LA-UR- 11-01305

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Title: Relevance of fcc-bcc Interface Structure to Defect Properties at Interfaces in Irradiation Environment

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Intended for: 2011 TMS Annual Meeting & Exhibition

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Form 836 (7/06)

2011 TMS Annual Meeting & Exhibition:
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Abstract:
Nanolayered Cu-Nb composites exhibit high strength and enhanced radiation damage tolerance. To understand the relevance of interface structure to interface properties in fcc-bcc systems, tunable potentials offer a fairly simple way to selectively vary parameters independently. In this work, the parameterization of the EAM interatomic potential in fcc-bcc system is modified to understand the interface properties. We first change the dilute heats of mixing between Cu and Nb and investigate the effect on interface structure and defect formation energies near interface. To understand the interface behavior in different lattice misfit environment, the relative lattice constants between Cu and the bcc crystal are varied. Interface dislocation analysis based on Frank-Bilby formulation is to be presented, together with atomistic simulation result. Defect-interface interactions are studied with molecular dynamics (MD) and accelerated MD method, to predict the radiation damage tolerance of these interface systems.

Relevance of fcc-bcc Interface Structure to Defect Properties at Interfaces in Irradiation Environment

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Acknowledgement:

Los Alamos National Laboratory Directed Research and Development program

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

Experimental background

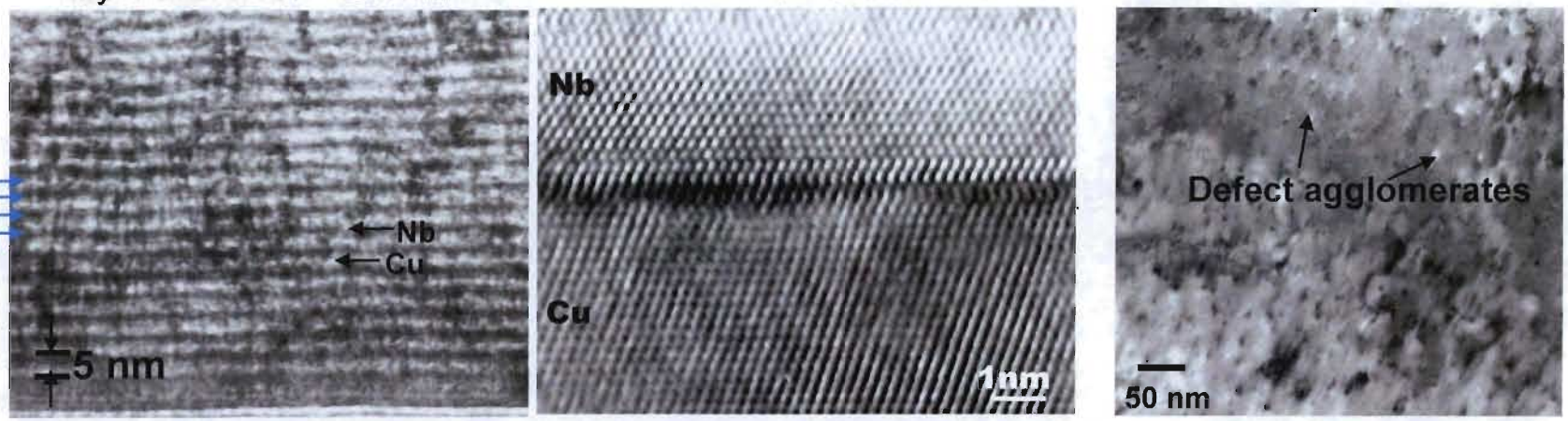
Cu-Nb multilayers

bulk Cu

layer thickness = 2.5 nm

t = 5 nm

layer interfaces provide sinks for defects

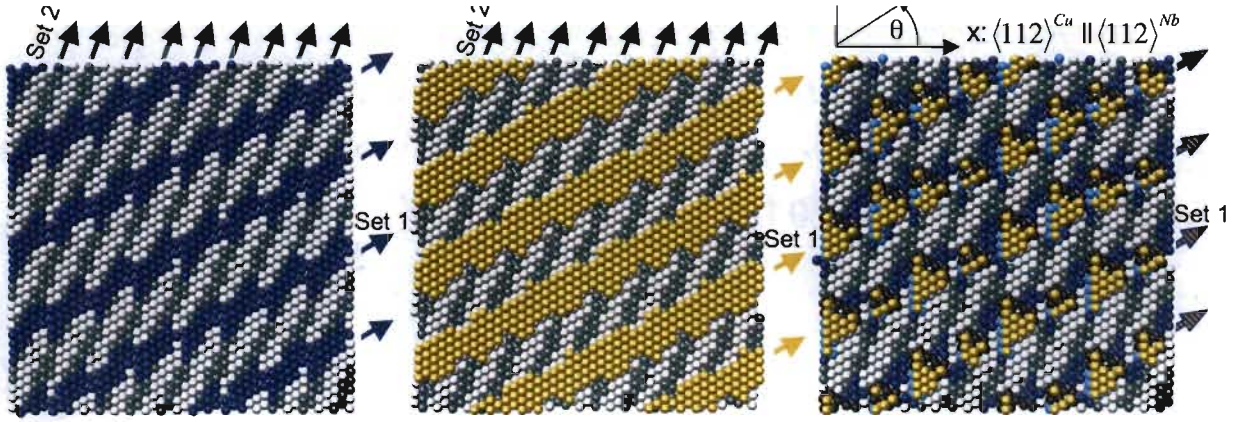


Room temperature He implantation, Energy: 150 keV, Dose: 1 x 10^{17} /cm^2 (7dpa)

Understanding of the defect properties at interfaces in irradiation environment is key to predictive design of radiation tolerance materials

Previous modeling effort and current work

Demkowicz et al, PRL 100, 136102 (2008)



How does the interface variation influence interface sink strength?

Need a way to systematically vary atomic structure without changing anything else and then explore the sink strength of interfaces with different atomic structure.

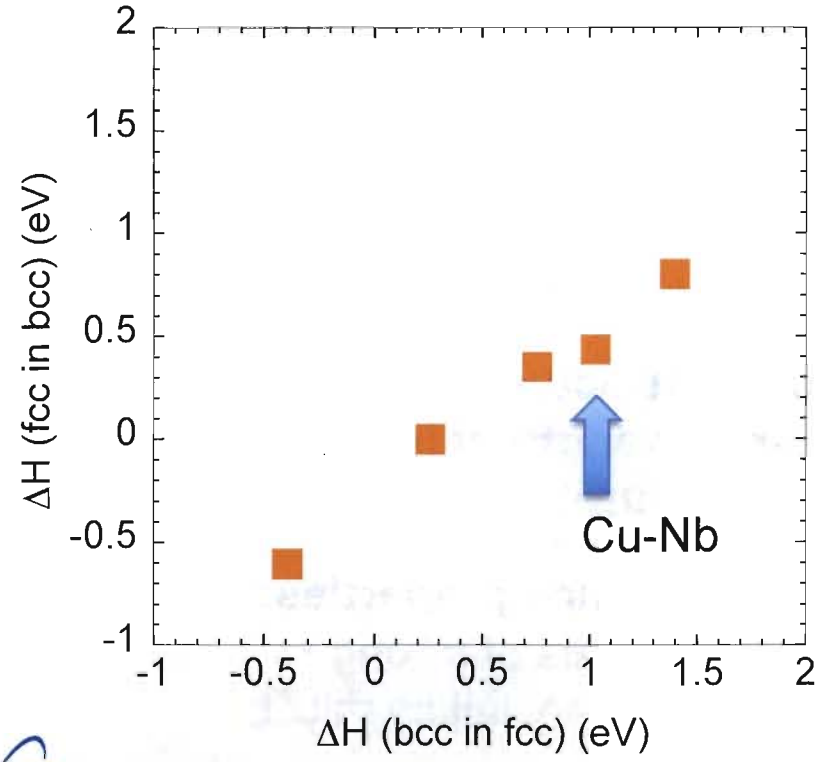
Use a "tunable" potential approach to vary interface properties:

- Keep lattice misfit constant, systematically vary heats of mixing,
- Or, keep heats of mixing constant, systematically vary lattice misfit.

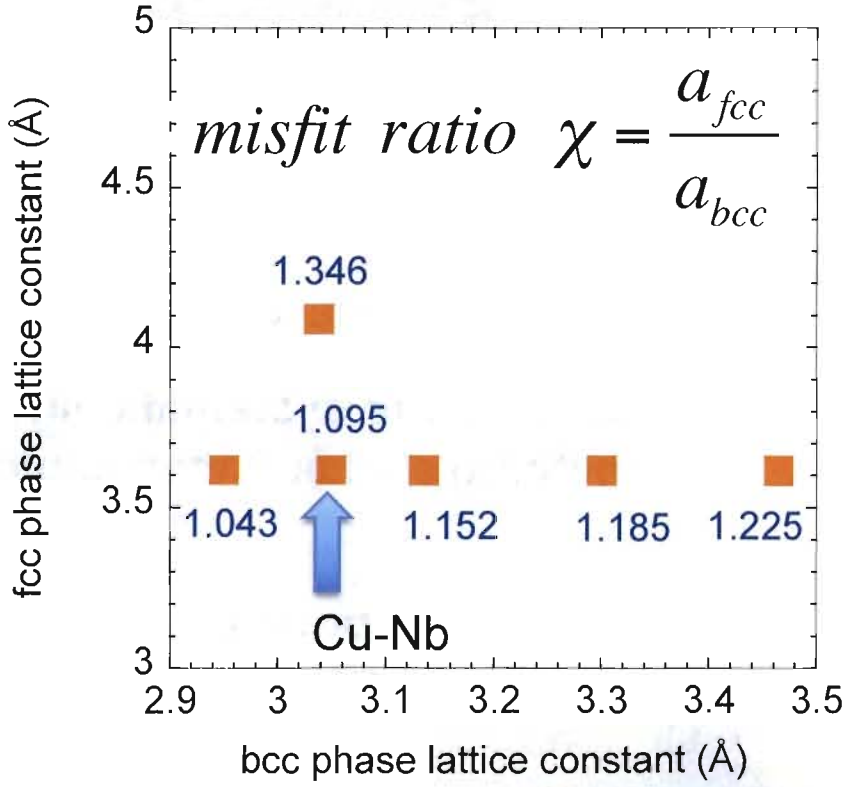
Tunable-potential approach

Tune the parameterizations of the interatomic potential describing fcc-bcc metallic material.

a.) Interface energetics (heats of mixing) **(results published in Liu et al, Acta Mater. 58, 4549 (2010).)**



b.) Variation of lattice mismatch (or misfit) at interface **(this talk)**

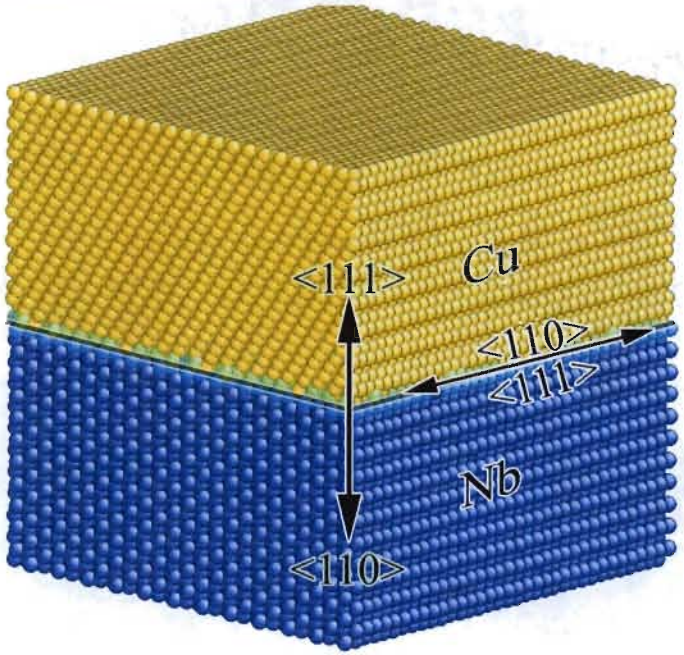


Fitting of interatomic potentials

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	-	-

Modeling consideration

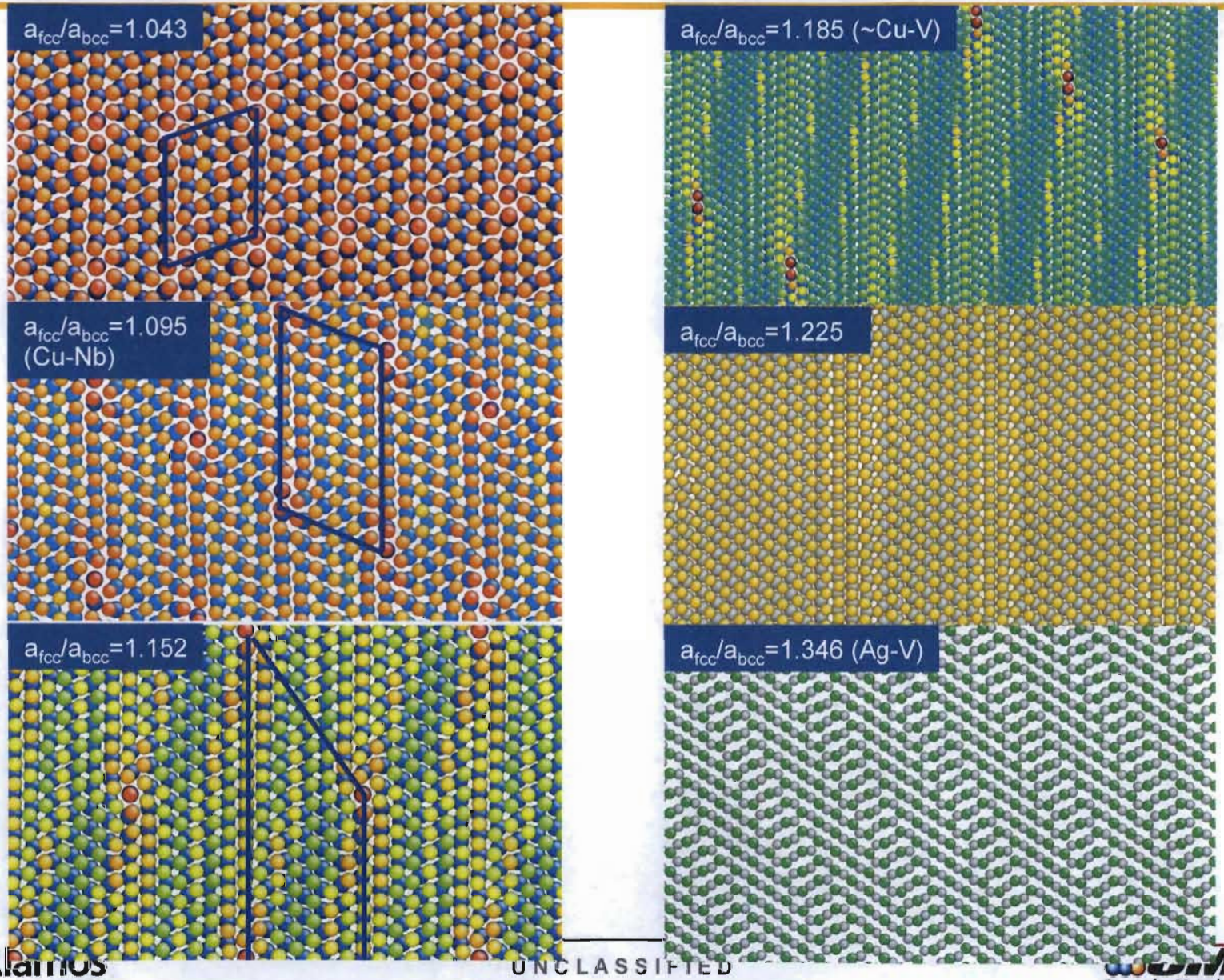


Kurdjumov-Sachs (KS) orientation relation

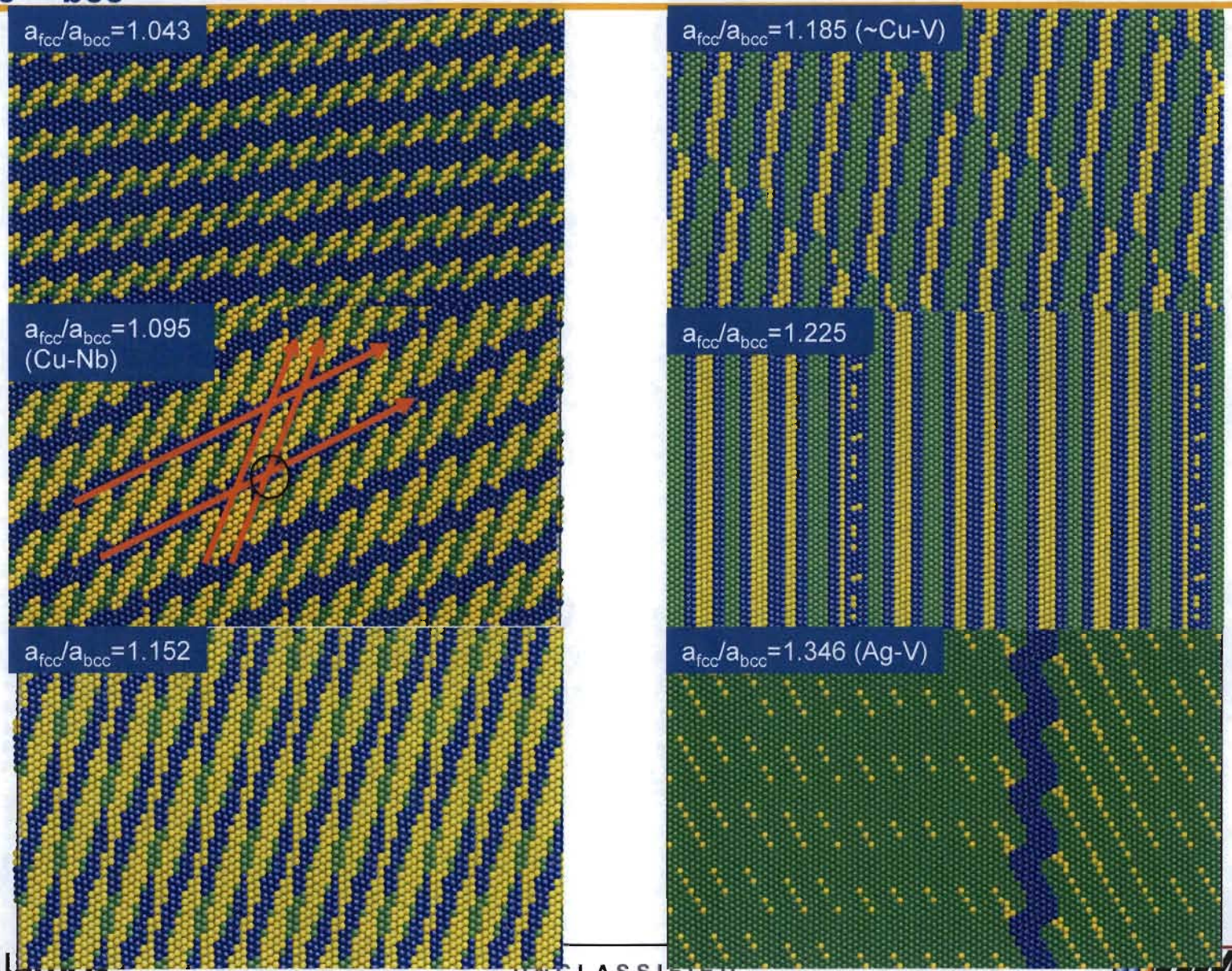
- $\{111\}_{fcc}||\{110\}_{bcc}$ || interface plane
- $<110>_{fcc}||<111>_{bcc}$ in interface plane

- In this work, extend our study to *general* fcc-bcc interface systems, and focus on KS orientation interfaces in this talk.

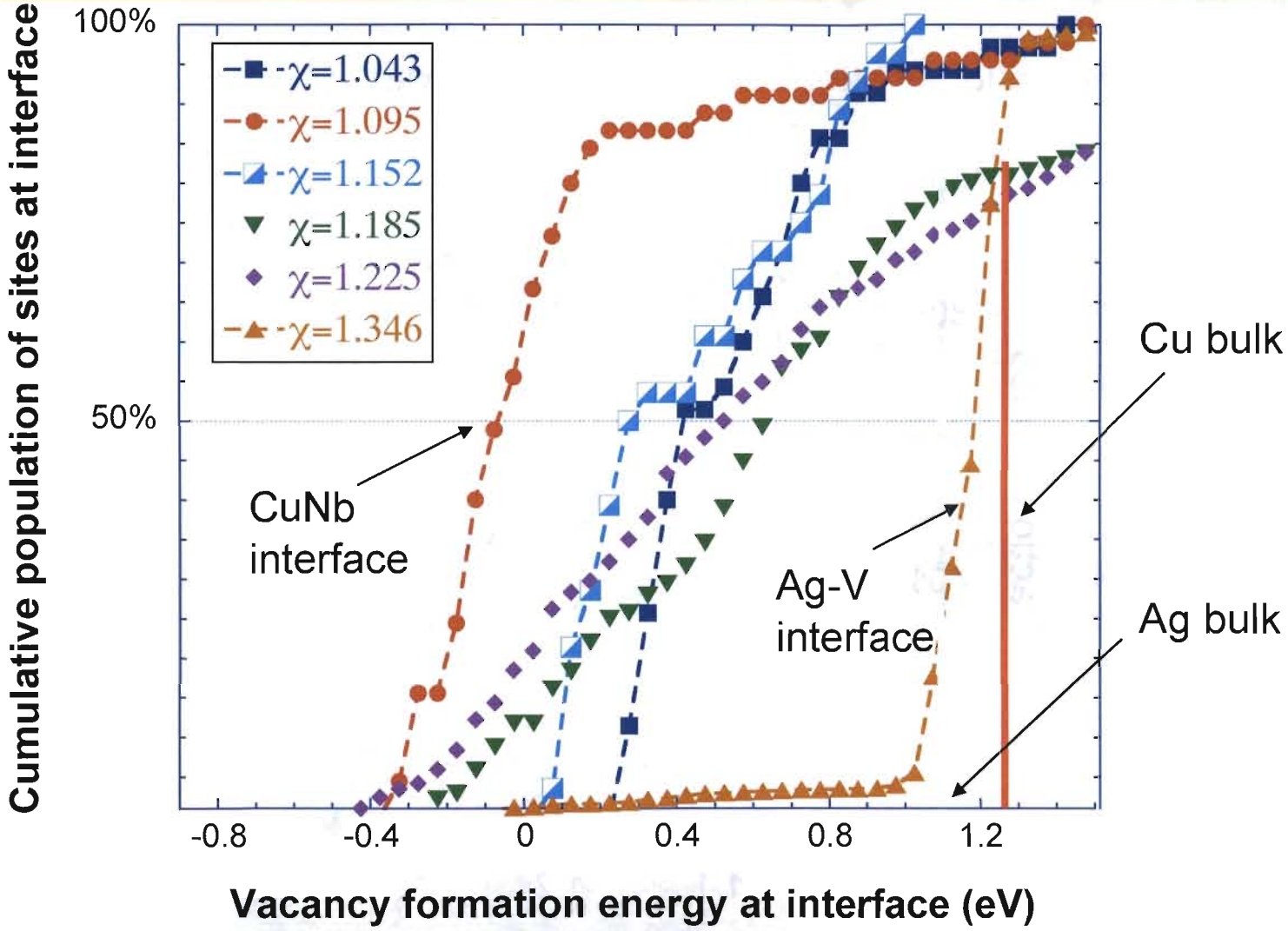
Interface structures with different lattice misfit at fcc-bcc interface



Misfit dislocation patterns vary substantially with a_{fcc}/a_{bcc}



Vacancy formation energies in fcc change substantially at different fcc-bcc interfaces



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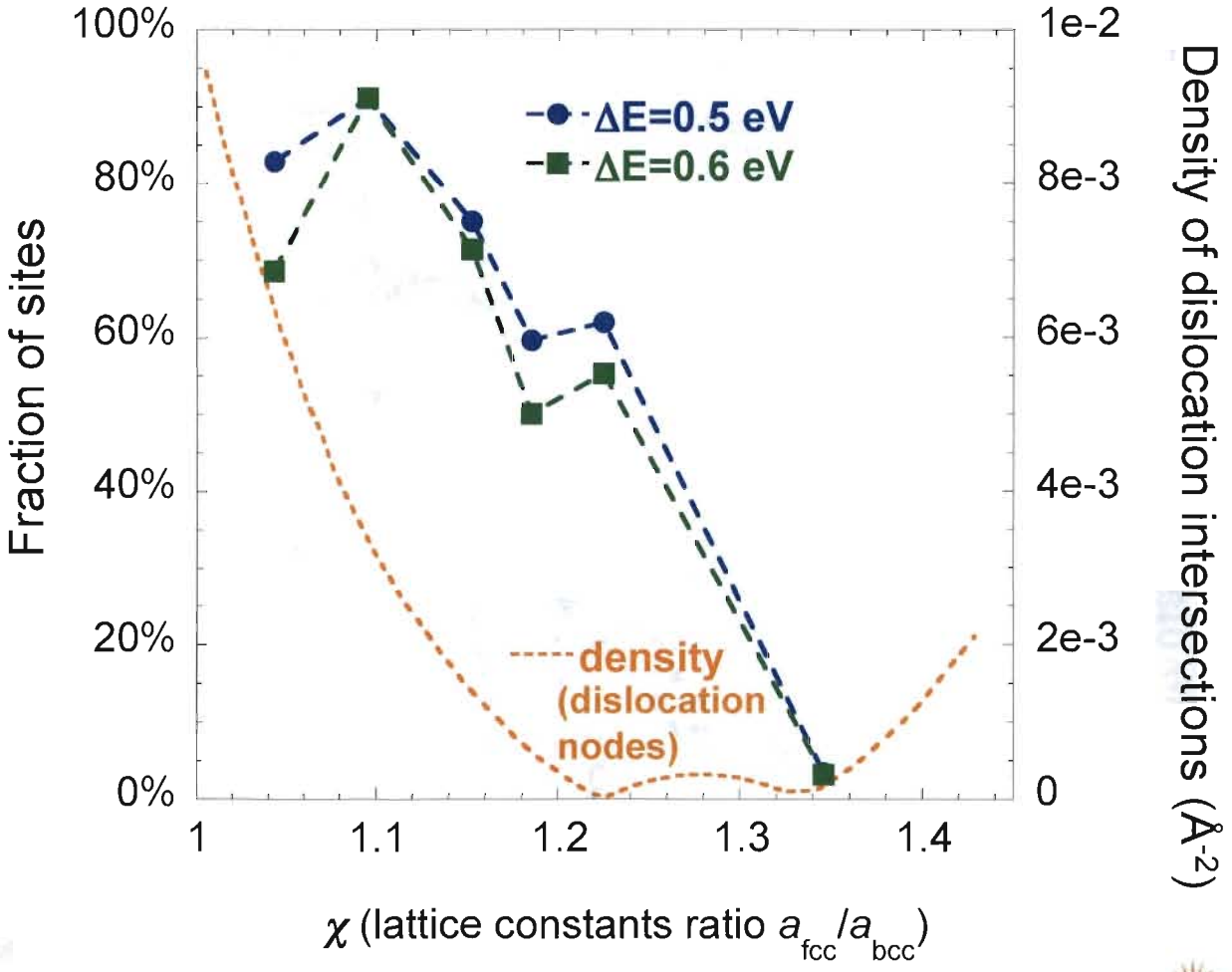
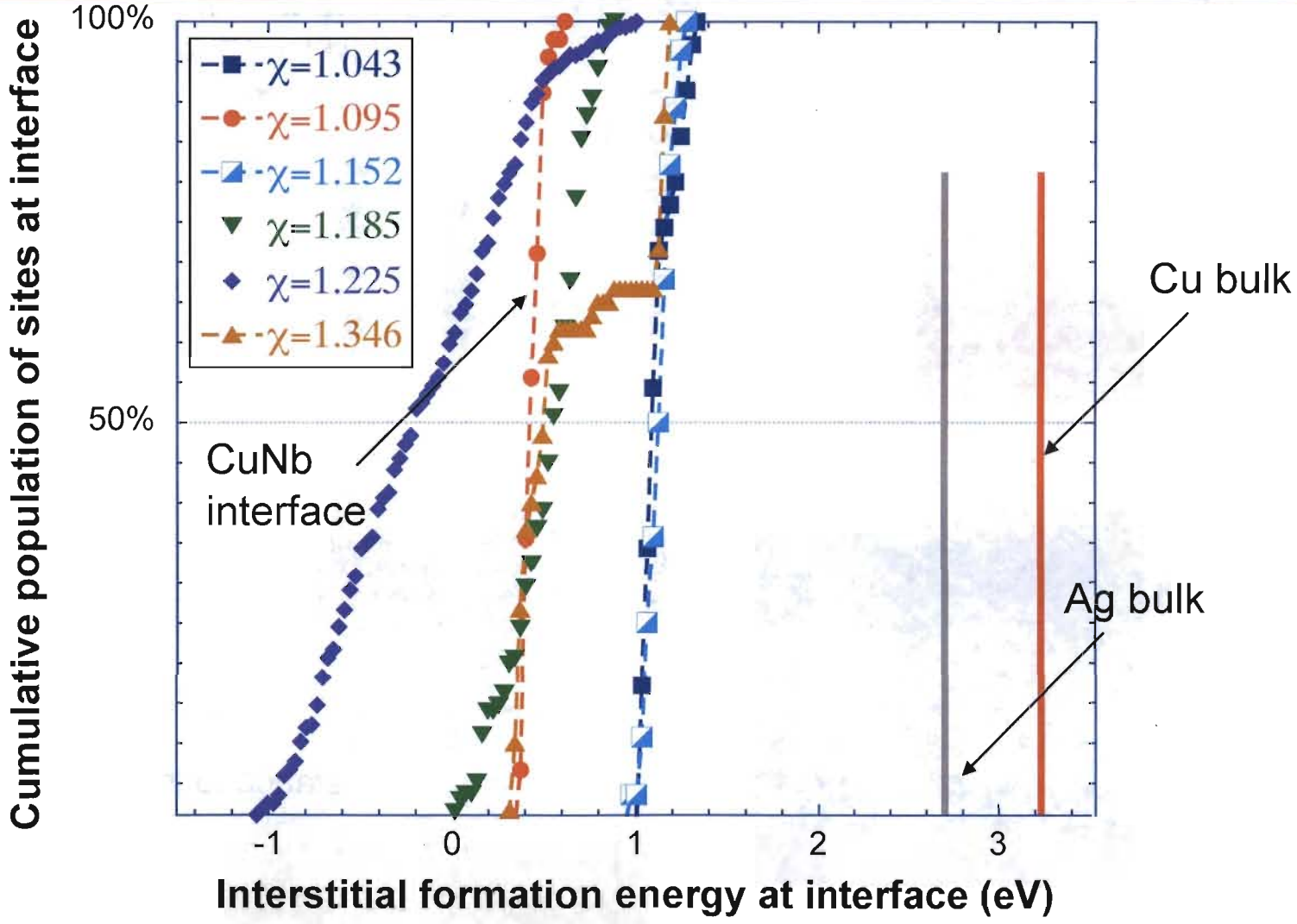
Vacancy formation energies in fcc change substantially at different fcc-bcc interfaces

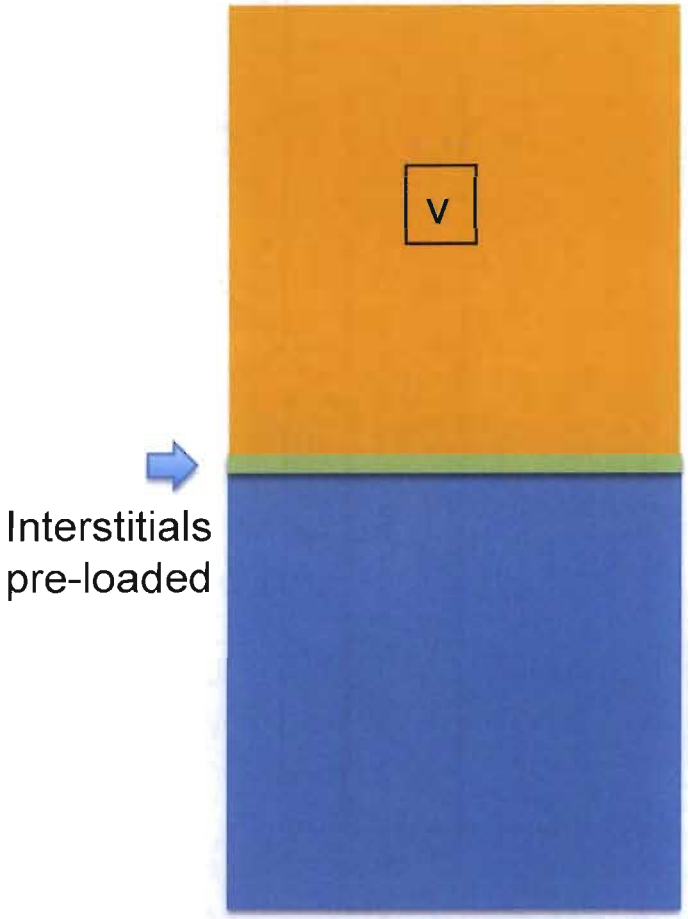
Calculation of interfacial sites fraction with $E_V^f \leq E_V^f(bulk) - \Delta E$

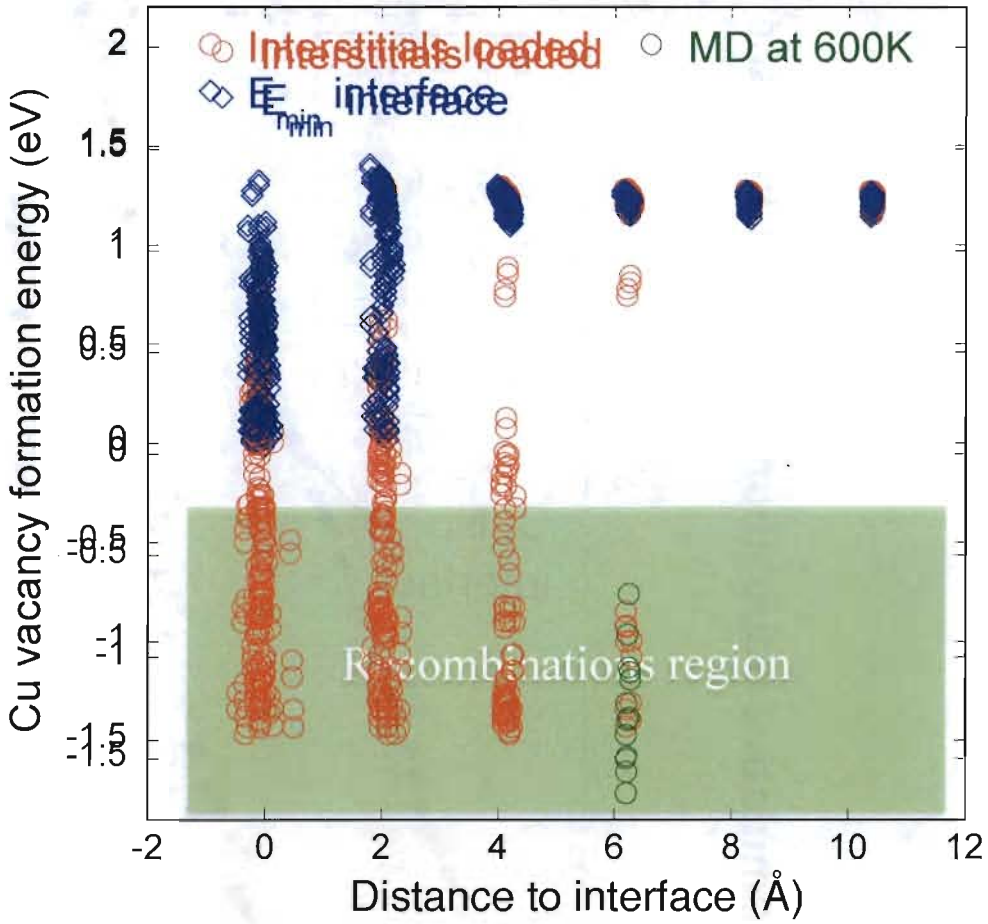


Interstitial formation energies in fcc are significantly lower compared to bulk values at all KS interfaces



"Interstitial loading" has 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

- 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 KS orientation interfaces with different misfit reveals:

  a) Vacancy formation energies decrease with increasing misfit dislocation density,

  b) 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.