energy (J/m^2)	0.5687	0.5675	0.5414
Areal density($atoms/nm^2$)	17.74	17.58	16.82

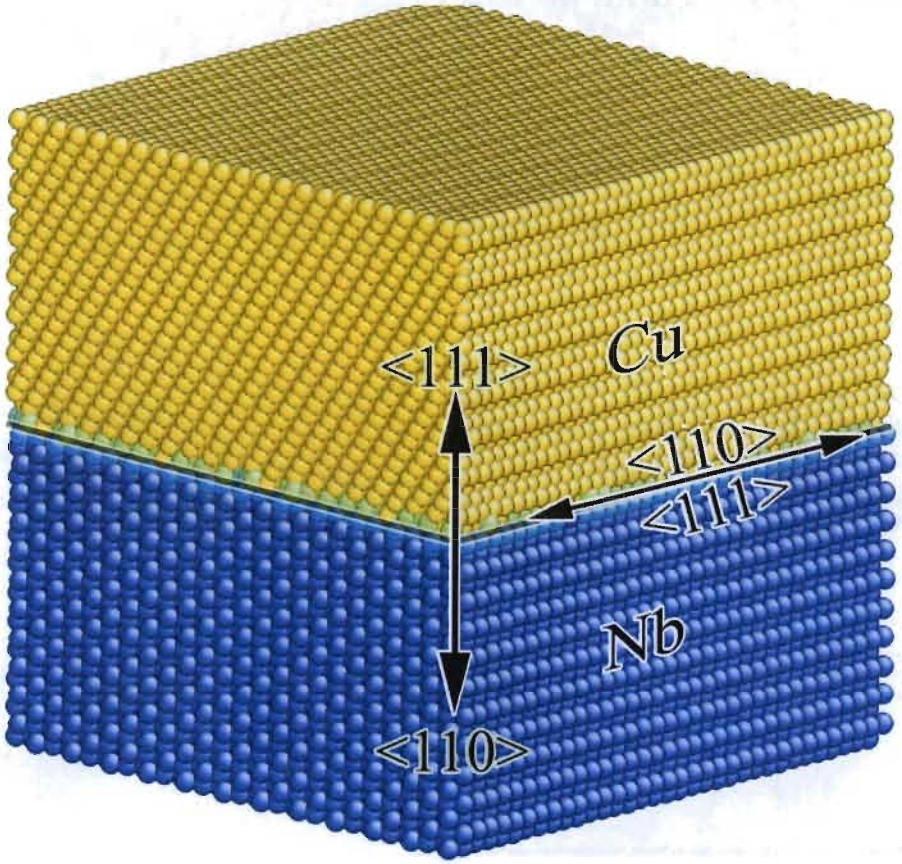
Shear strength of interfaces depends on their atomic structures and is anisotropic



Two-dimensional flow strength of Cu/Nb interfaces

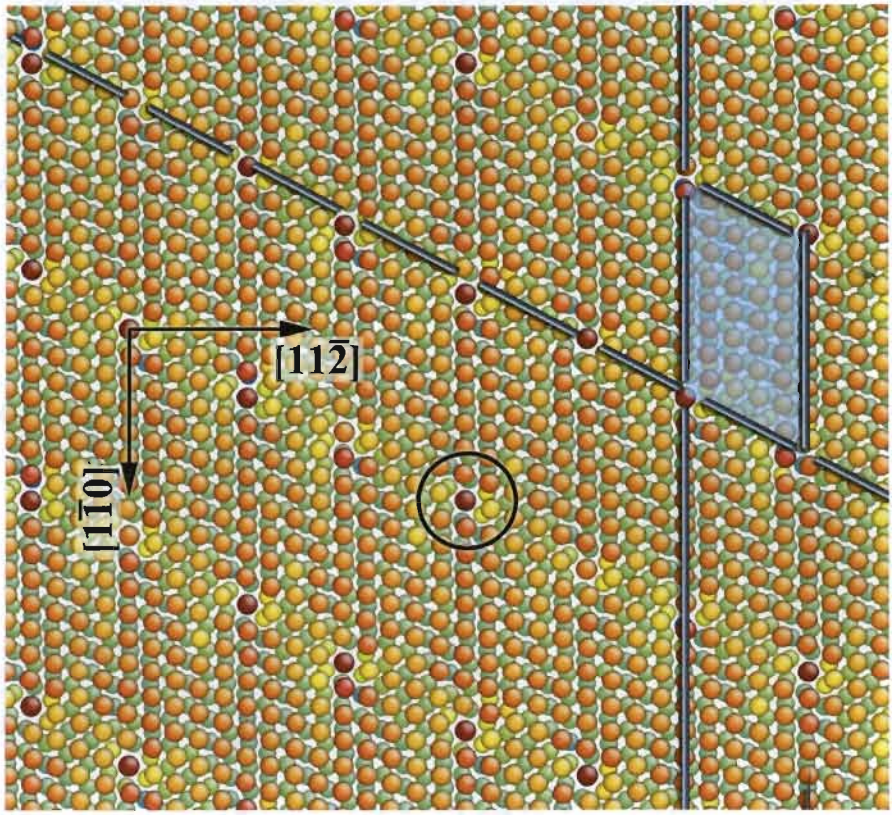
Shear strength is lower than the theoretical shear strength in Cu and Nb.

Atomic structure of interfaces is mainly determined by crystallographic orientation relationship



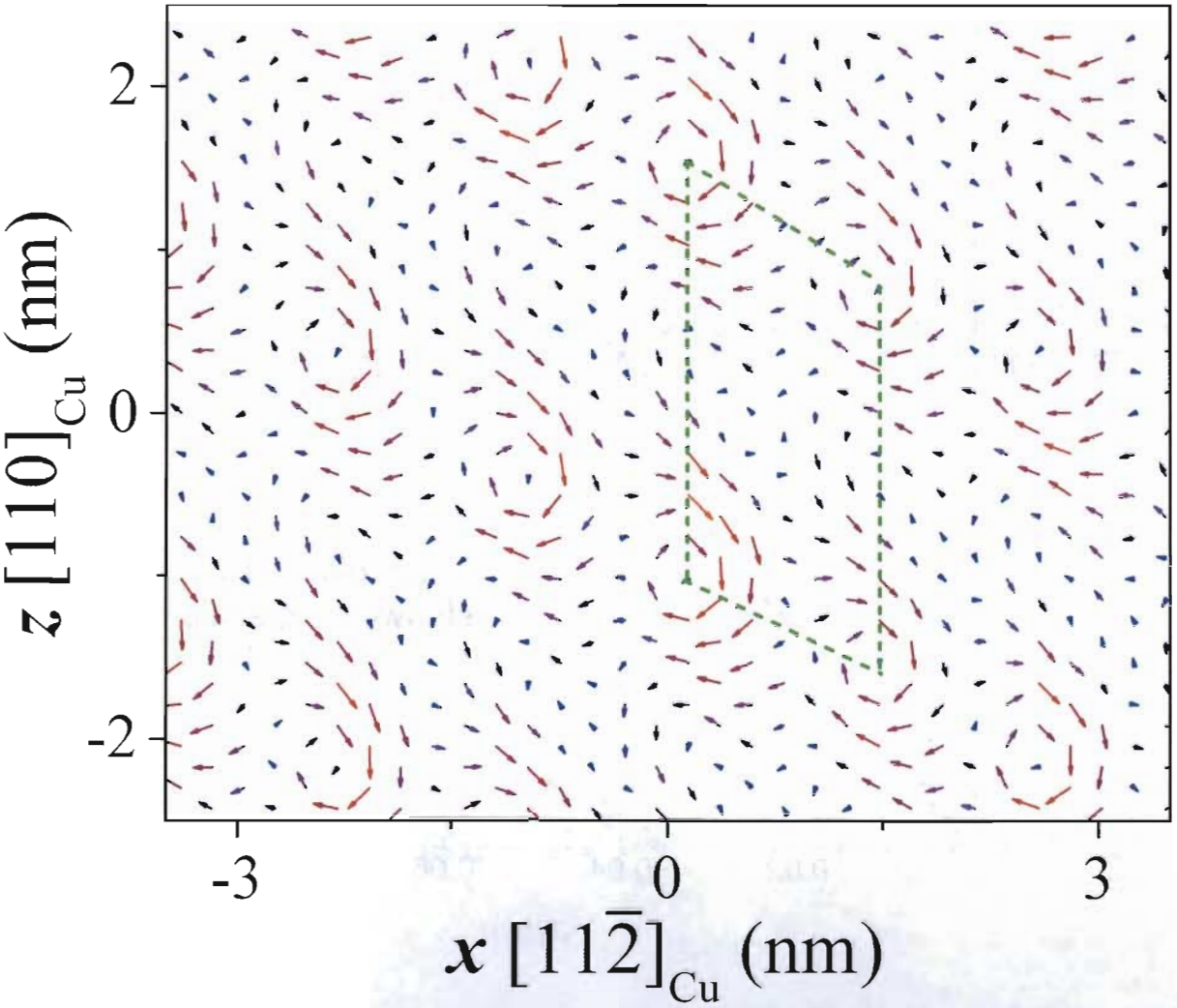
Kurdjumov-Sachs (KS) orientation relation

- $\{111\}_{Cu}$ II $\{110\}_{Nb}$ II interface plane
- $<110>_{Cu}$ II $<111>_{Nb}$ in interface plane



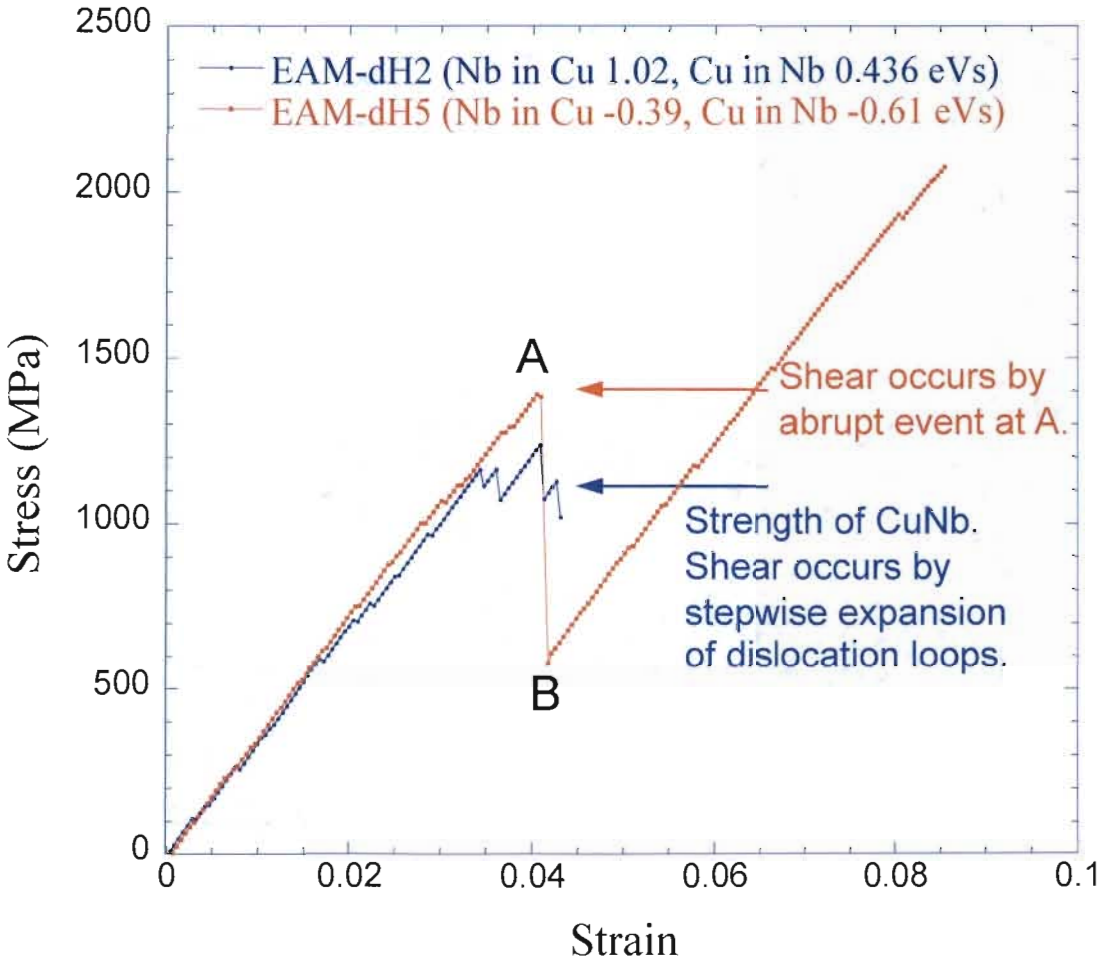
Plan view of atomic structure of interface

Atomic structure of interfaces is mainly determined by crystallographic orientation relationship

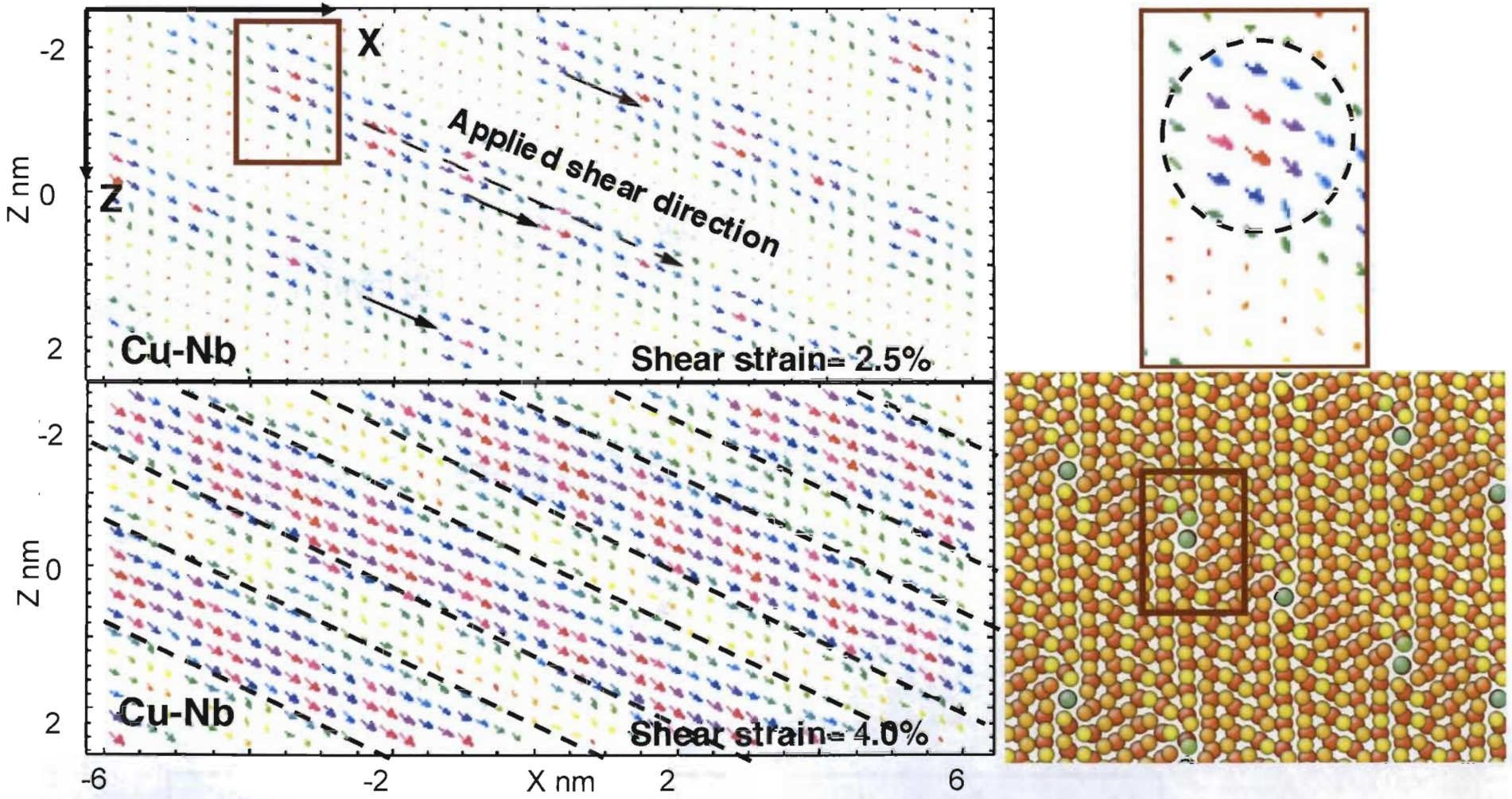


Vector plot of the relative displacement of Cu atoms

Heat of mixing variation changes active shear mode of interface

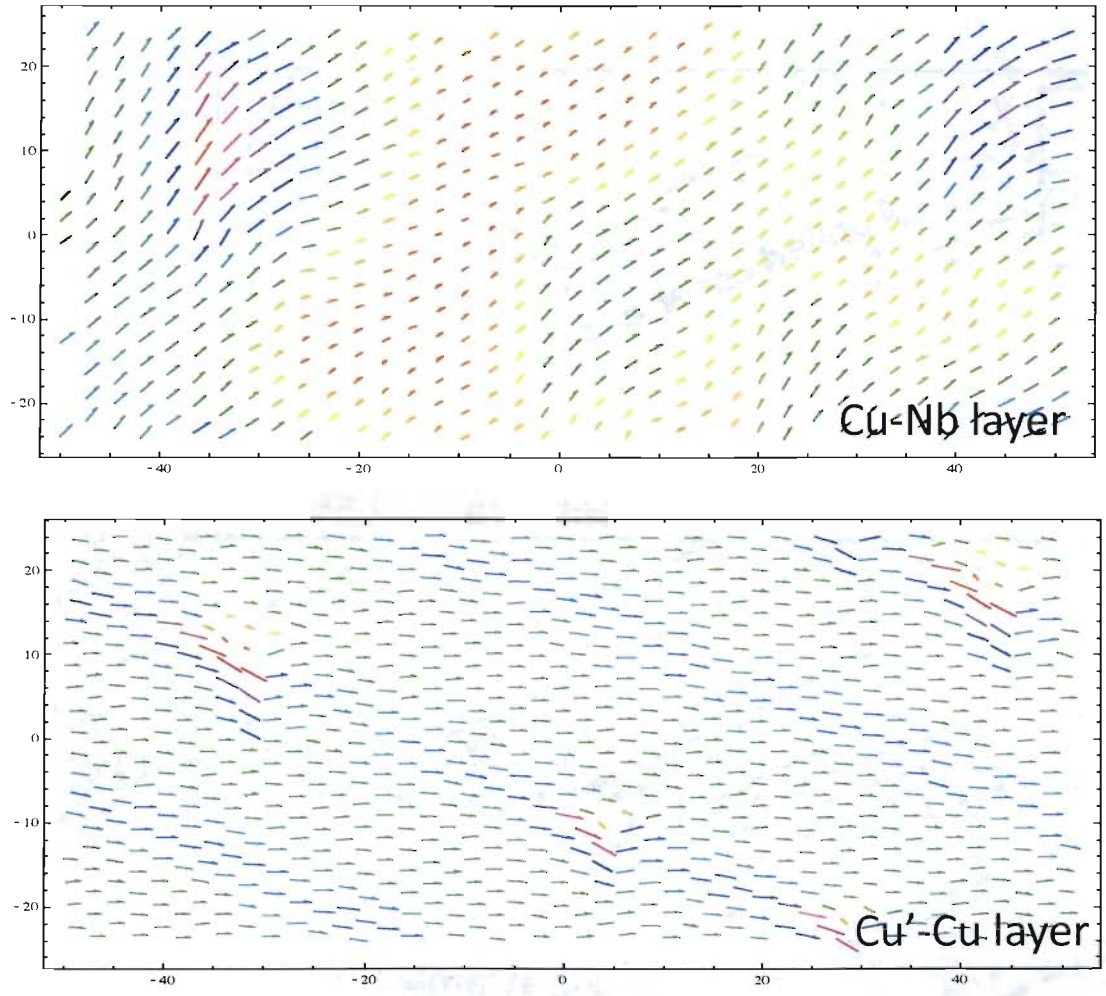


Low shear resistance results from the ease of creation and glide of interface dislocations



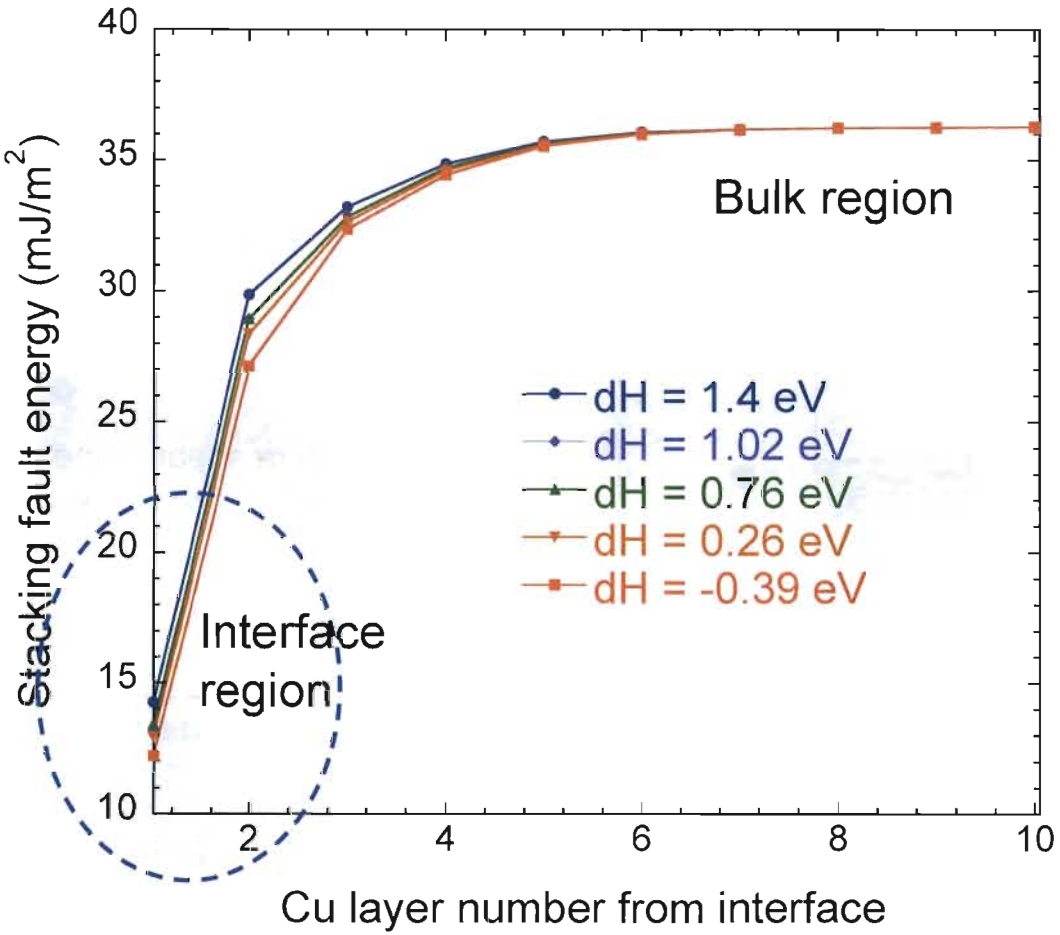
Vector plot of disregistry across the Cu-Nb interface plane

Shearing of fcc'-fcc layers at strong interface



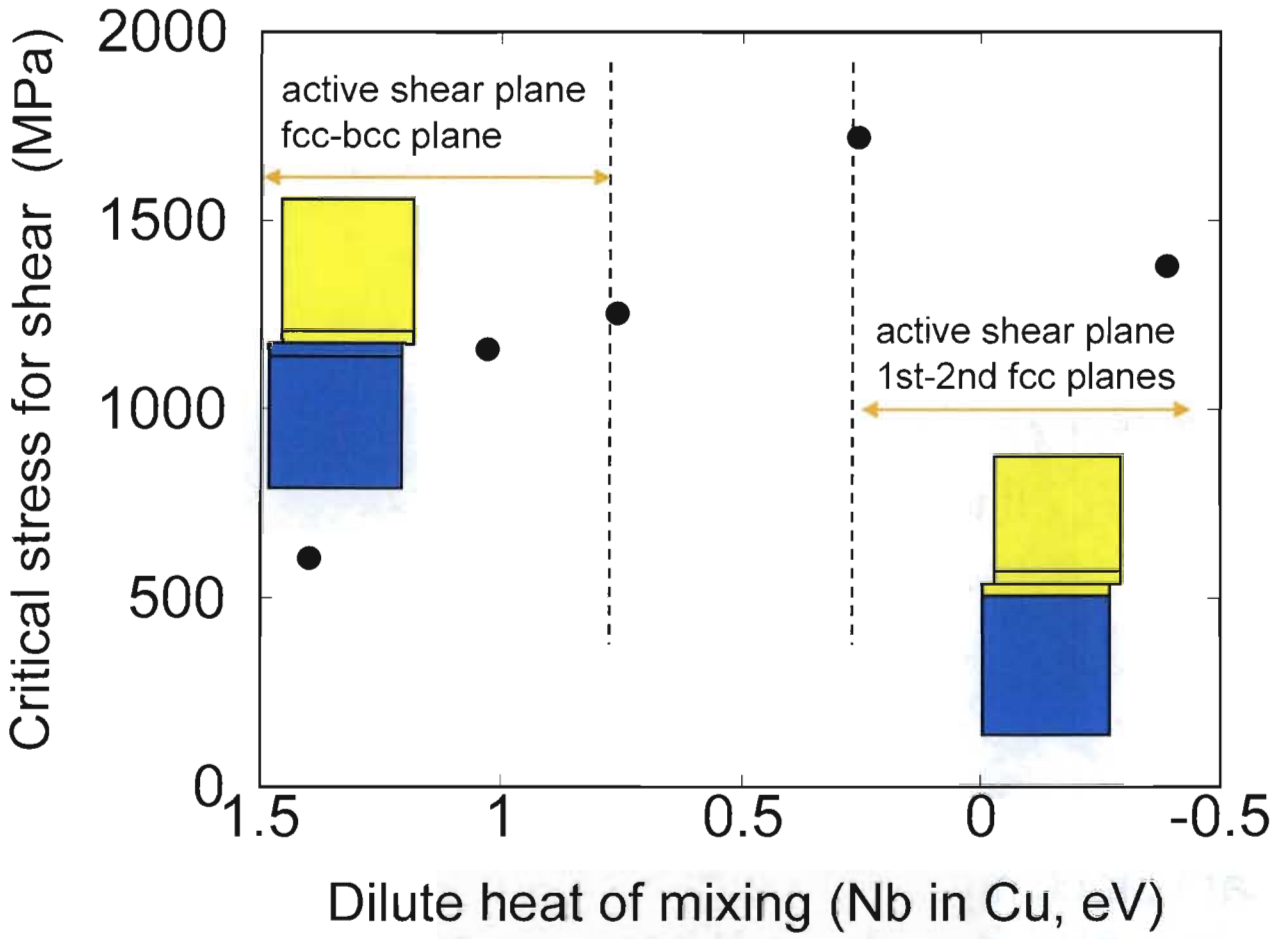
Atoms in 2nd fcc layer near the interface are displaced by Shockley partial ***b***

Why shear mode change?

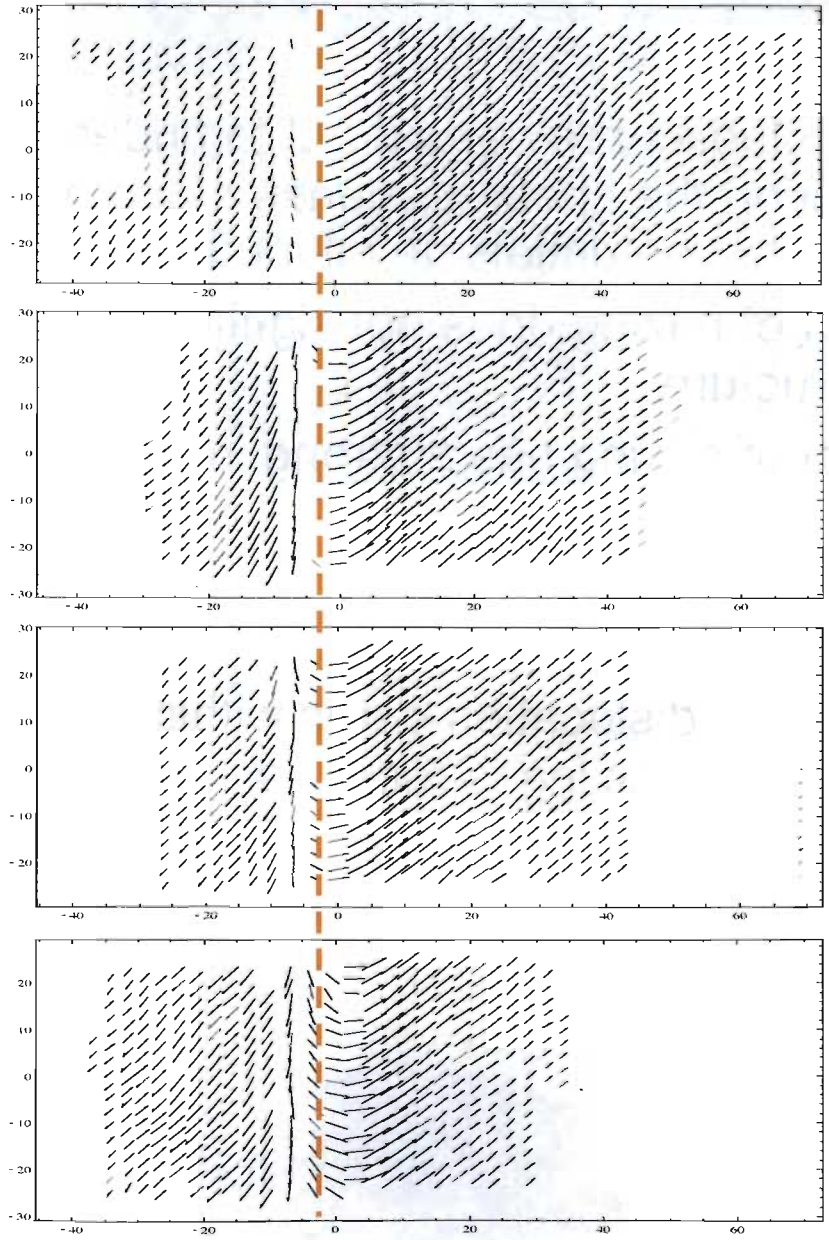


Significant stacking fault energy change at fcc layers near interface (KS_1). This provides physical basis for stacking sequence change under stresses.

Shear strength of fcc/bcc interface (KS_1)



The spreading extent of dislocation cores within interfaces is dependent on HOM



dh=1.40

dh=1.03

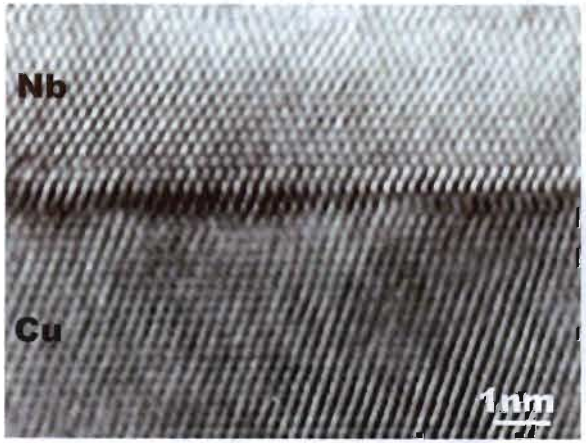
dh=0.26

dh=-0.39

Summary of Part I

- Atomistic modeling studies are carried out to understand the heat of mixing effect on the shear response of fcc-bcc interfaces using tunable potentials developed.
- Variation of the heat of mixing does not significantly alter the fcc-bcc interface structure.
- Variation of the heat of mixing has a strong influence on the interfacial shear strength.
- The active shear plane at the interface may also change as the heat of mixing is reduced.
- The spreading extent of dislocation cores within interfaces decreases as the heat of mixing is reduced.

Part II: relevance of fcc-bcc interface structure to defect properties at interfaces in irradiation environment



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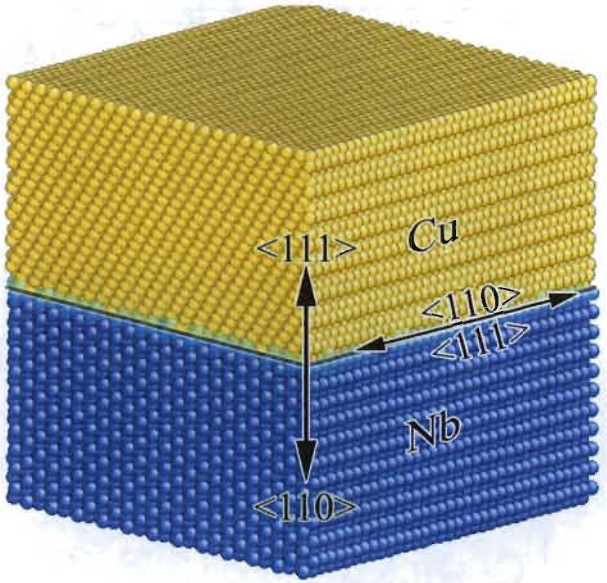


Systematically vary atomic structure and explore the sink strength of interfaces

- Keep heats of mixing unchanged from those of Cu/Nb,
- Vary interface misfit by changing the lattice constant of the bcc phase, and keep the lattice constant of the fcc phase*.

* In the case of lattice constants ratio (a_{fcc}/a_{bcc}) equals to 1.346, Ag/V material system is modeled.

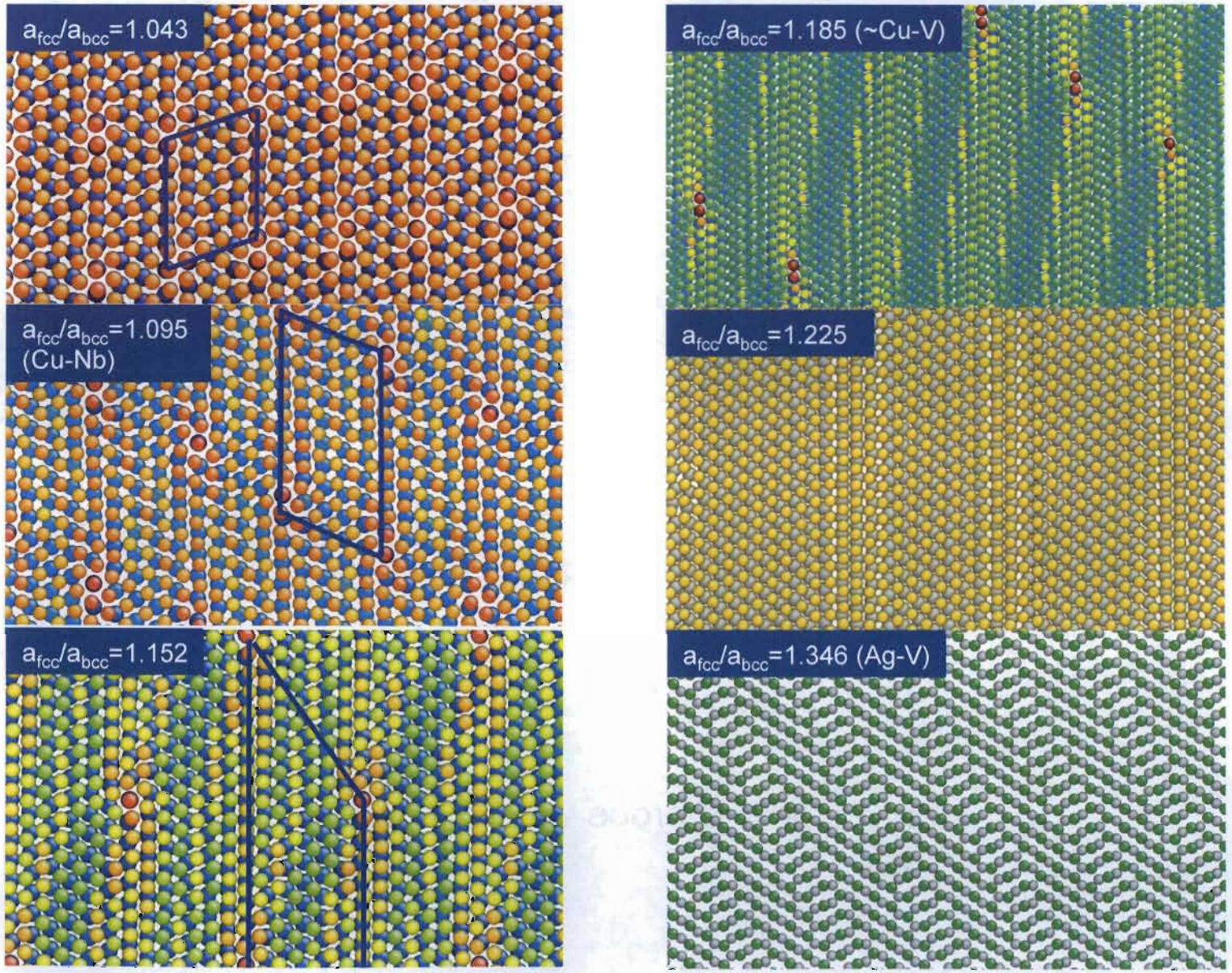
Fitting of interatomic potentials

A series of EAM (embedded-atom-method) potentials are developed

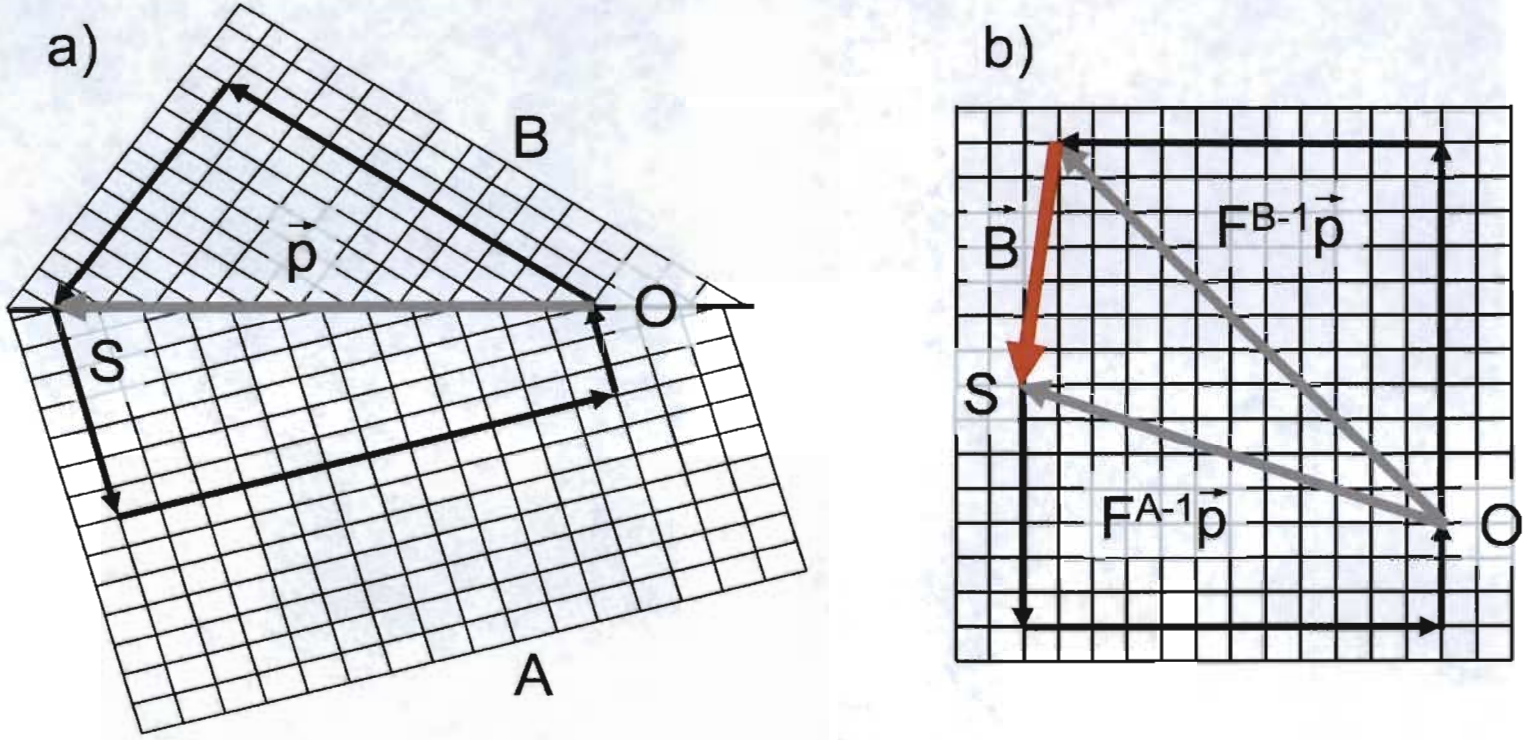
	a_{fcc}(Å)	a_{bcc}(Å)	χ	ΔH (eV) (bcc in fcc)	ΔH (eV) (fcc in bcc)	E_{CsCl}(eV)	B_{CsCl}(GPa)
Expt./DFT (Cu-Nb)	3.615	3.301		1.02	0.48	-	168 (VASP)
Cu-bcc1	3.615	3.465	1.043	1.09	0.497	-10.98	188
Cu-Nb	3.615	3.301	1.095	1.03	0.436	-10.95	188
Cu-bcc2	3.615	3.137	1.152	1.01	0.488	-10.60	189
Cu-bcc3	3.615	3.050	1.185	1.00	0.501	-10.56	188
Cu-bcc4	3.615	2.951	1.225	1.02	0.498	-10.62	188
Ag-V	4.090	3.039	1.346	1.16	0.872	-	-

$$misfit\ ratio\ \chi = \frac{a_{fcc}}{a_{bcc}}$$

Kurdjumov-Sachs interface structures with different lattice misfits at fcc-bcc interface



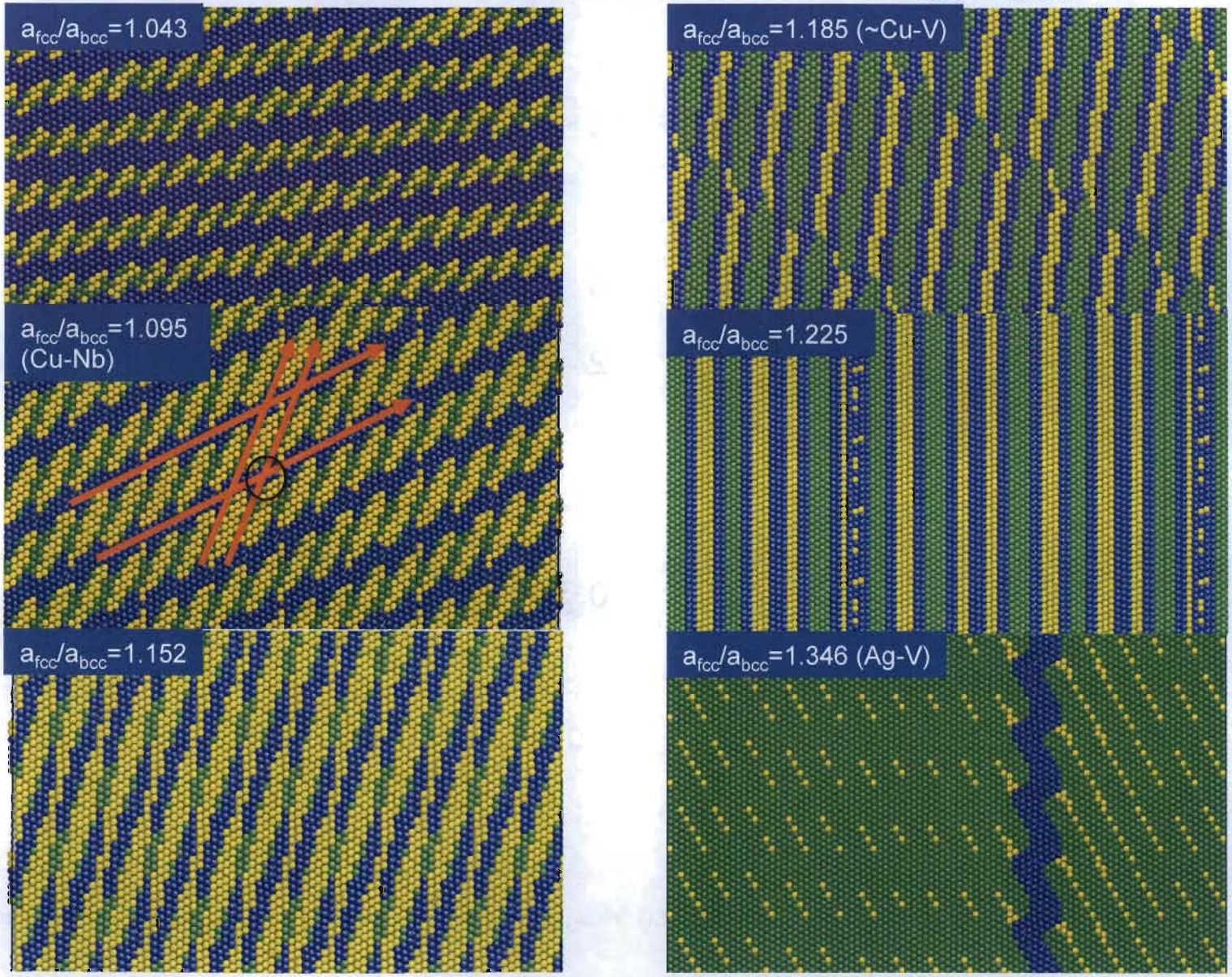
Frank-Bibly Approach (to analysis interface misfit dislocations)



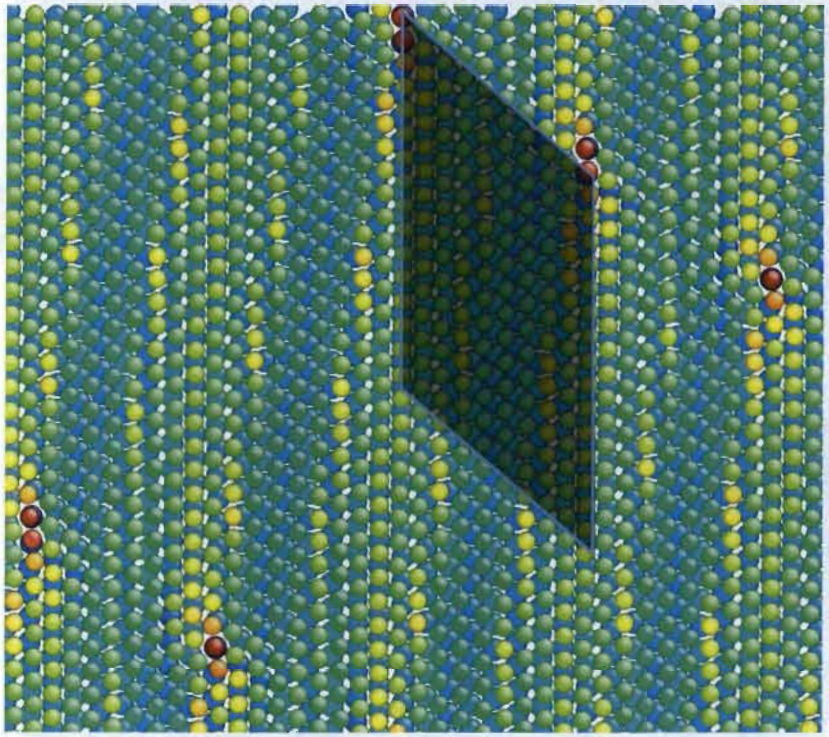
$$\vec{B} = (F^{A-1} - F^{B-1})\vec{p}$$

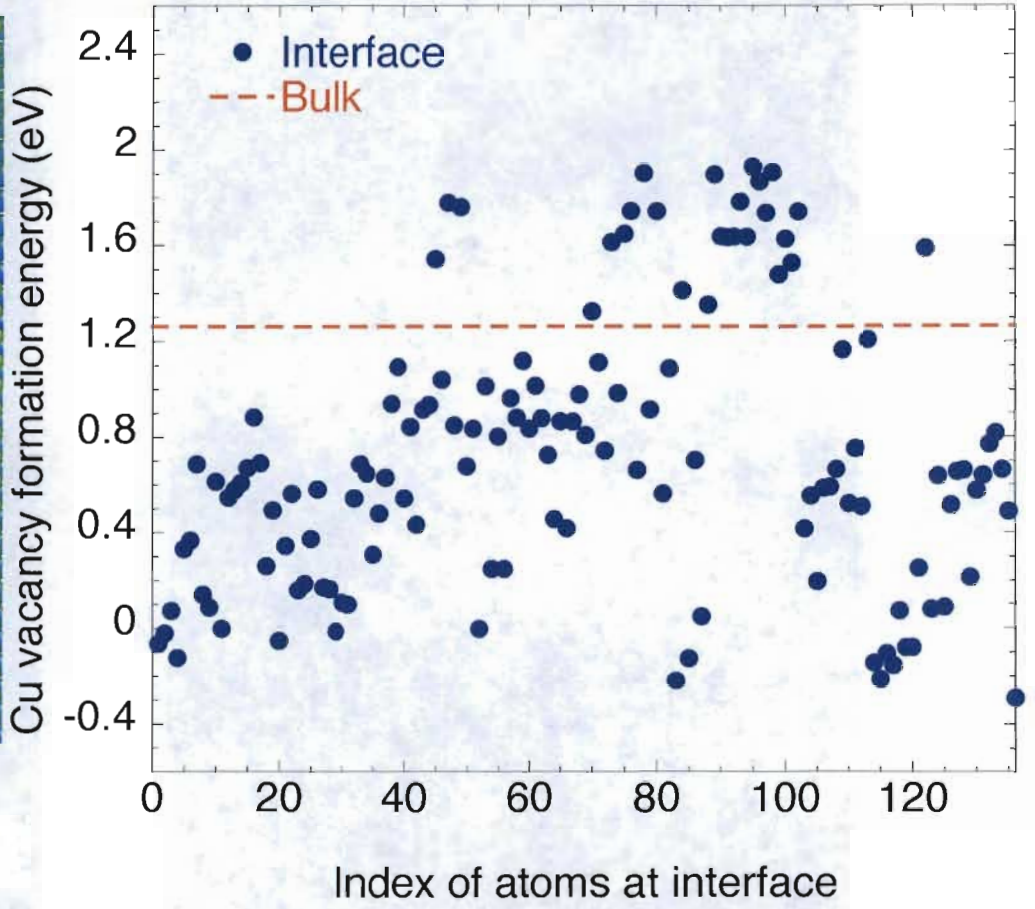
Unit vector $\vec{p}$ is probe vector; $\vec{B}$ is total Burgers vector.

Kurdjumov-Sachs interface misfit dislocation patterns vary substantially with a_{fcc}/a_{bcc}



Vacancy formation energies change substantially at fcc-bcc interfaces with different lattice misfits





X.-Y. Liu, R.G. Hoagland, M.J. Demkowicz, M. Nastasi, A. Misra, submitted.

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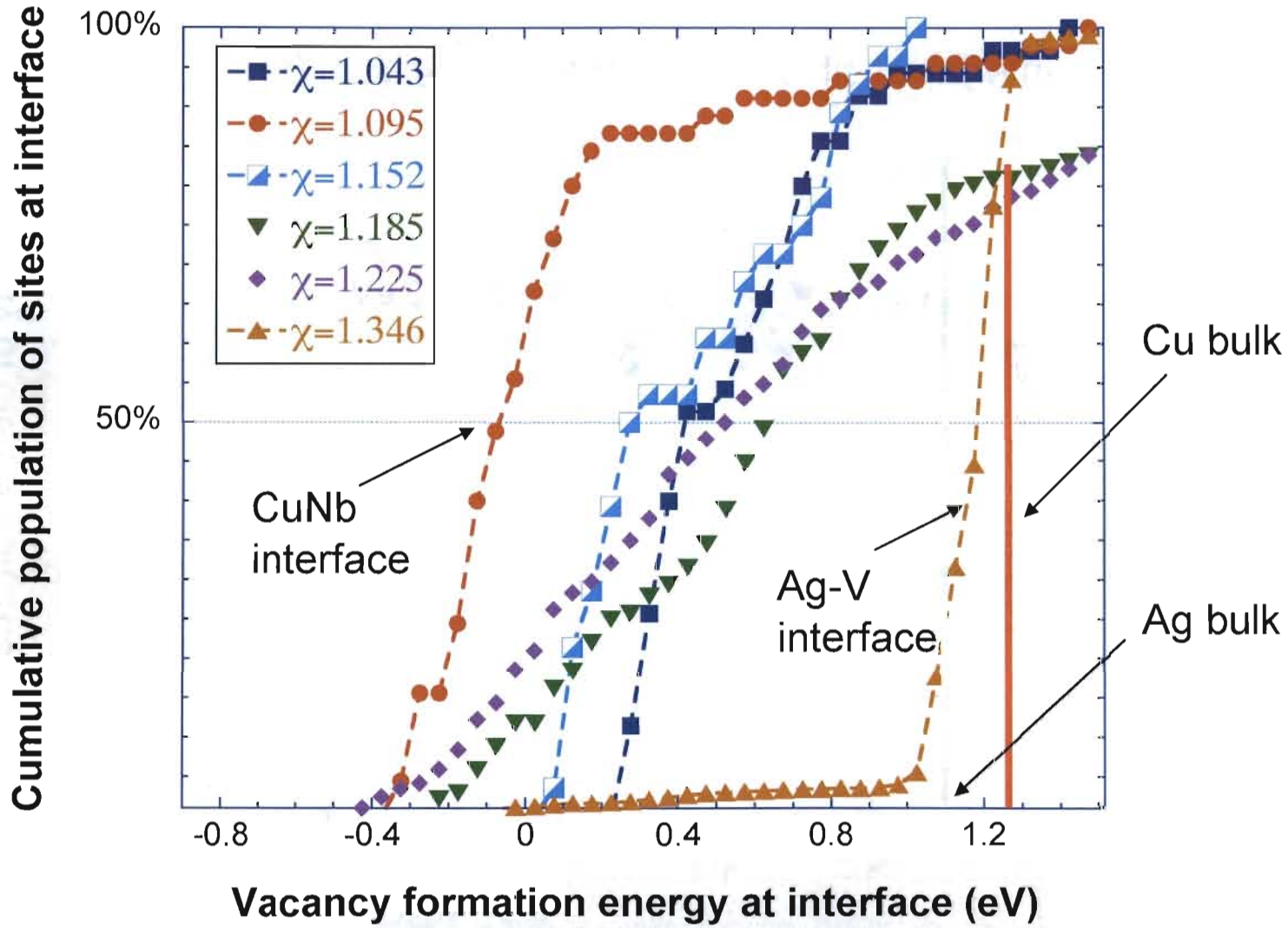
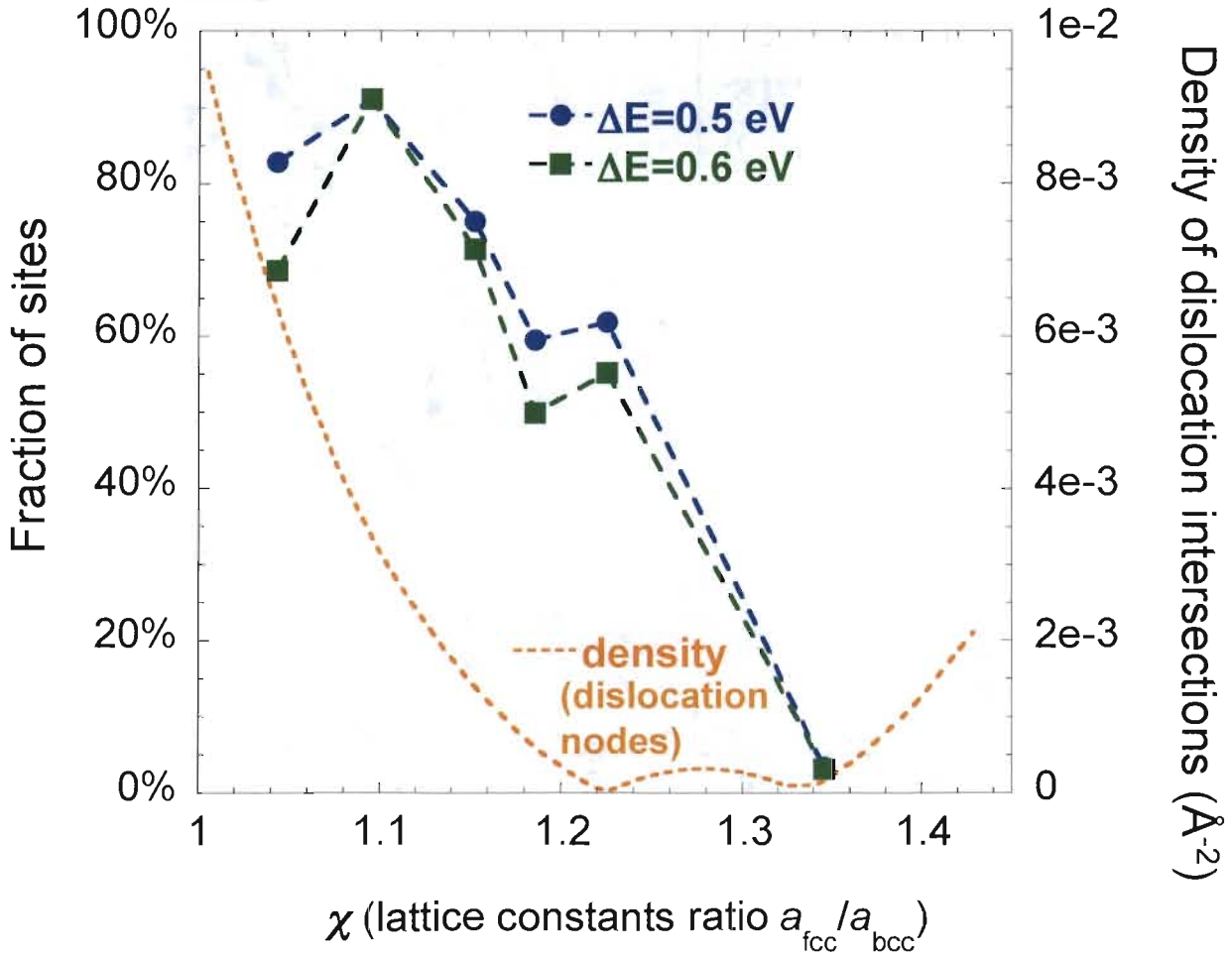


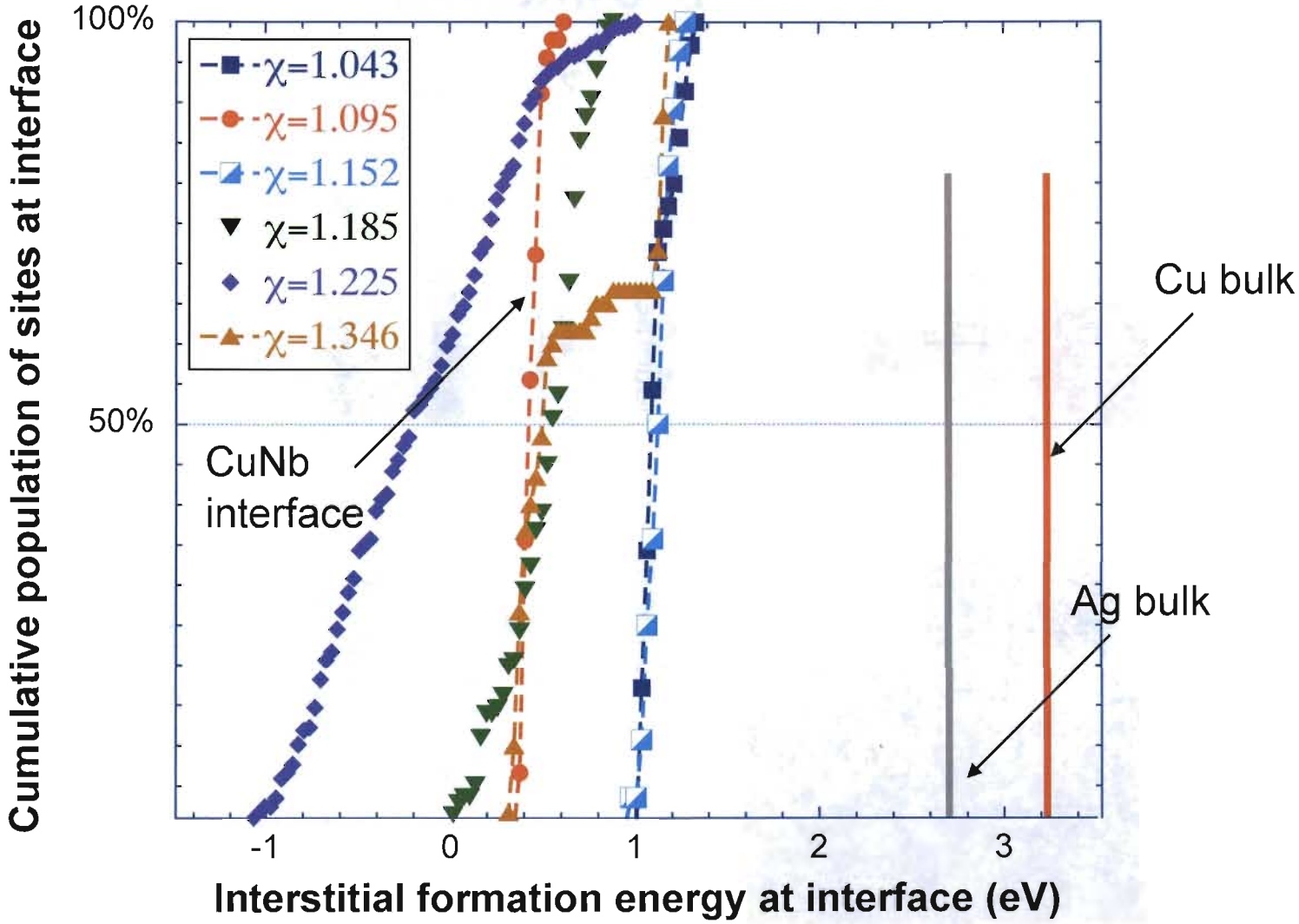
X.-Y. Liu, R.G. Hoagland, M.J. Demkowicz, M. Nastasi, A. Misra, submitted.

Vacancy formation energies change substantially at fcc-bcc interfaces with different lattice misfits

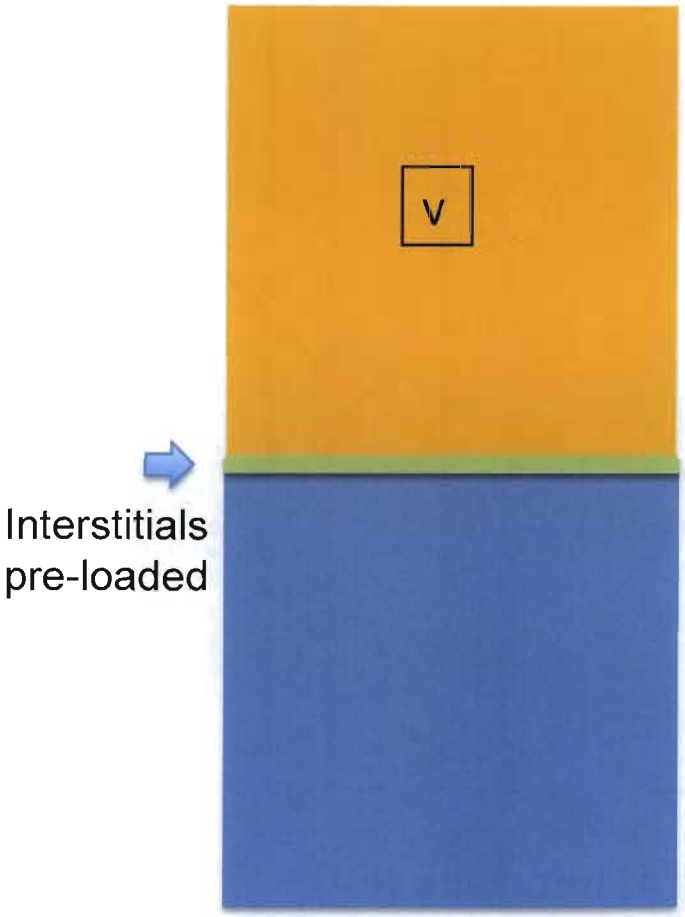
Interfacial sites fraction with $E_V^f \leq E_V^f(bulk) - \Delta E$

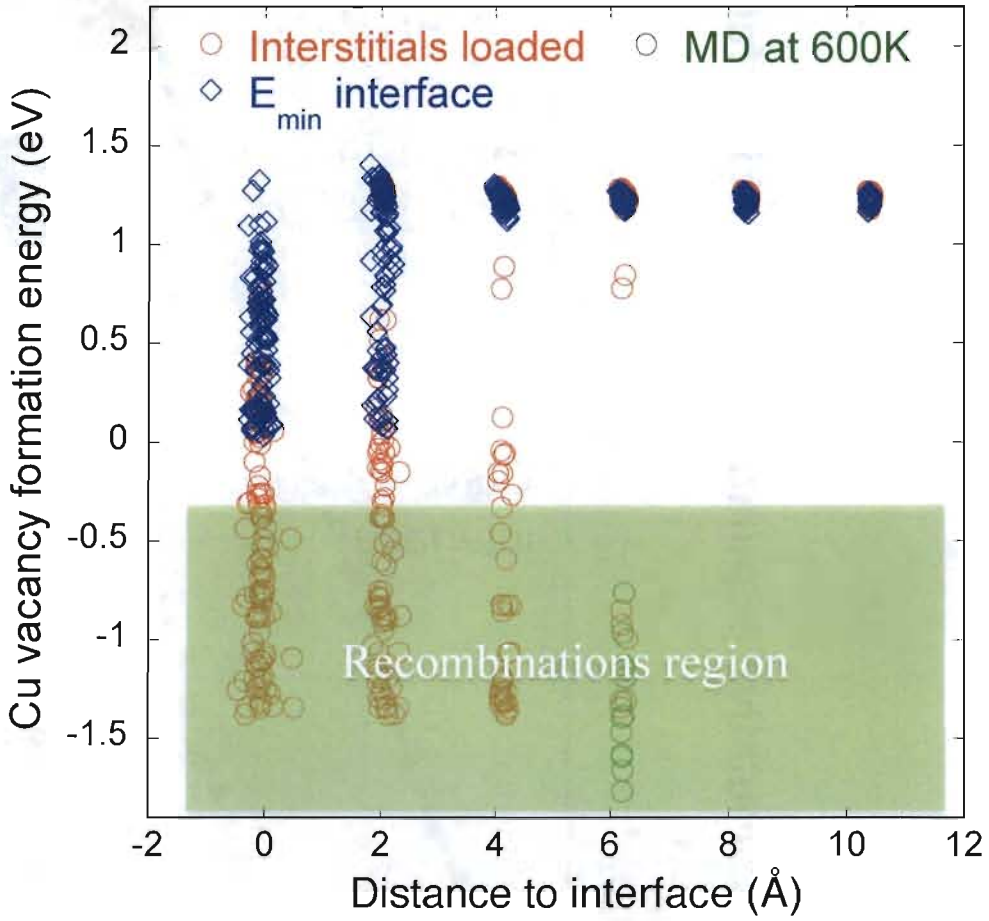


Interstitial formation energies are significantly lower at fcc-bcc interfaces compared to bulk values



"Interstitial loading" has significant effect on vacancy formation, migration via interstitial emissions at fcc-bcc interface





90% migration barriers probed through MD
< 0.38 eV (bulk Cu 0.69 eV)

*** Mechanism similar to at Cu GBs, Bai et al, Science 327, 1631 (2010).**

Summary of Part II

- Tunable EAM potentials are developed to model general fcc-bcc interfaces with different lattice misfits from 1.043 to 1.346, to investigate the relevance of fcc-bcc interface structure to defect properties.

- Study of Kurdjumov-Sachs orientation interfaces with different misfit reveals:

  - Vacancy formation energies decrease with increasing misfit dislocation density,

  - Interstitial formation energies are substantially below the bulk value, and depend on the interface misfit in a complex way.

- "Interstitial loading" at fcc-bcc interface lowers vacancy formation and migration energetics via interstitial emissions, which may bear significance for 2-3 nm layer-thickness multi-layer structures in irradiation environments.