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Title:	Interface structures, defects, and mechanical properties at fcc-bcc interfaces from "tunable" potentials
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2012 TMS Annual Meeting:
Solid-State Interfaces II: Toward an Atomistic-Scale Understanding of Structure, Properties, and Behavior Through Theory and Experiment

Title:
Interface structures, defects, and mechanical properties at fcc-bcc interfaces from "tunable" potentials

Authors:
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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 change the dilute heats of mixing between Cu and Nb and investigate the effect on interface structures, defect formation energies, and 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, to examine effects on interface dislocations and defect formation energetics. Defect-interface interactions are studied with MD and other methods, to predict the radiation damage tolerance of these interface systems.

Interface Structures, Defects, and Mechanical Properties at fcc-bcc Interfaces from "Tunable" Potentials

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MIT: Michael J. Demkowicz

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Interface structure

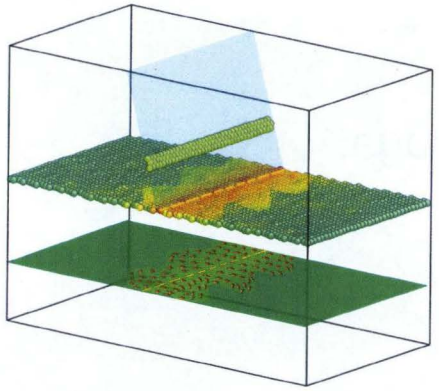
relevance to

Deformation

•Control deformation by interacting with dislocations

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

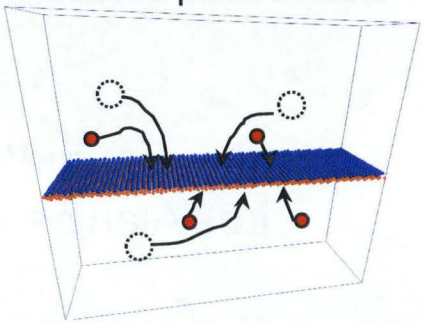
Important for understanding
- yield strength - work hardening
- recovery - fracture



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).
J. Wang, R.G. Hoagland, J.P. Hirth, A. Misra, Acta Mater. 56, 5685 (2008).
A. Misra, M.J. Demkowicz, X. Zhang, R.G. Hoagland, JOM 59(9), 62 (2007).

Goals of this study

- 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.

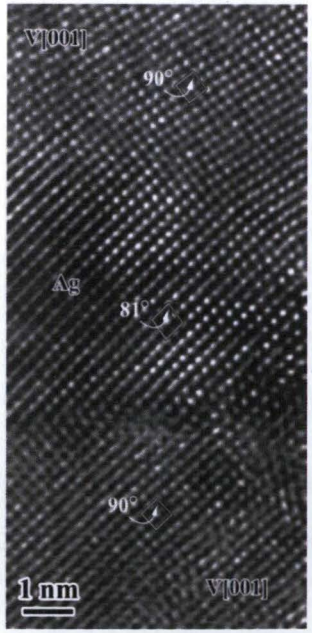
How to "represent" heterophase interface?

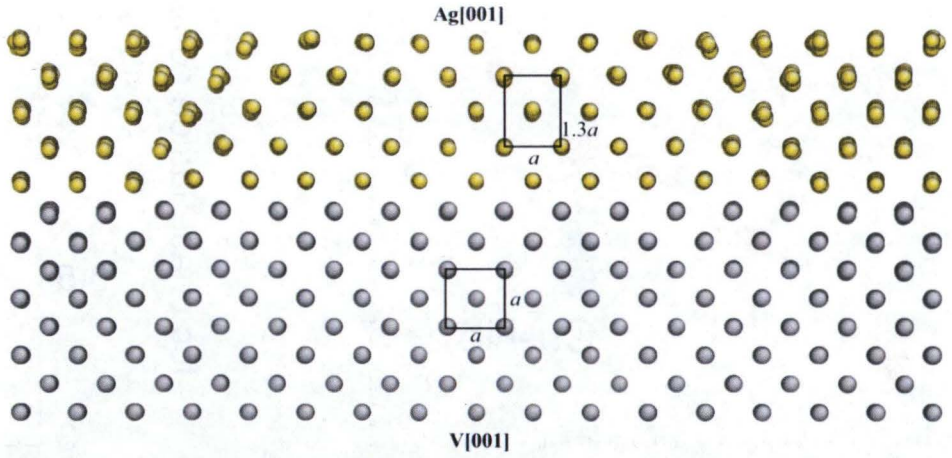
Geometry

- 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





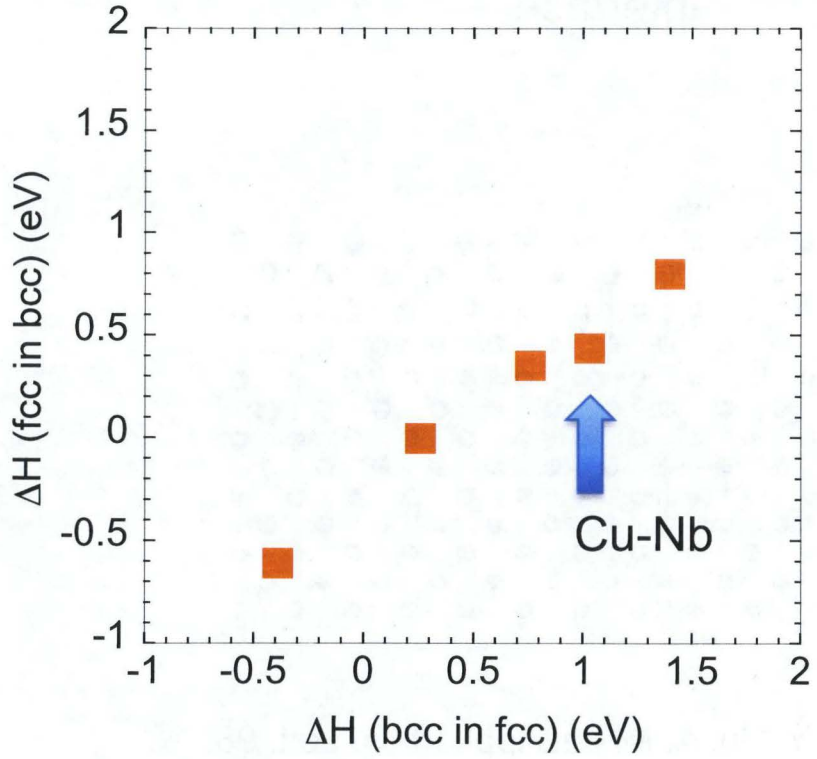
* Q.M. Wei, X.-Y. Liu, A. Misra, Appl. Phys. Lett. 98, 111907 (2011).

Manipulating interface properties via tunable potentials

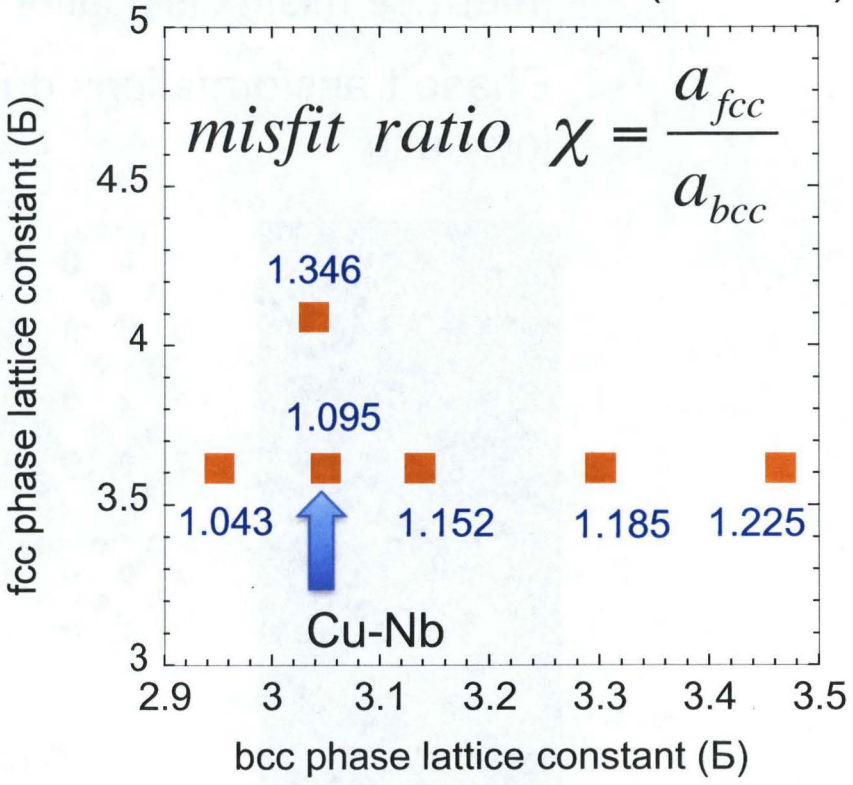
- Keep geometry constant, systematically vary heats of mixing
- Or keep heats of mixing constant, systematically vary geometry

⇨ Tune the parameterizations of the interatomic potentials for fcc-bcc

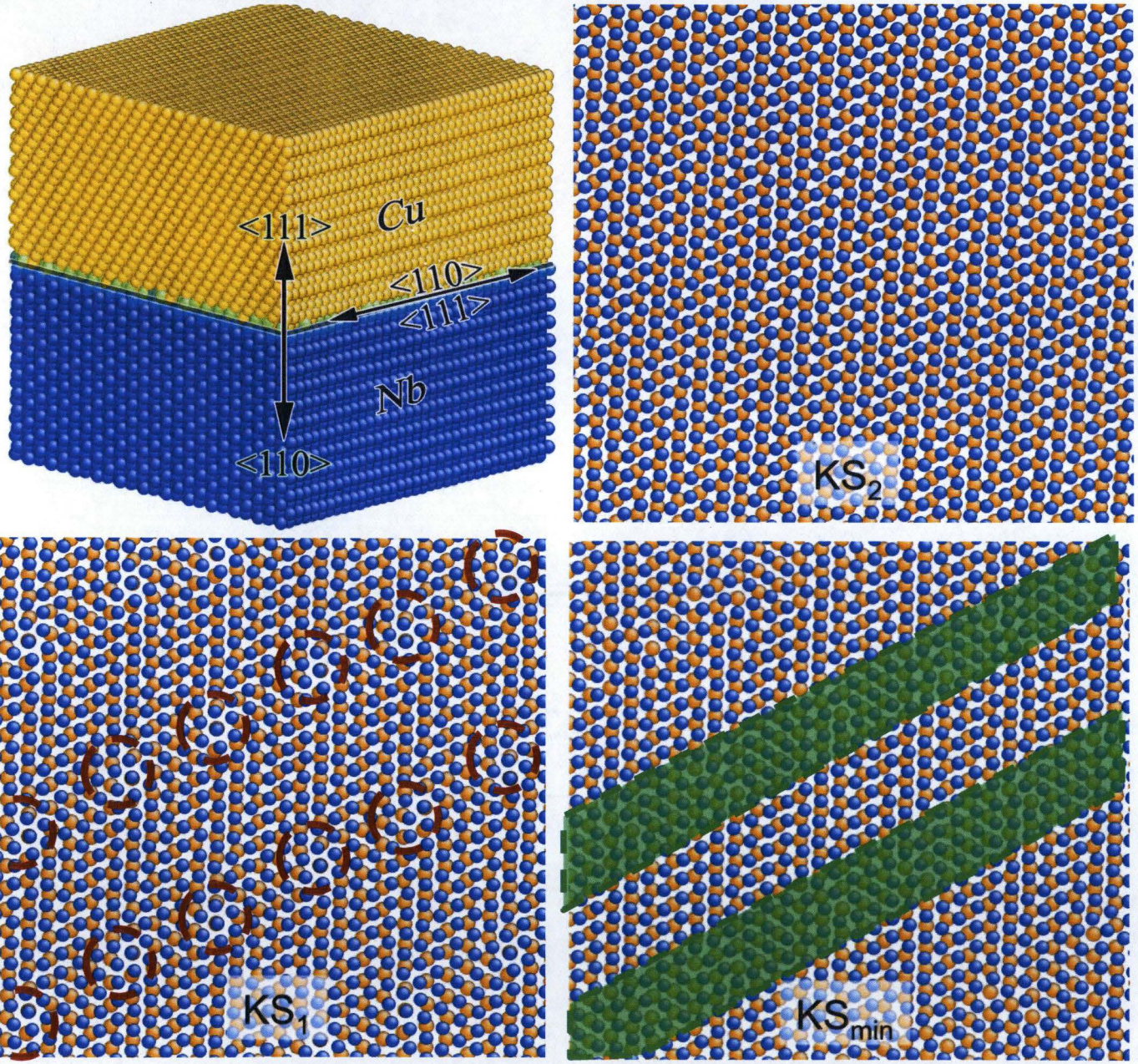
- Interface energetics (heats of mixing)



- Variation of lattice mismatch (or misfit)



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

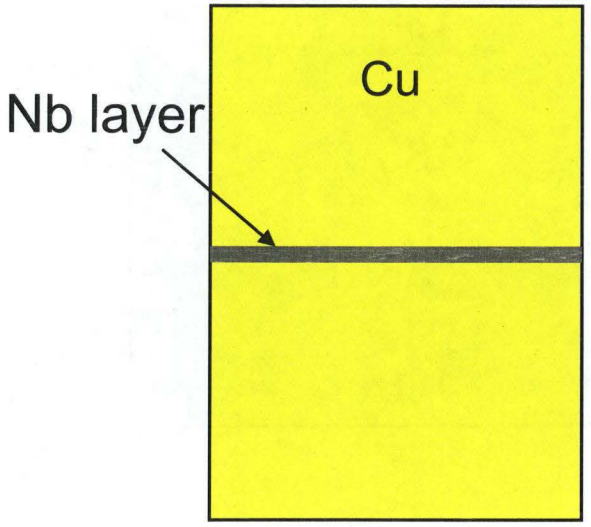
Construction of EAM potentials – variation of heats of mixing

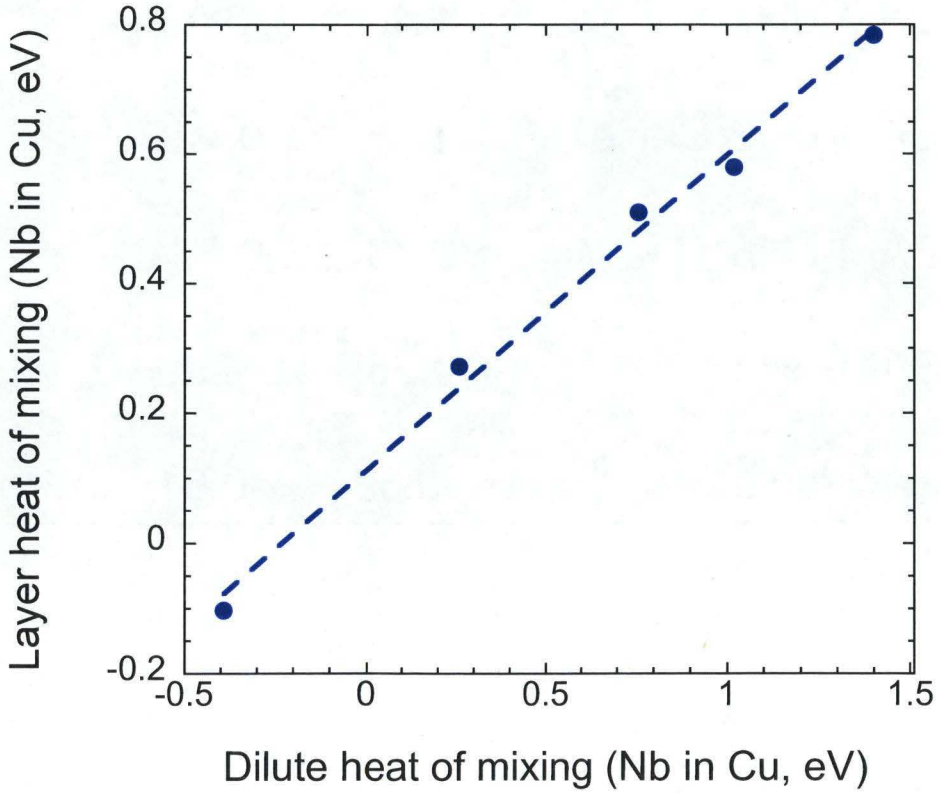
	ΔH (Nb in Cu) (eV)	ΔH (Cu in Nb) (eV)	a_{CsCl}(Å)	B_{CsCl}(GPa)
Expt. / VASP	1.02	0.48	3.22 (VASP)	168 (VASP)
EAM-dH1	1.40	0.80	3.19	188
EAM-dH2(CuNb)	1.03	0.436	3.19	188
EAM-dH3	0.76	0.351	3.17	188
EAM-dH4	0.26	-0.004	3.16	188
EAM-dH5	-0.39	-0.61	3.16	188

Heats of mixing (HOM): dilute and layer HOM

How good is dilute HOM (single impurity atom in host matrix) in defining the interface bond change?

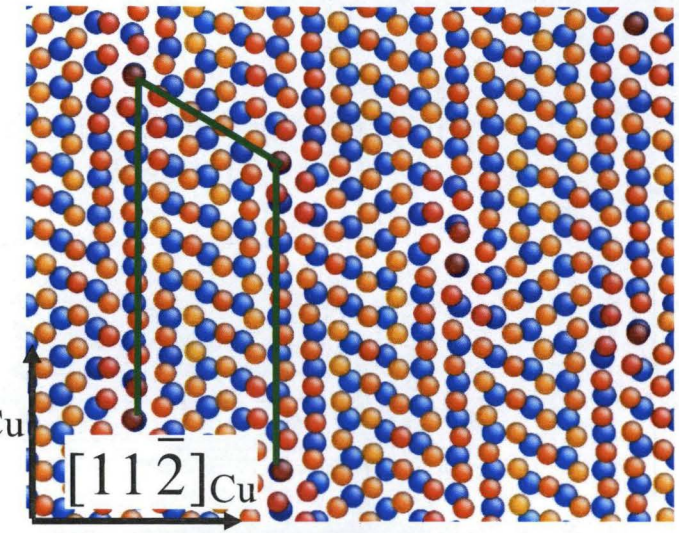
Check with layer HOM calcs.

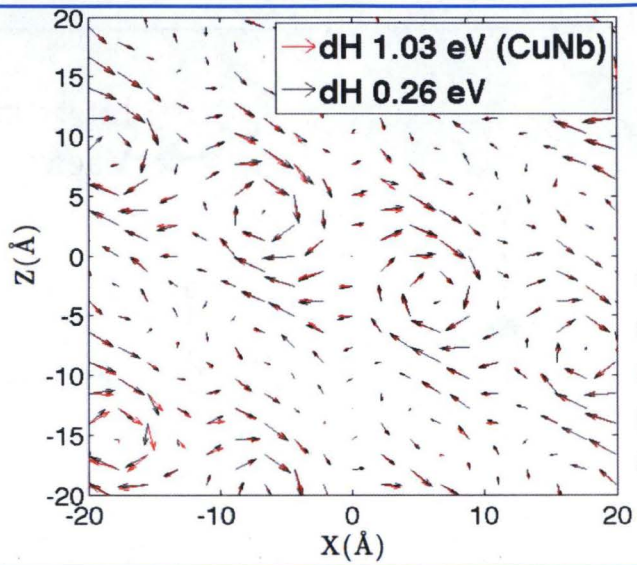




HOM variation does *not* significantly alter the structures

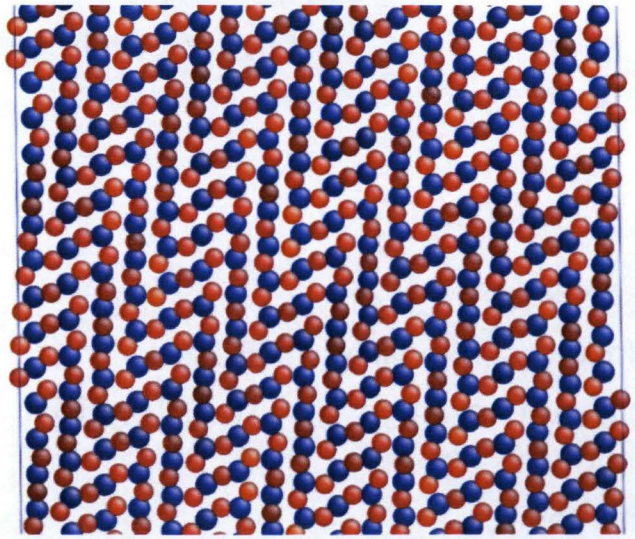
KS1

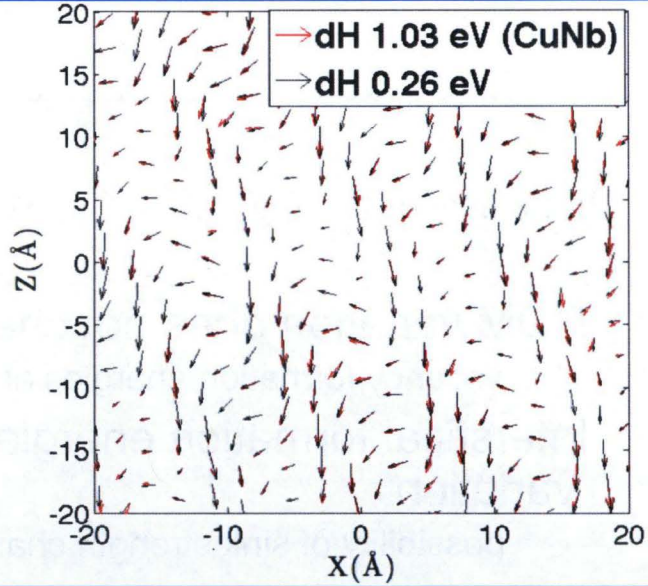




Cu layer displacement upon relaxation at interface

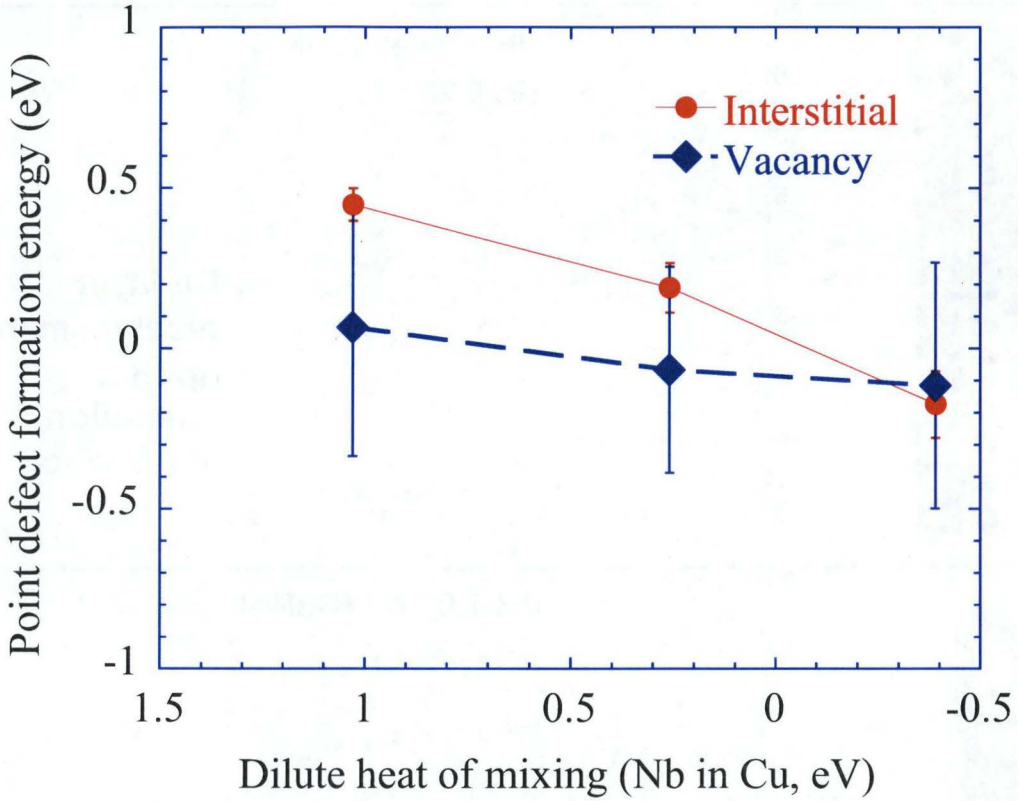
KS2



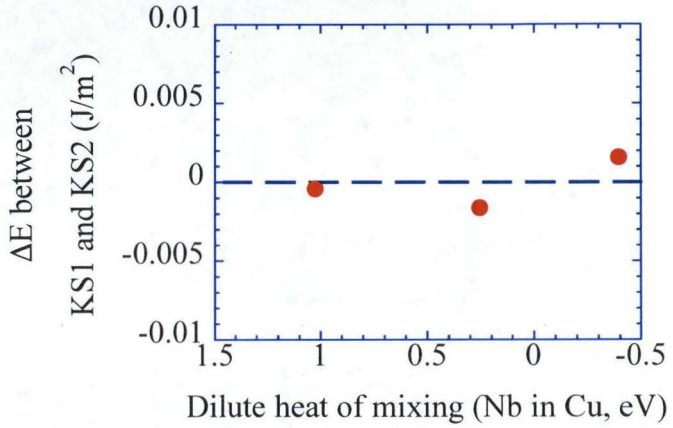


* The dH value is bcc atom in fcc phase

HOM variation modifies defect formation energies

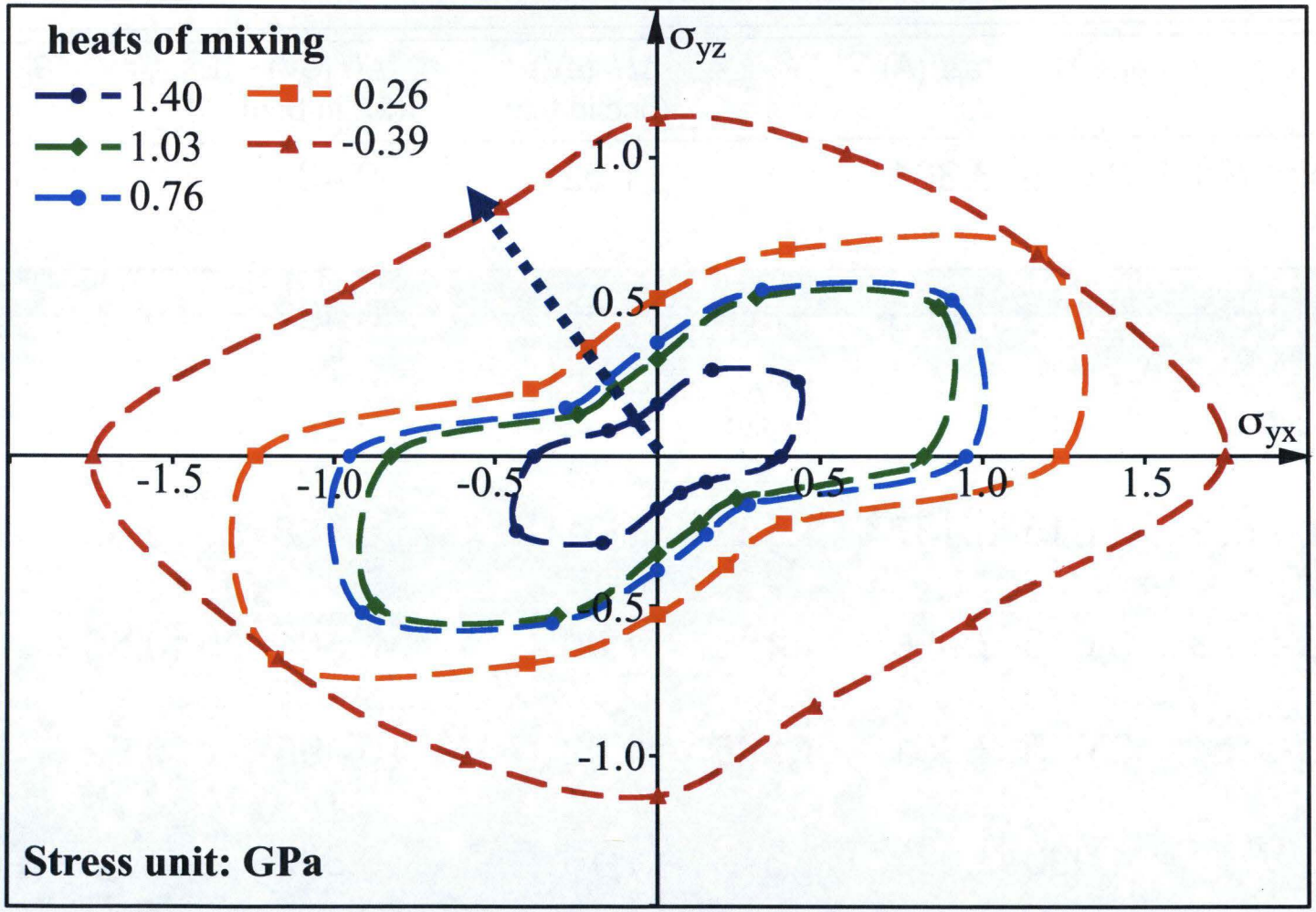


Interface energy difference between KS1 and KS2



- HOM variation does not change the multiplicity of interface states
  - vacancy formation energies at interface are *insensitive* to HOM.
- Interstitial formation energies at the interface are modified by HOM variation
  - possibility of sink strength change at interface.

Shear strength of interfaces increases with the decrease of HOM and is anisotropic



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

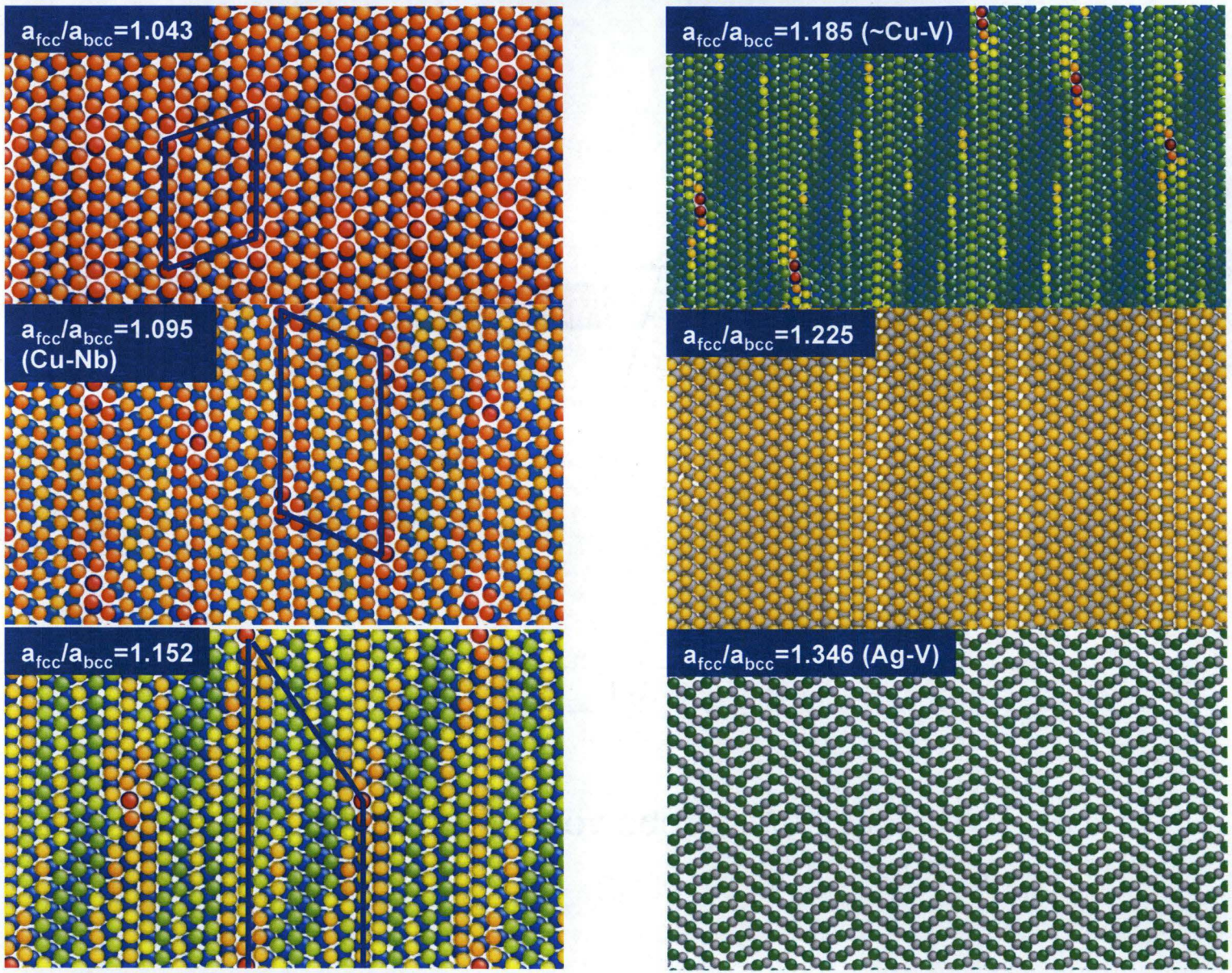
* J. Wang, R.G. Hoagland, X.-Y. Liu, A. Misra, Acta Mater. **59**, 3164 (2011).

Construction of EAM potentials – variation of lattice misfits

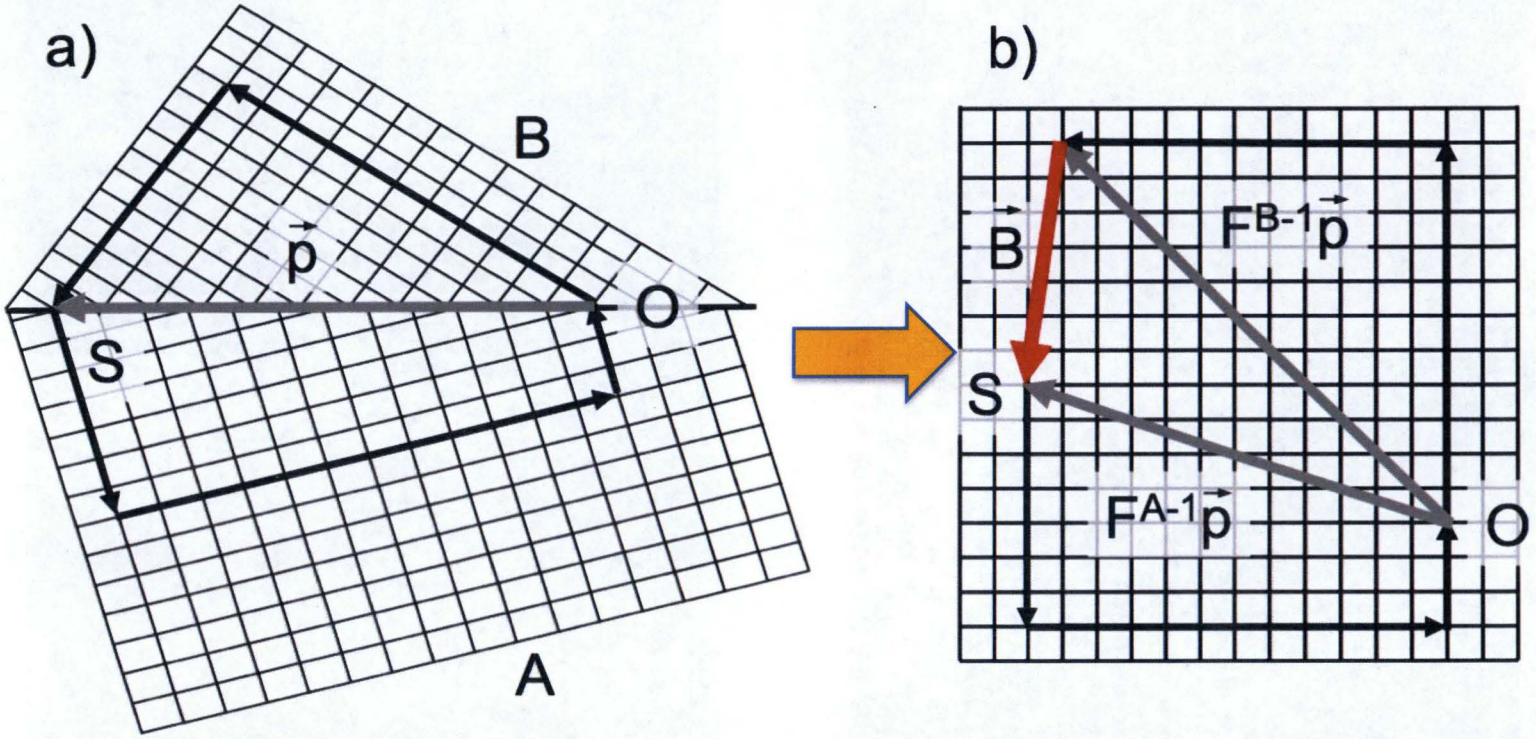
	a_{fcc}(Å)	a_{bcc}(Å)	χ	ΔH (eV) (bcc in fcc)	ΔH (eV) (fcc in bcc)	E_{CsCl}(eV)	B_{CsCl}(GPa)
Expt./DFT (Cu-Nb)	3.615	3.301		1.02	0.48	-	168 (VASP)
Cu-bcc1	3.615	3.465	1.043	1.09	0.497	-10.98	188
Cu-Nb	3.615	3.301	1.095	1.03	0.436	-10.95	188
Cu-bcc2	3.615	3.137	1.152	1.01	0.488	-10.60	189
Cu-bcc3	3.615	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



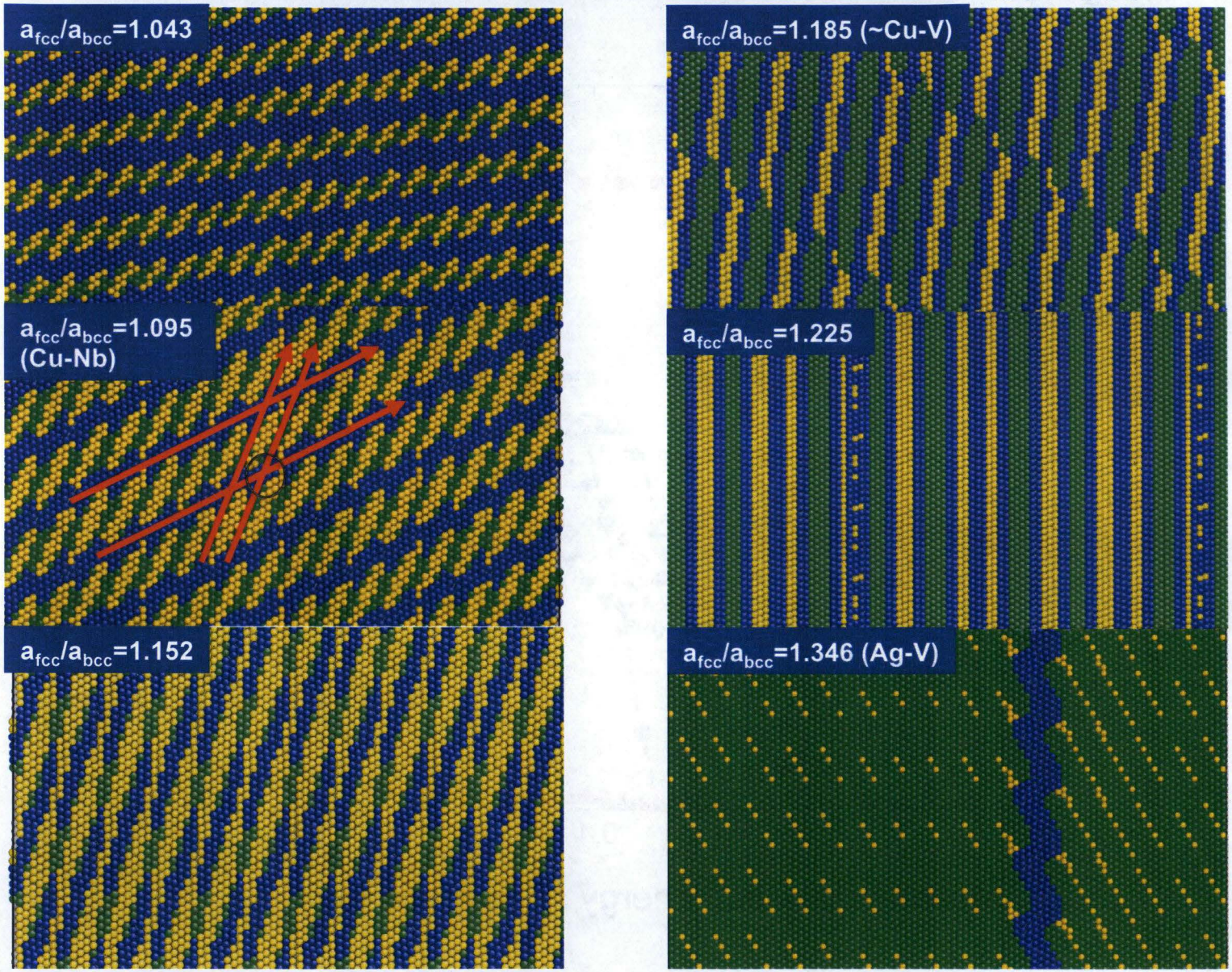
The Frank-Bibly equation to analyze interface misfit dislocations



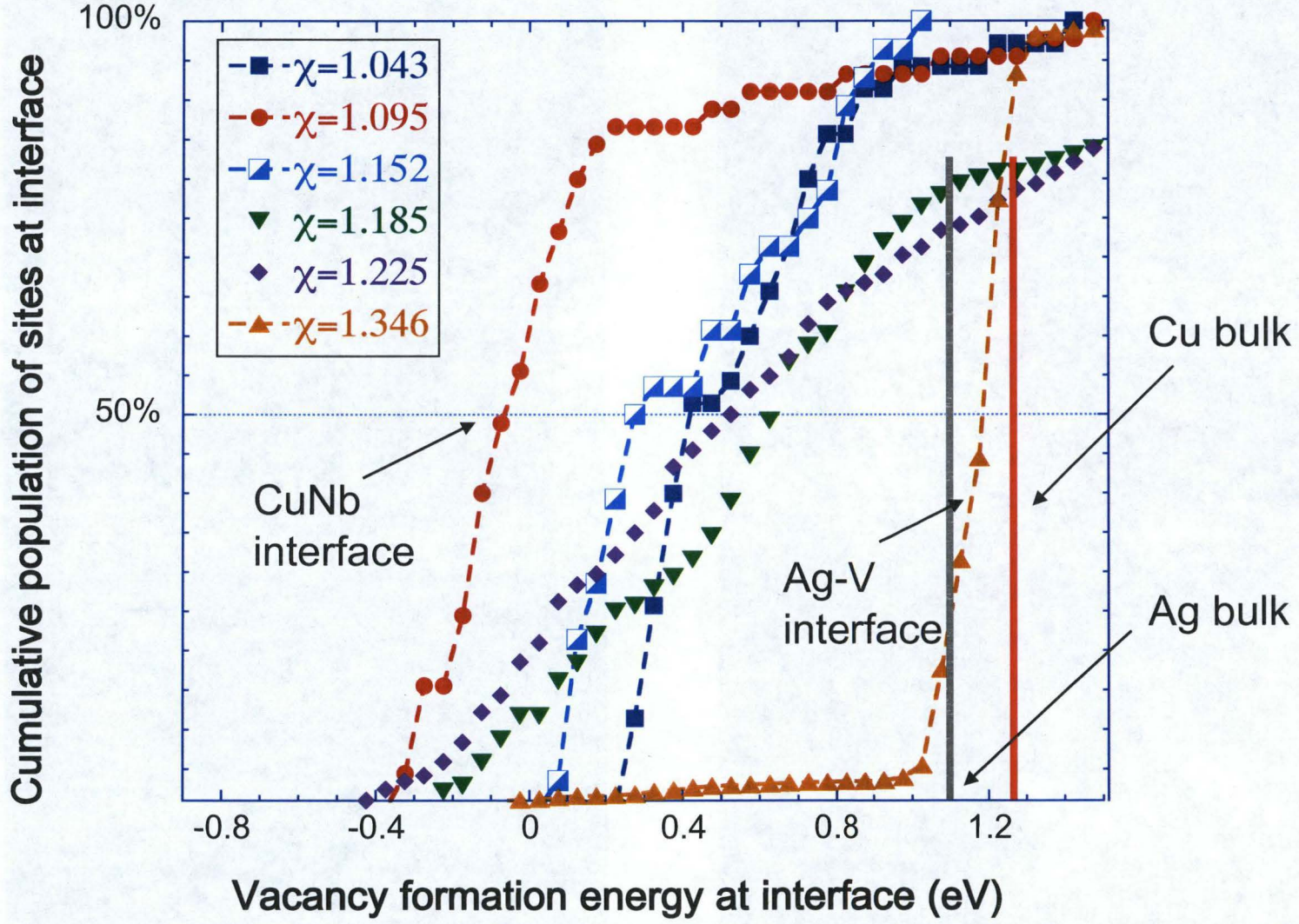
$$\vec{B} = (F^{A-1} - F^{B-1})\vec{p}$$

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

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



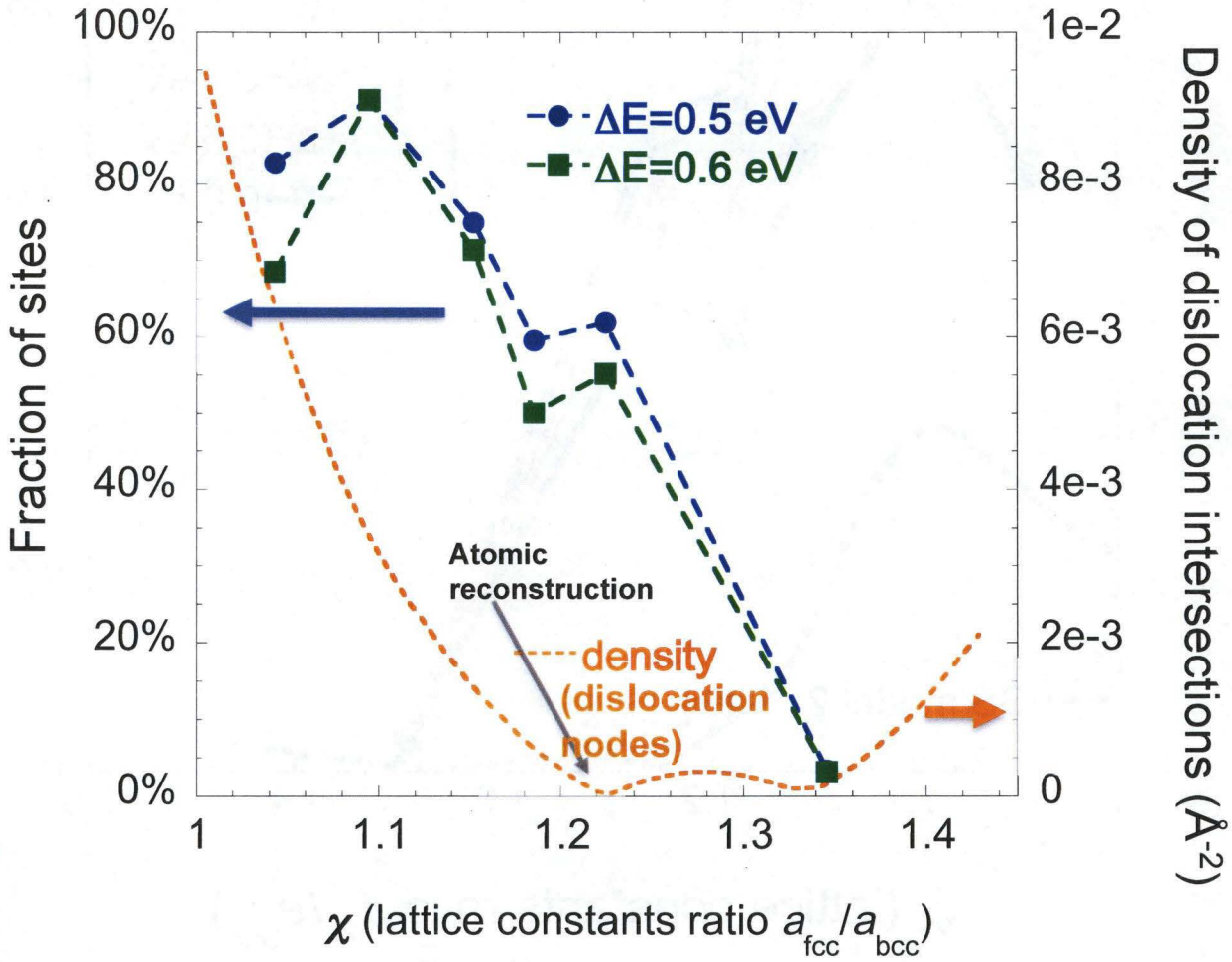
Vacancy formation energies change substantially at fcc-bcc interfaces with different lattice misfits



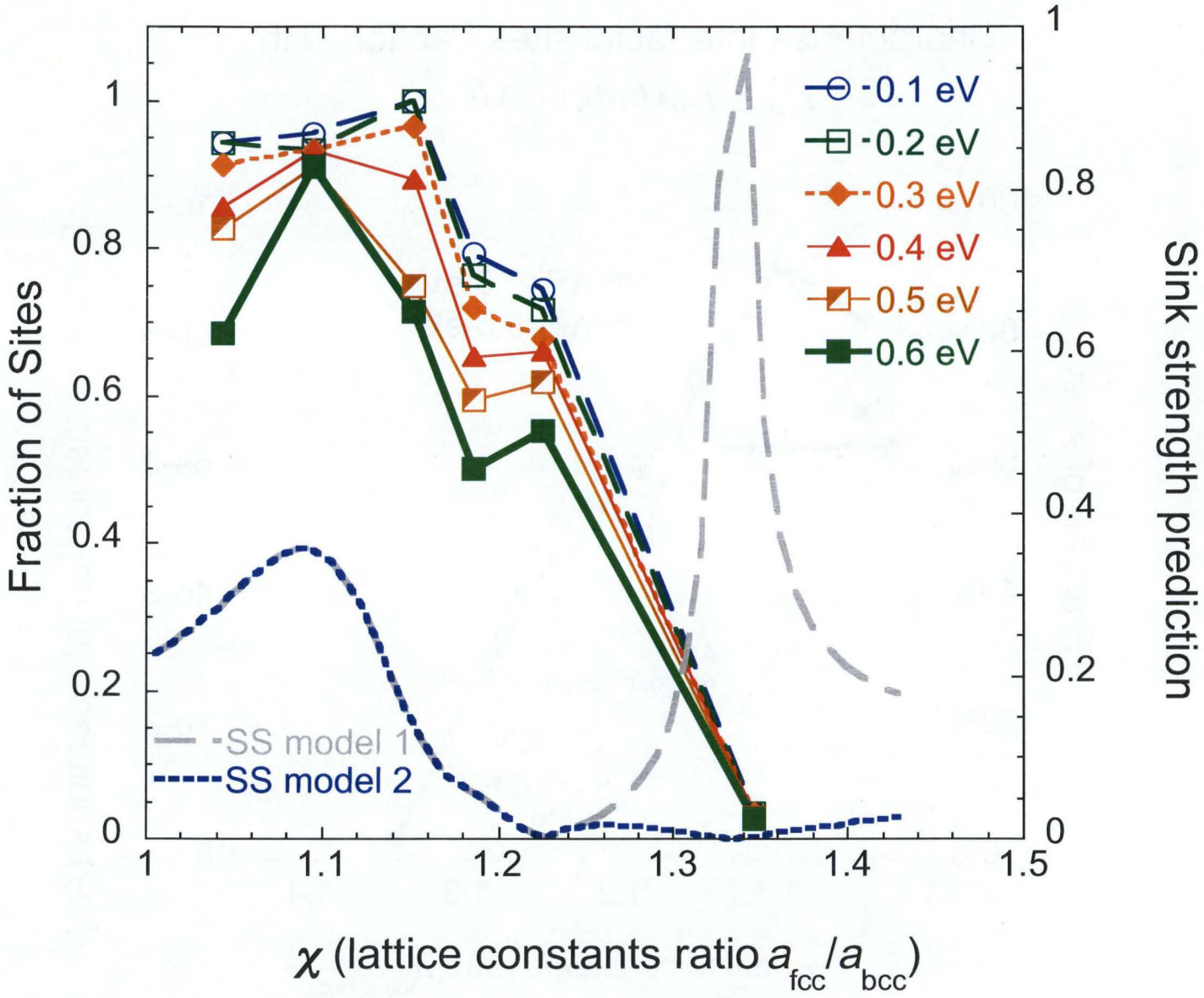
Correlation between vacancy formation energies and structural features

Characterize interfacial sites fraction with

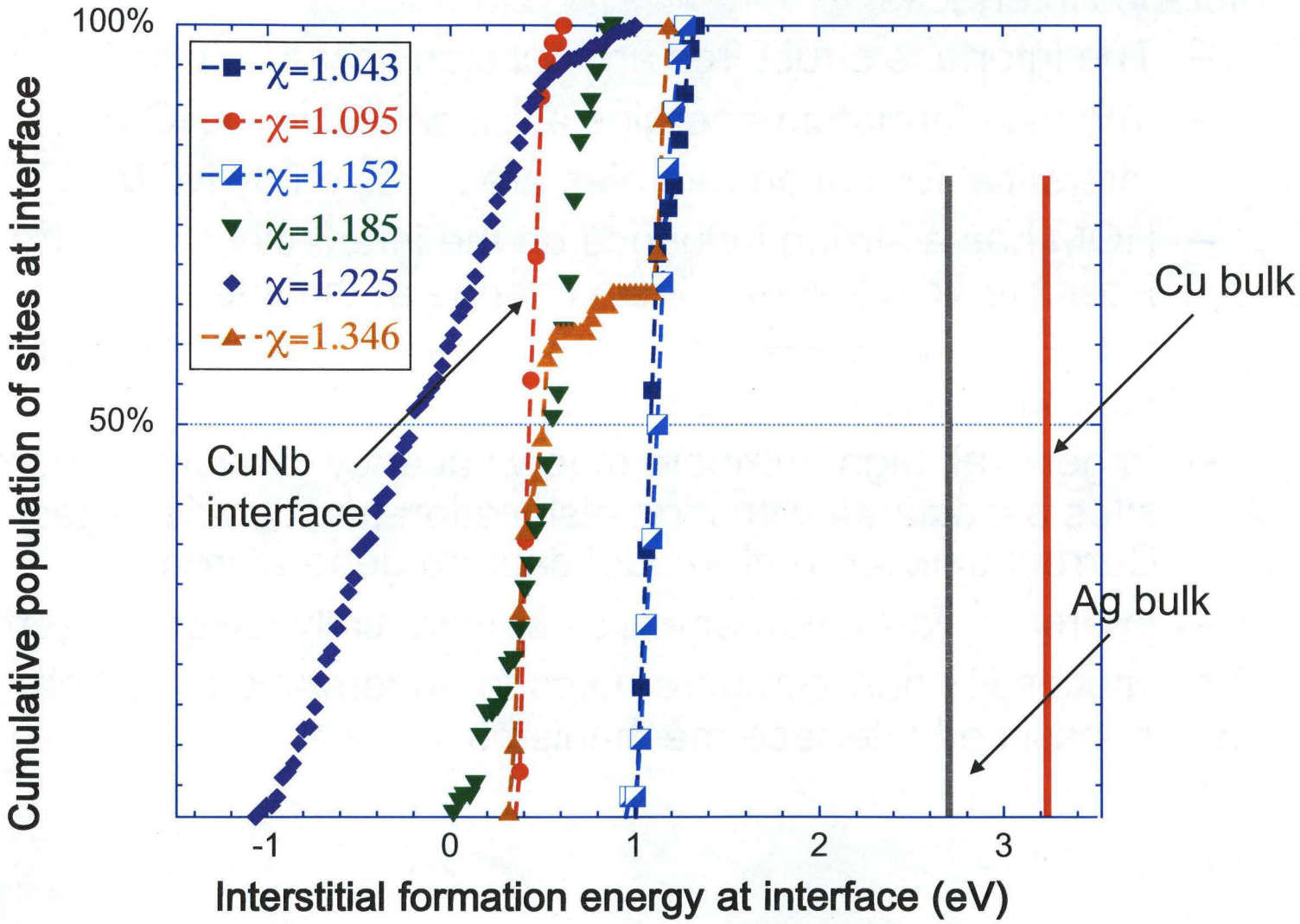
$$E_V^f \le E_V^f(bulk) - \Delta E$$



Interface sink strength model based on dislocation densities



Interstitial formation energies are significantly lower at interfaces: implication on interstitial-vacancy recombination mechanisms at and near interface



Summary

- Tunable EAM potentials on variation of heats of mixing (HOM) at fcc-bcc interfaces
  - The interface structures are not significantly altered.
  - Vacancy formation energies are insensitive to HOM.
  - Interstitial formation energies are modified by HOM.
  - HOM has a strong influence on the interfacial shear strength. Possible active shear plane change at the interface too.
- Tunable EAM potentials on fcc-bcc interfaces with different lattice misfits from 1.043 to 1.346 range
  - In general, high numbers of low vacancy-formation-energy sites associated with high dislocation-junction densities. Current sink strength model capture general trend.
  - Interstitial formation energies substantially lower at interfaces.
- The atomistic approach here helps to understand the different defect assisted interface mechanisms.