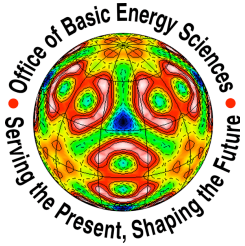
Massachusetts Institute of Technology



Design of composite materials for outgassing of implanted He

M. J. Demkowicz

MIT Department of Materials Science and Engineering,
Cambridge, MA 02139

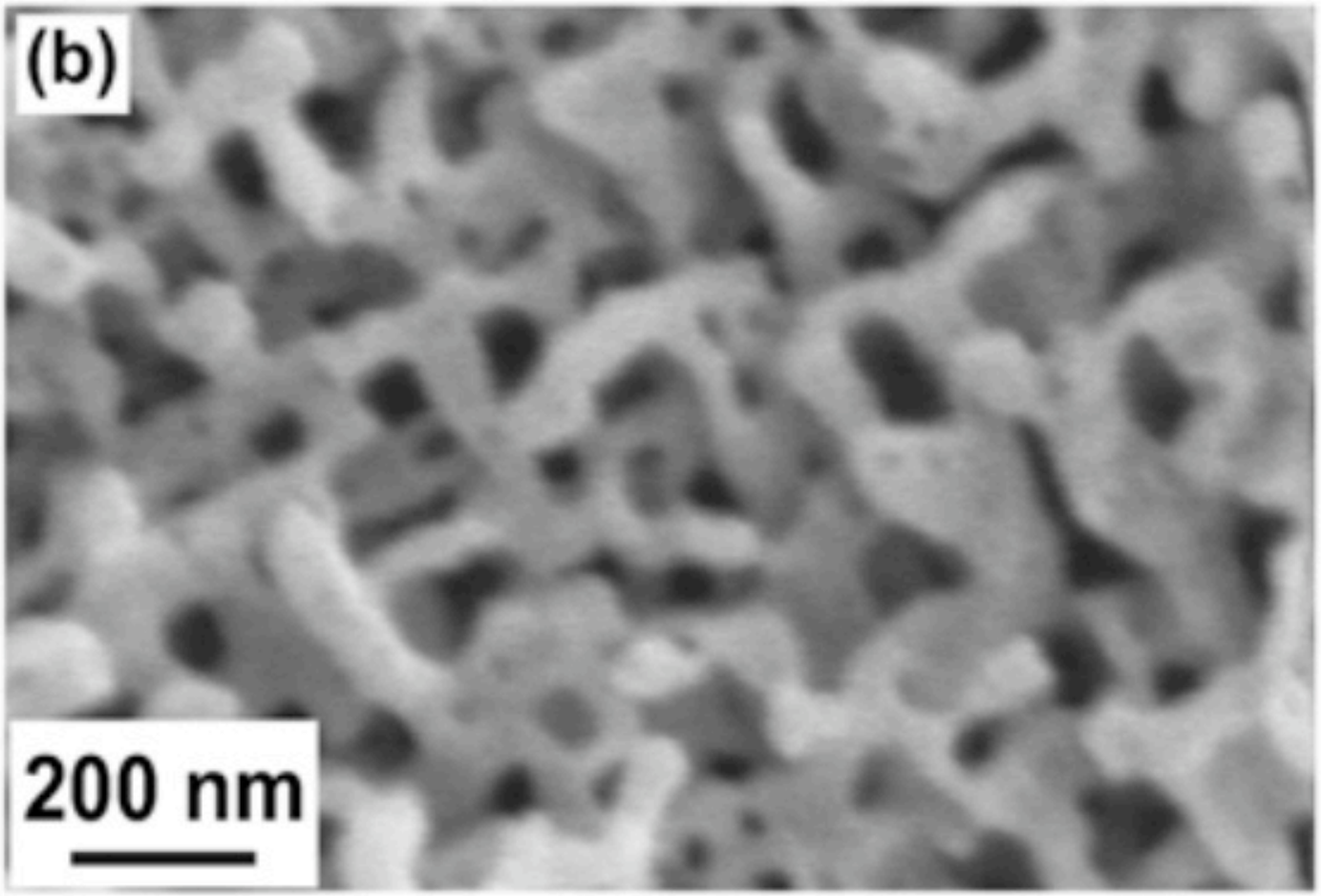
Sponsors:
• CMIME, an Energy Frontier Research Center funded by DOE, Office of Science under Award Number 2008LANL1026
• LANL LDRD program

ICTP-IAEA 2014
Trieste, Italy

Acknowledgements:
A. Kashinath, D. Yuryev,
P. Wang, J. Majewski, A. Misra,
X. Zhang, D. Bhattacharyya, …

He-induced damage

He-implanted W, T=1000-2000K

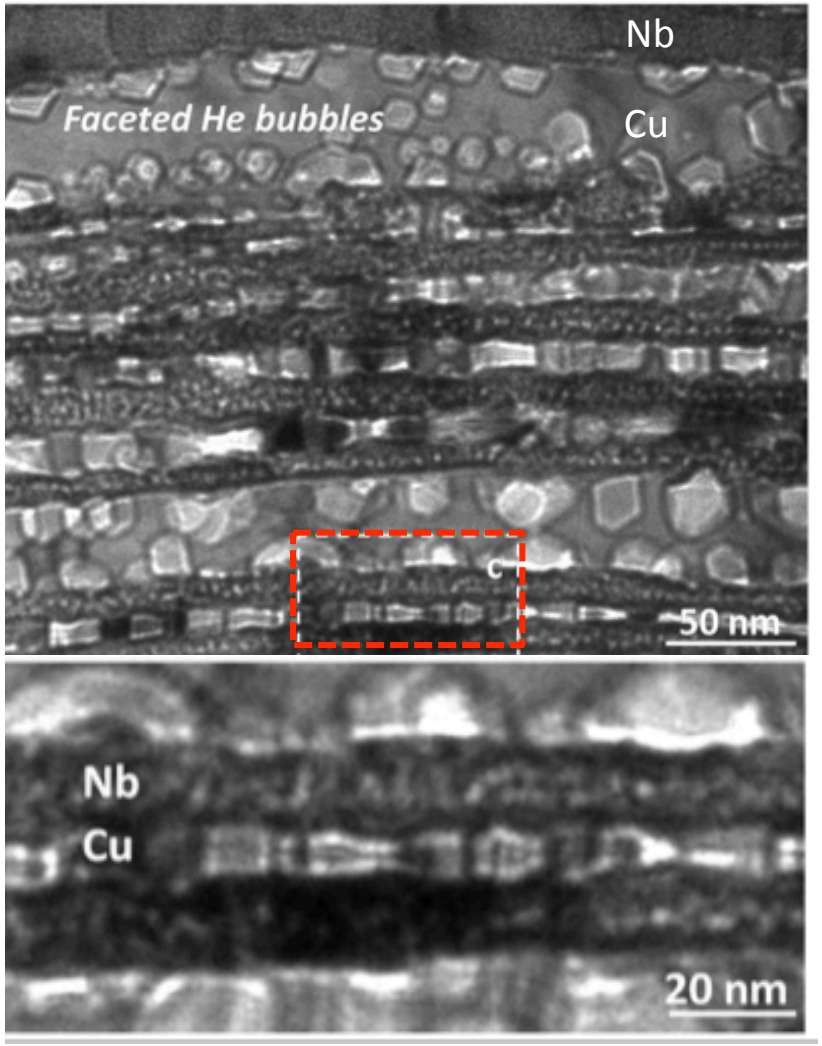


S. Kajita *et al.*, Nucl. Fus. **49**, 095005 (2009)

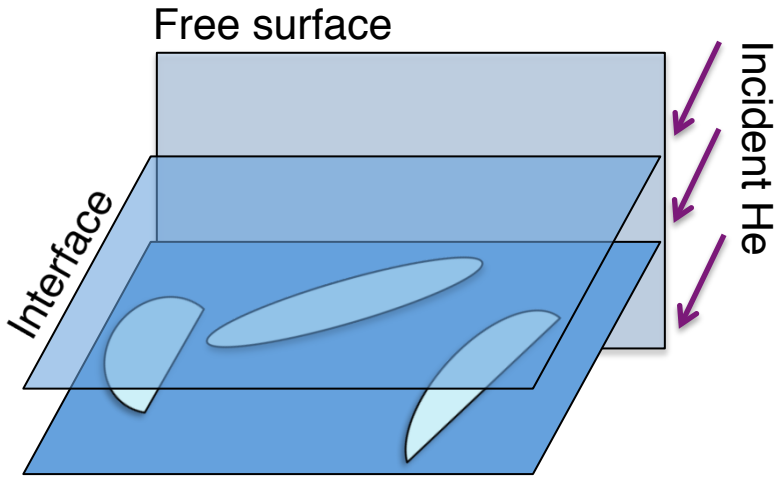
Can we design a materials where this sort of damage does not occur?

Channels for continuous He outgassing

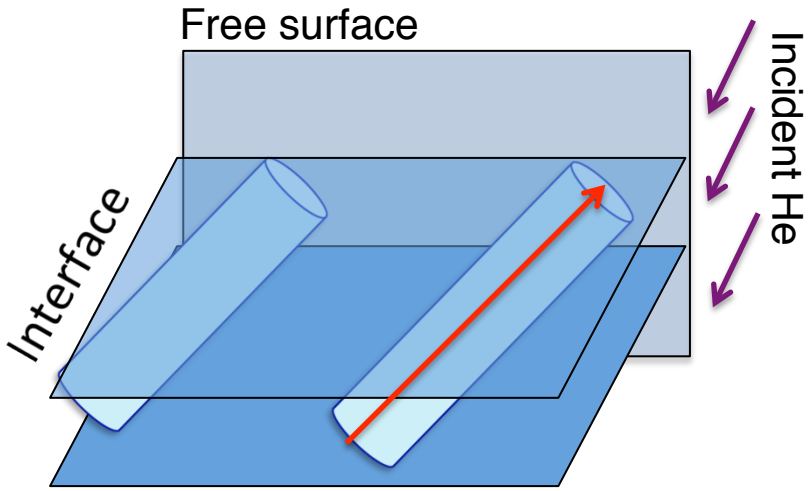
Cu-Nb layered composites



W. Z. Han *et al.*, J. Nucl. Mater. **452**, 57 (2014)



No design: uncontrolled precipitation



Design: channels for He outgassing

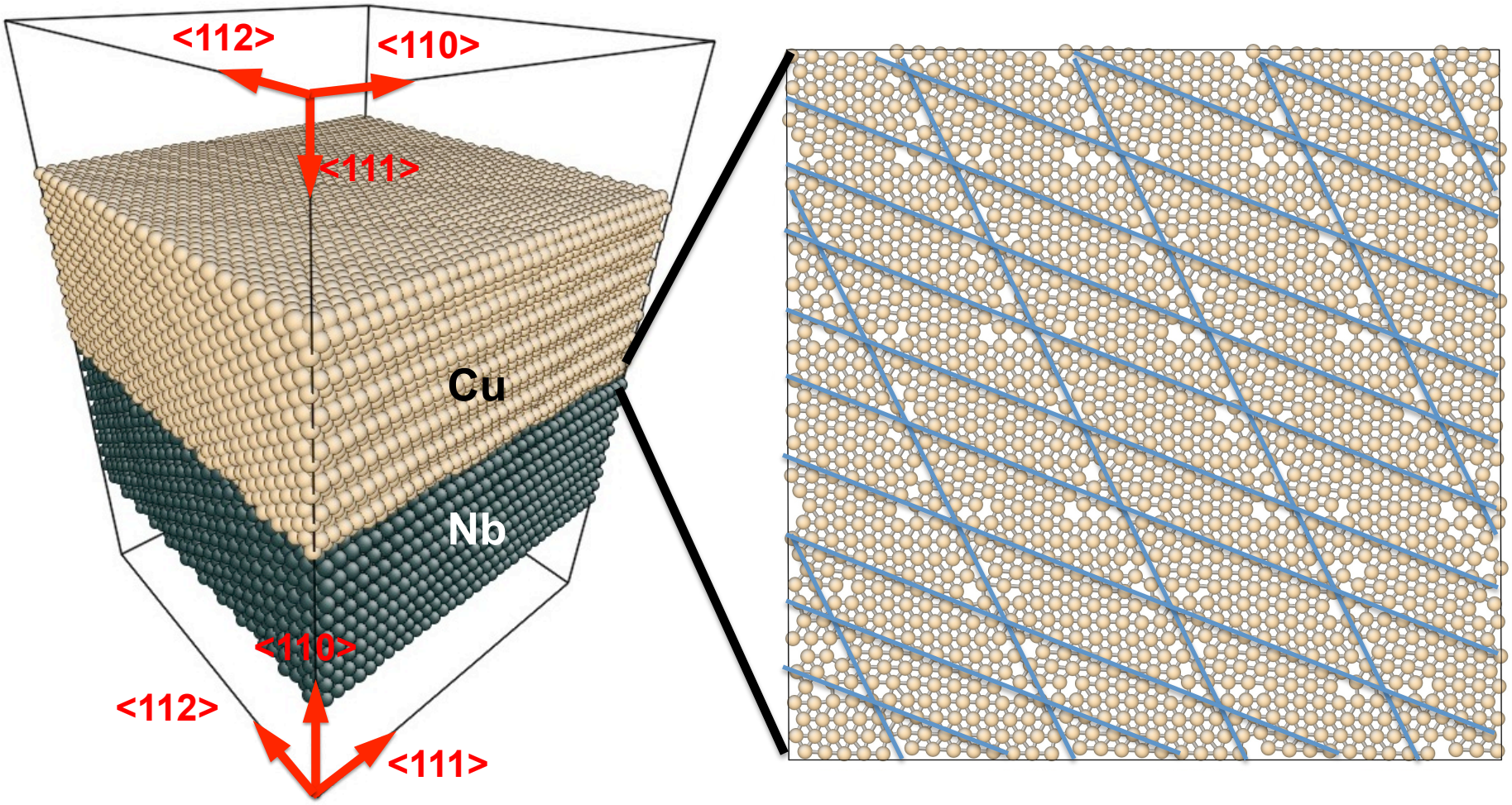
D. V. Yuryev *et al.*, APL **under review** (2014)

Outline

- ***Modeling He precipitation in metal multilayers***
- Experimental validation of modeling results
- Design of metal composites for He outgassing

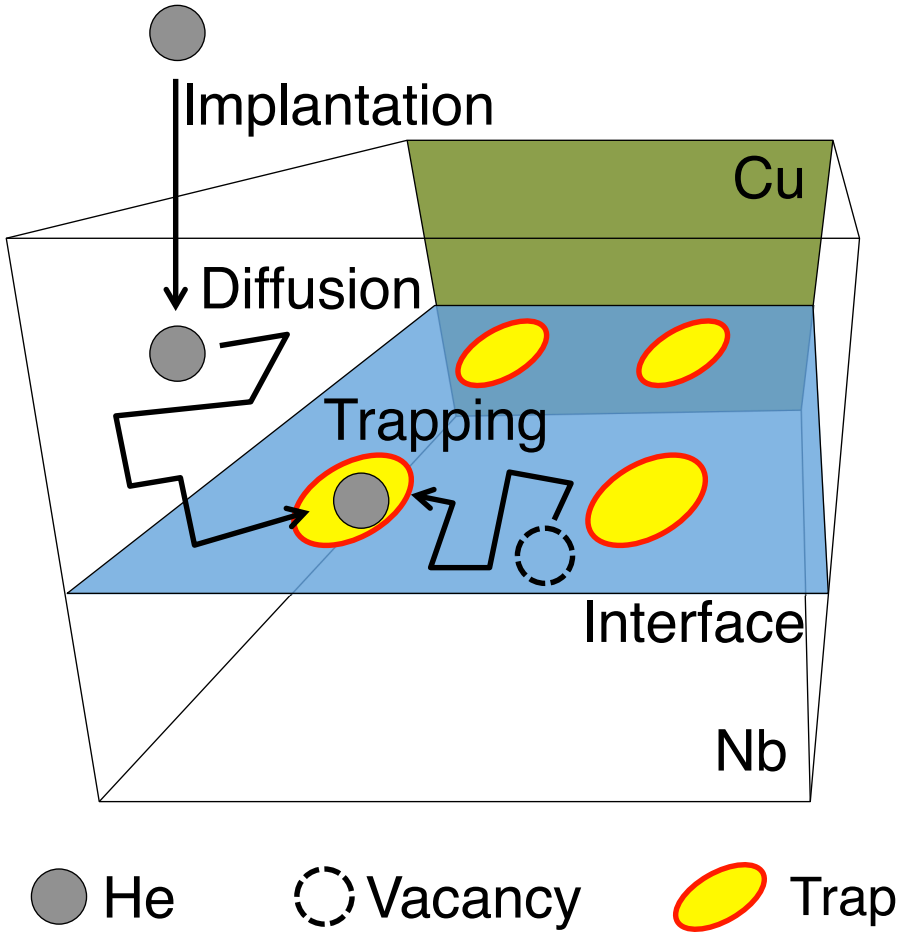
Misfit dislocation patterns at Cu-Nb interfaces

All Cu-Nb interfaces in magnetron sputtered composites have the same crystallography: $\{111\}_{fcc} \,||\, \{110\}_{bcc}$ and $\langle 110\rangle_{fcc} \,||\, \langle 111\rangle_{bcc}$



He trapping at Cu-Nb interfaces is quasi-static

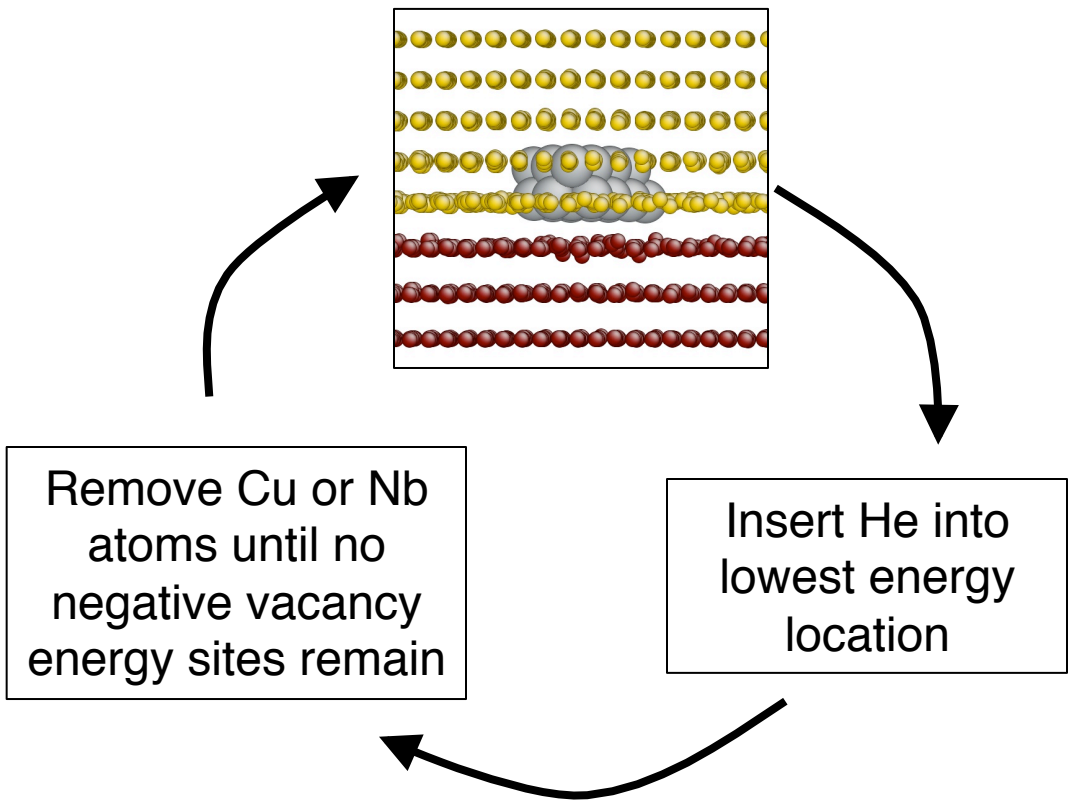
- 35 keV He ions are implanted to a dose of $10^{17}/cm^2$ in 3 hours => 1 He atom reaches the vicinity of a trap every ~12 minutes
- He migration energy at the interface is ~0.1 eV => time to find the trap <1ns
- Vacancy migration energy at the interface is ~0.4 eV => time to equilibrate vacancy concentration <1s



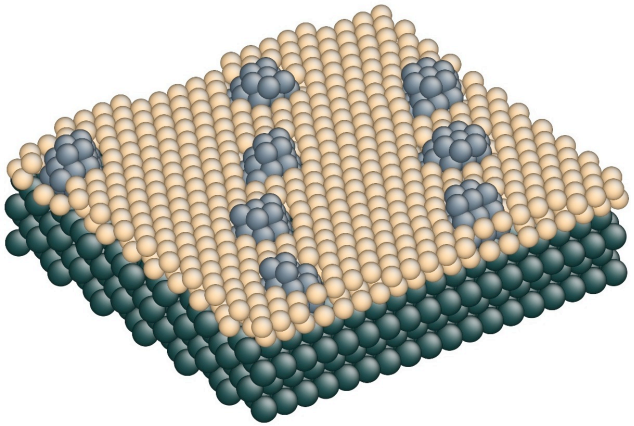
[1] A. Y. Dunn *et al,* JNM **435** 141 (2013); [2] K. Kolluri *et al*, PRB **84**, 104102 (2011)

Atomic-level modeling of He trapping
at a Cu-Nb interface using a custom-made EAM potential

Iterative method for introducing He into interface:



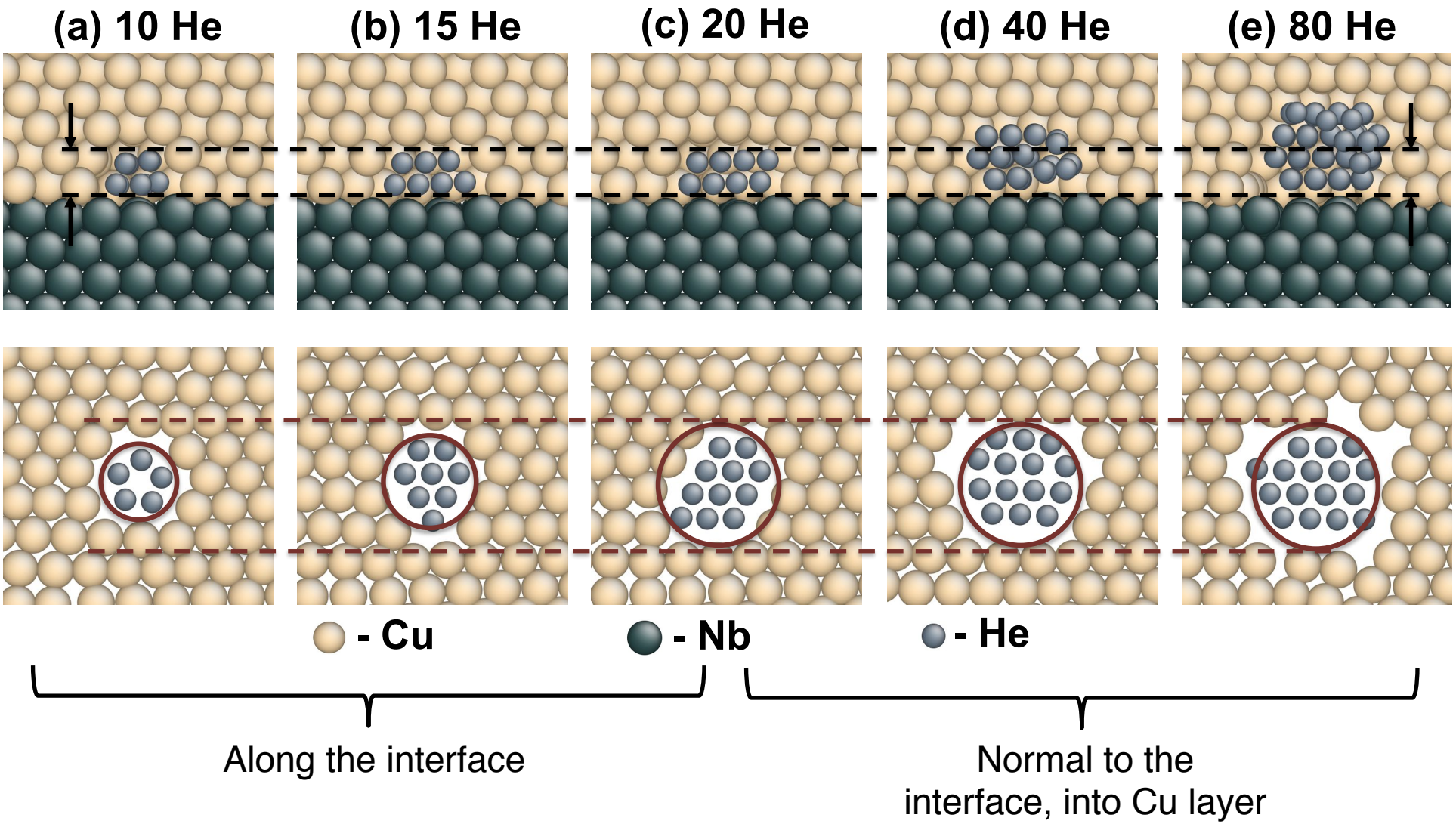
Outcome: He clusters grow at MDIs on Cu side of interface



- There is a thermodynamic driving force for clusters to coalesce, but the kinetics of coalescence is very slow.
- He/vacancy ratio ≈ 1

A. Kashinath *et al.*, PRL **110**, 086101 (2013)

Two modes of He cluster growth

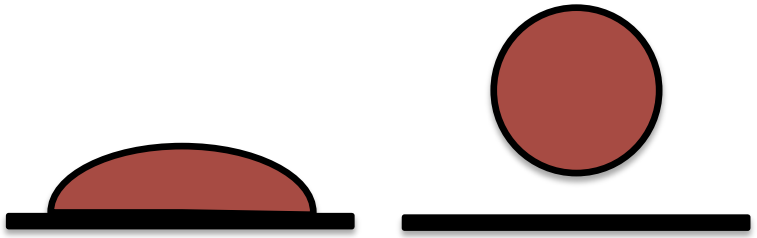


A. Kashinath *et al.*, PRL **110**, 086101 (2013)

Mechanism of interfacial He precipitation:
wetting at misfit dislocation intersections

Wetting Coefficient:

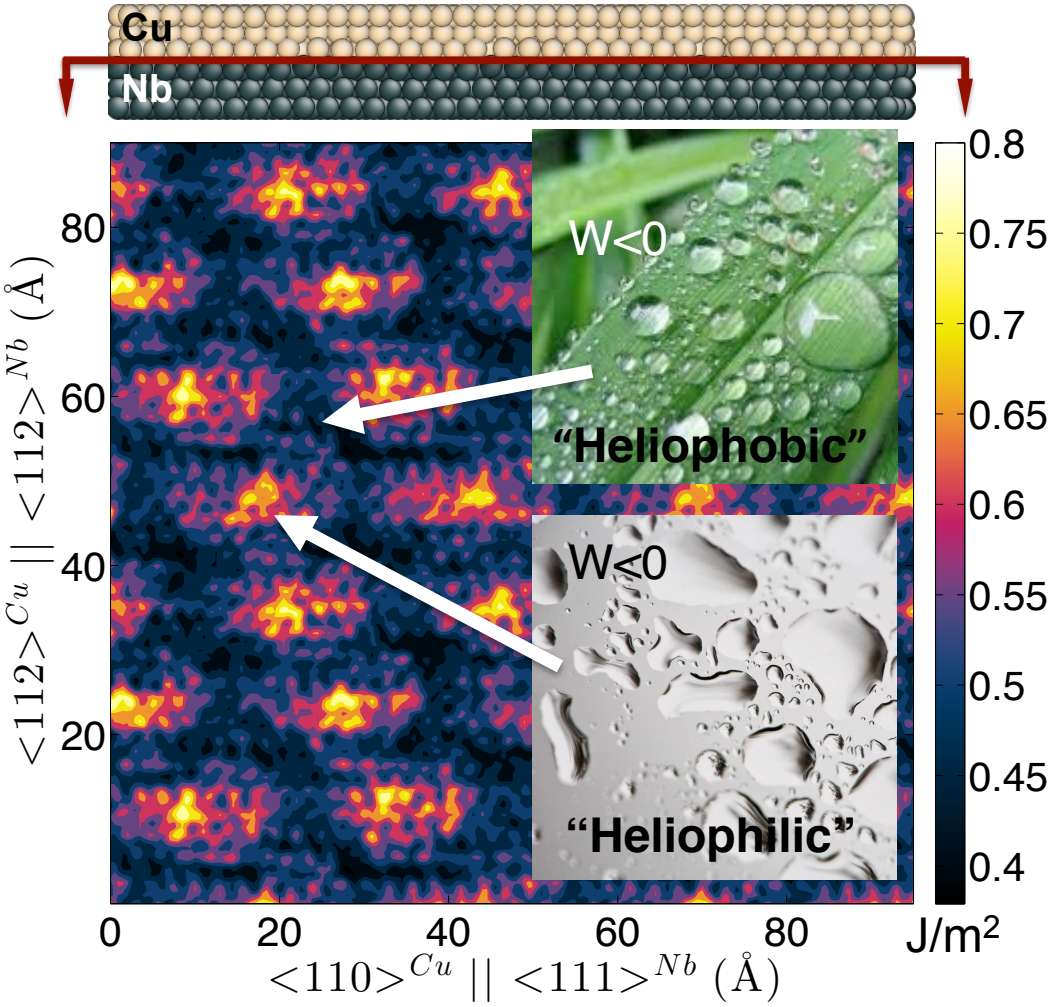
$$W = \gamma_{Cu\text{-}Nb} + \gamma_{He\text{-}Cu} - \gamma_{He\text{-}Nb}$$



Wetting
$W > 0$

Non-wetting
$W < 0$

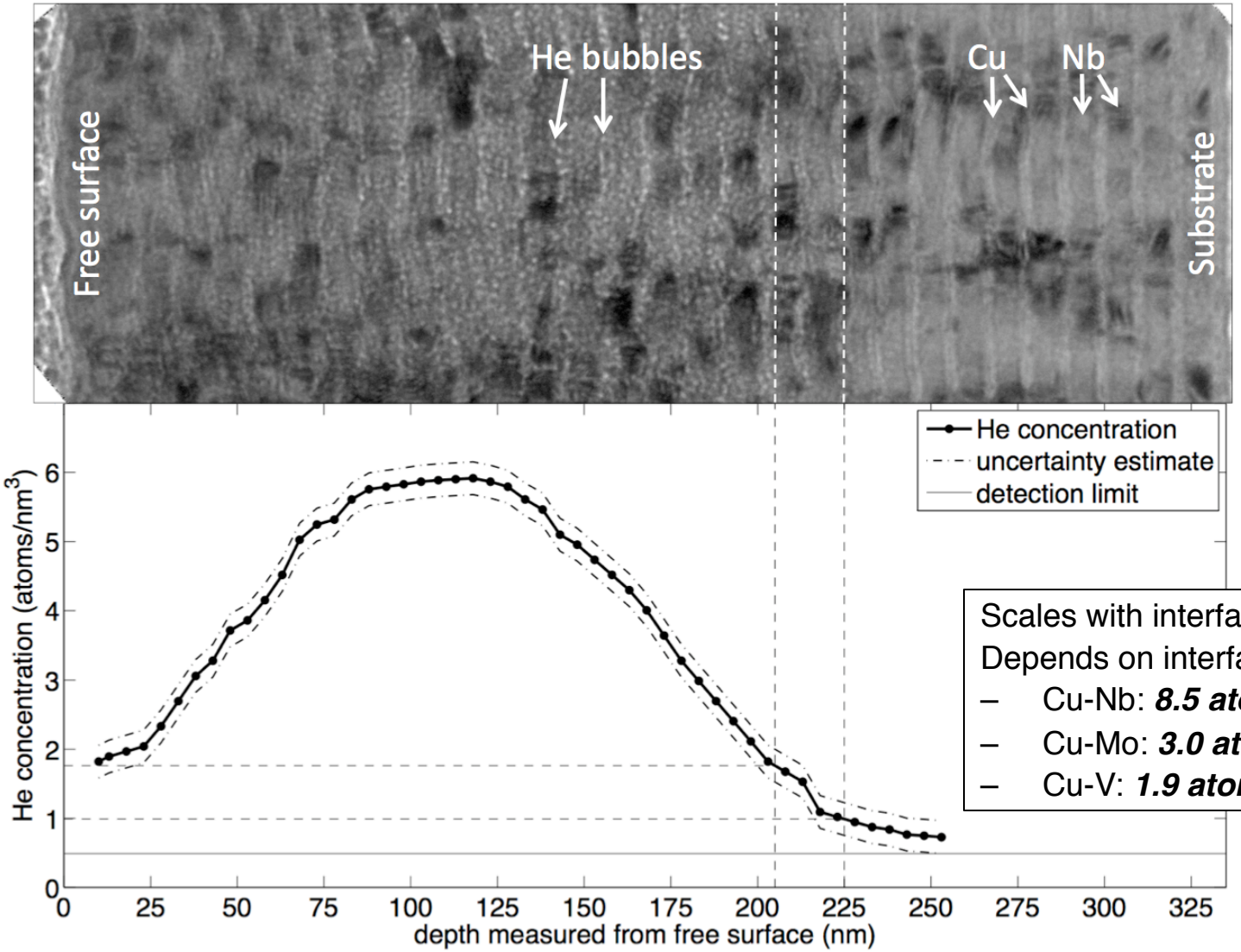
	Interface Energy (J/m²)
$\gamma_{He\text{-}Cu}$	1.93
$\gamma_{He\text{-}Nb}$	2.40
$\gamma_{Cu\text{-}Nb}$	Depends on location in the interface plane



Outline

- Modeling He precipitation in metal multilayers
- ***Experimental validation of modeling results***
- Design of metal composites for He outgassing

Critical He concentration to observe bubbles



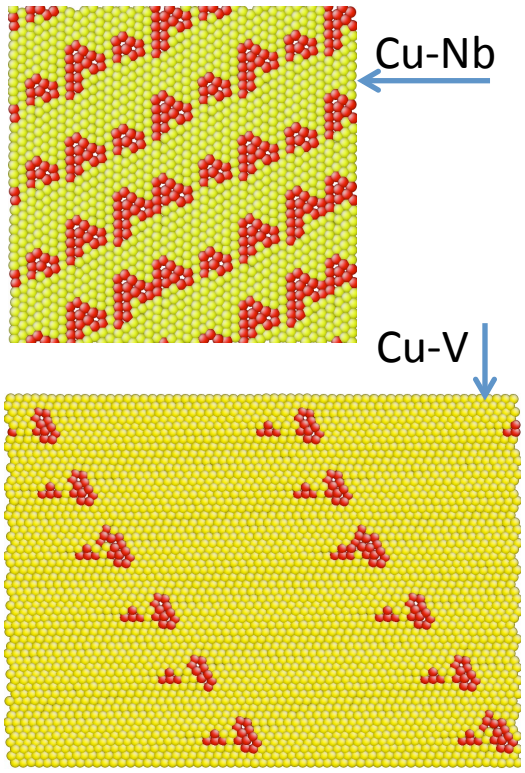
Scales with interface area/vol.
Depends on interface type:

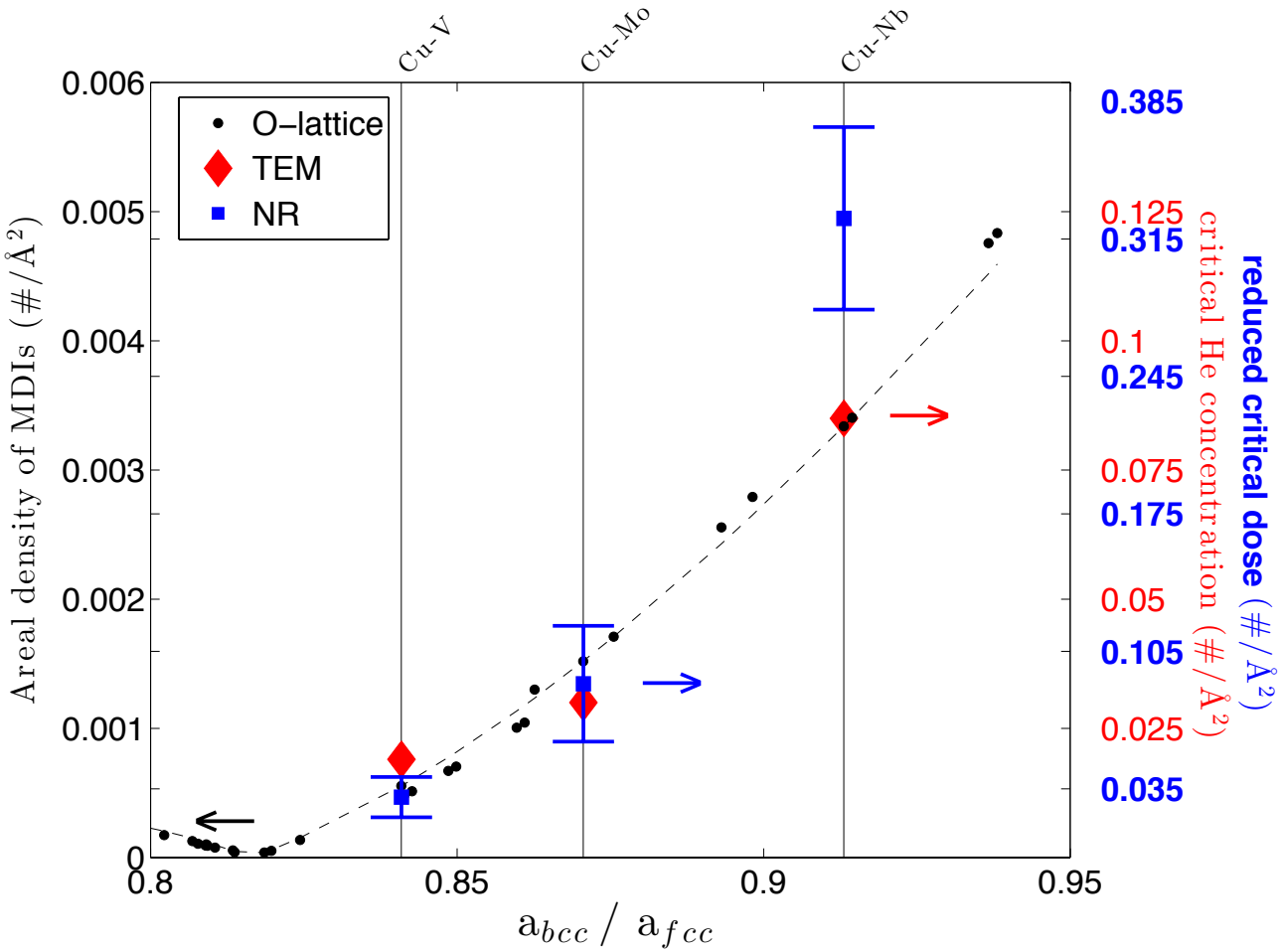
- Cu-Nb: ***8.5 atoms/nm^2***
- Cu-Mo: ***3.0 atoms/nm^2***
- Cu-V: ***1.9 atoms/nm^2***

M. J. Demkowicz *et al.*, Appl. Phys. Lett. **97**, 161903 (2010)

Agreement between model, TEM, and NR

Areal density, ρ, of heliophilic patches in





Kurdjumov-Sachs orientation relation, closest-packed interface planes

A. Kashinath *et al.*, JAP **114**, 043505 (2013)

Outline

- Modeling He precipitation in metal multilayers
- Experimental validation of modeling results
- ***Design of metal composites for He outgassing***

Designing interfaces that outgas He

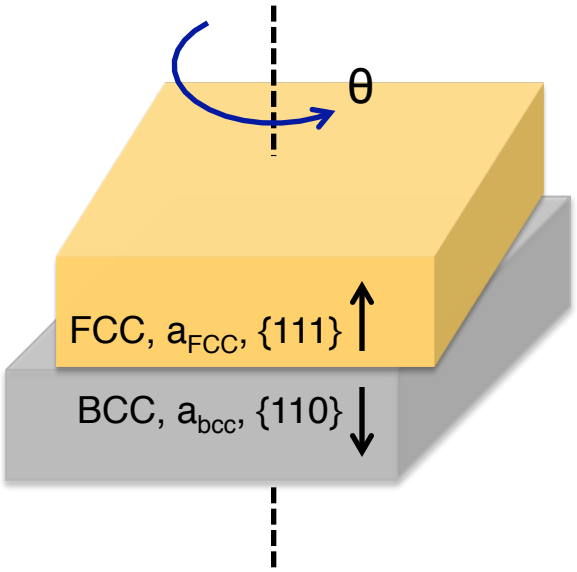
Model 2:
quantized Frank-Bilby equation
+ anisotropic elasticity

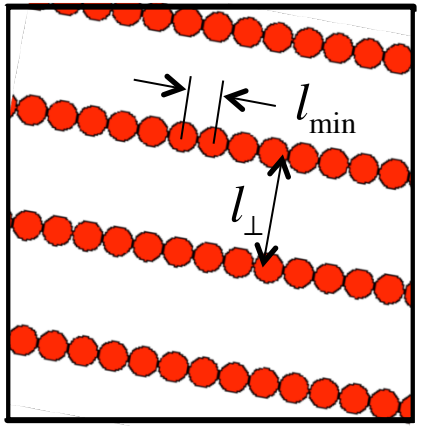
Model 2:
wetting of misfit
dislocation intersections

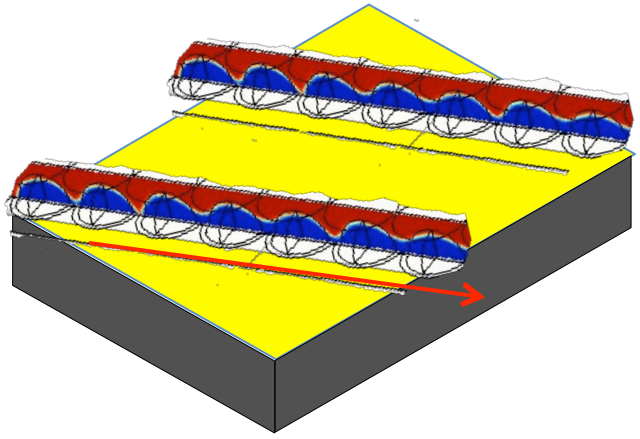
Interface composition and crystallography

Misfit dislocation intersections (MDIs) closely spaced in one direction and far apart in the perpendicular direction

Precipitation of linear He channels with MDI pattern as a template

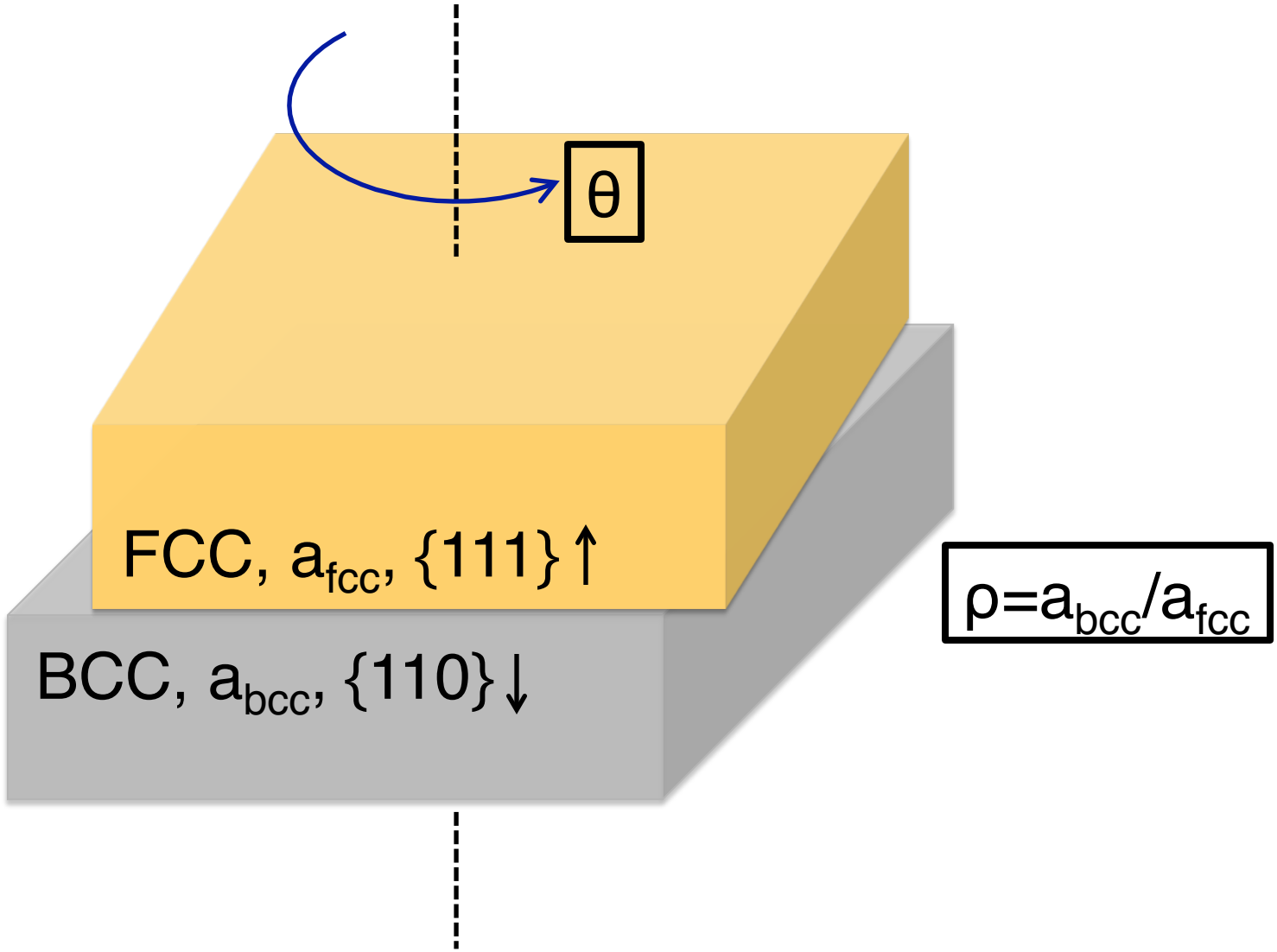






D. V. Yuryev and M. J. Demkowicz, APL **under review** (2014)

Two degrees of freedom: θ and ρ



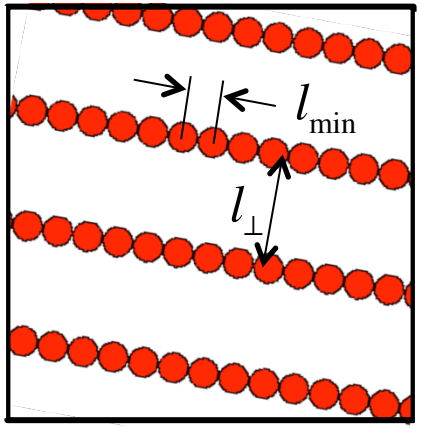
D. V. Yuryev and M. J. Demkowicz, APL **under review** (2014)

Design criteria

Criterion 1:

$$l_{\min} < l_{\min}^{cut}$$

Precipitates overlap along l_{min} prior to bubble-to-void transition

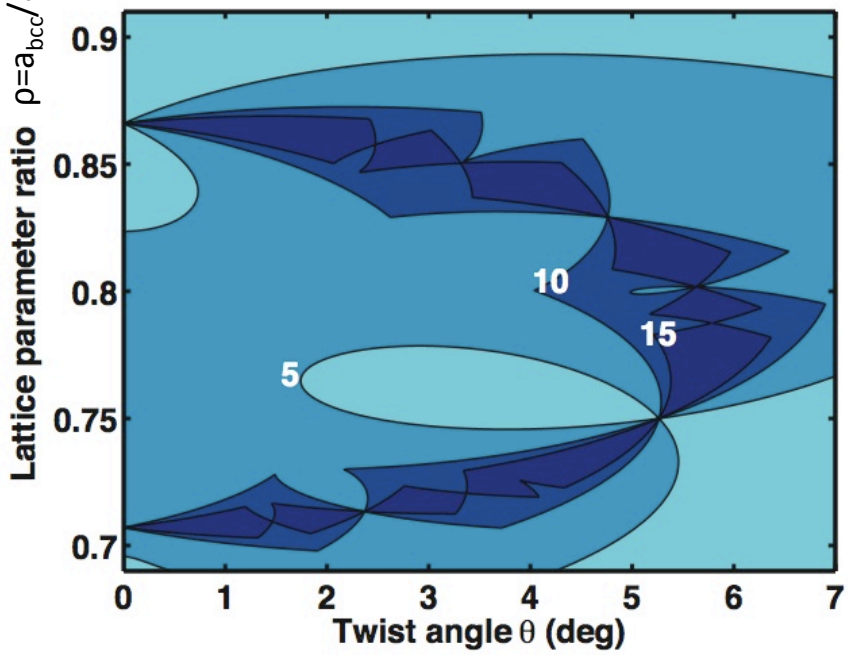


Criterion 2:

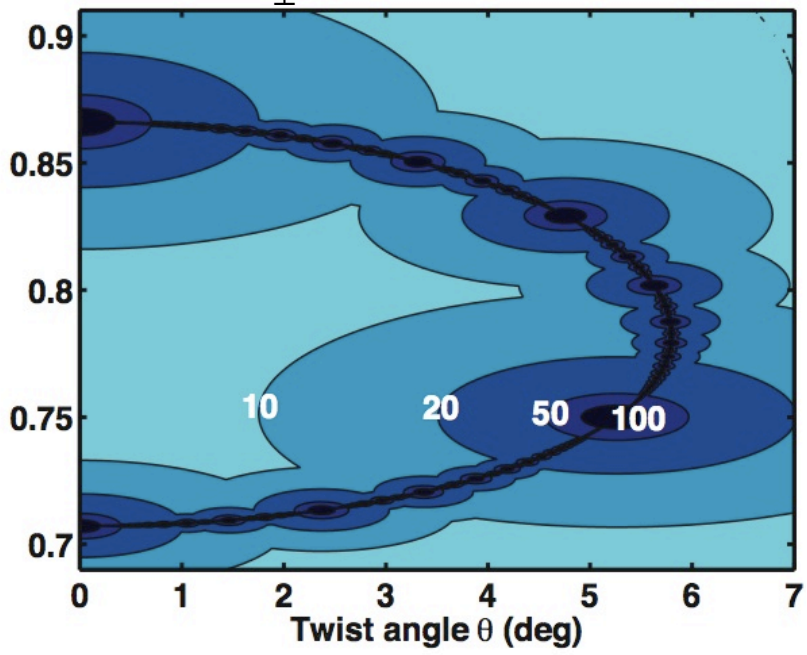
$$l_{\perp}^{lower} < l_{\perp} < l_{\perp}^{upper}$$

- $l_{\perp}^{lower}$: channels sufficiently far apart not to overlap
- $l_{\perp}^{upper}$: channels sufficiently close to getter He before it clusters

$l_{\min}$ (multiples of a_{fcc})



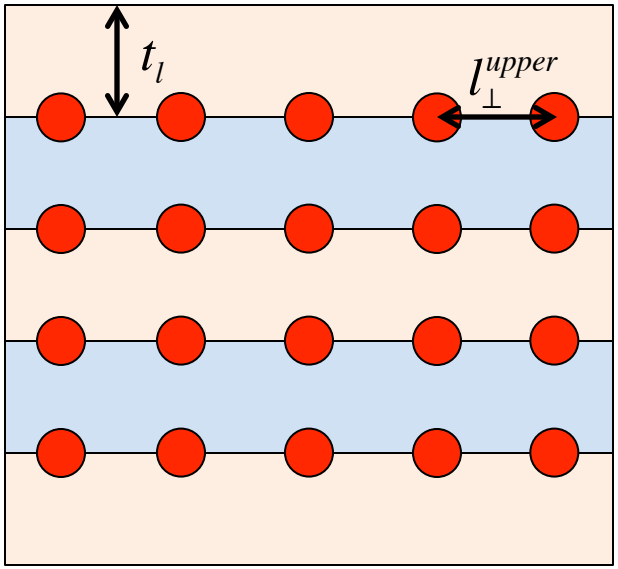
$l_{\perp}$ (multiples of a_{fcc})



D. V. Yuryev and M. J. Demkowicz, APL **under review** (2014)

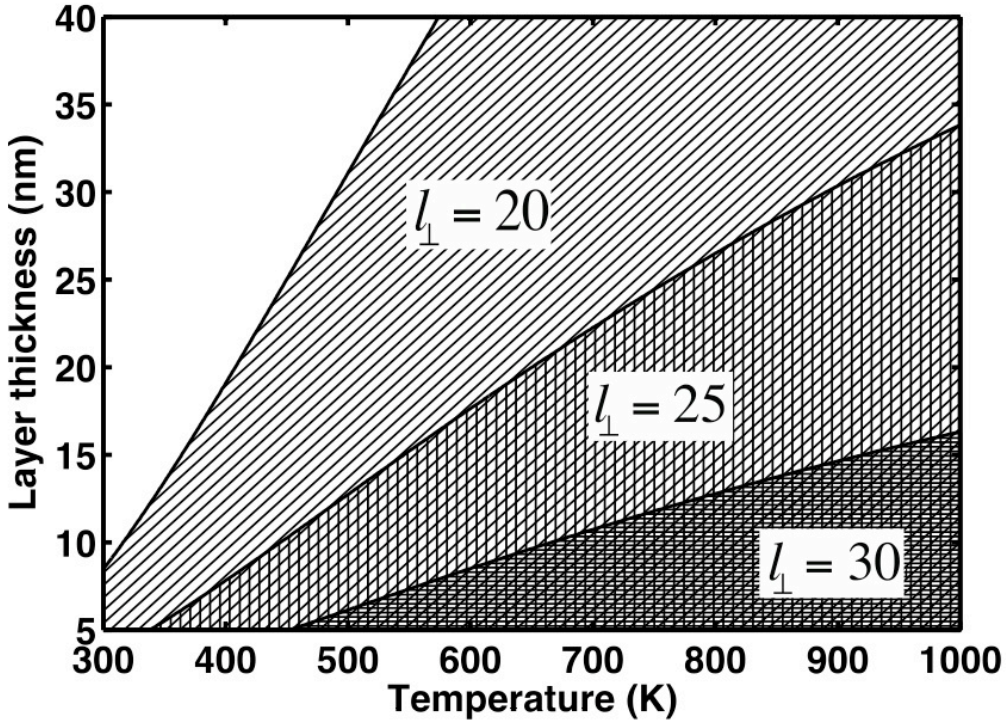
$l_{\perp}^{upper}$

Rate theory model for He clustering



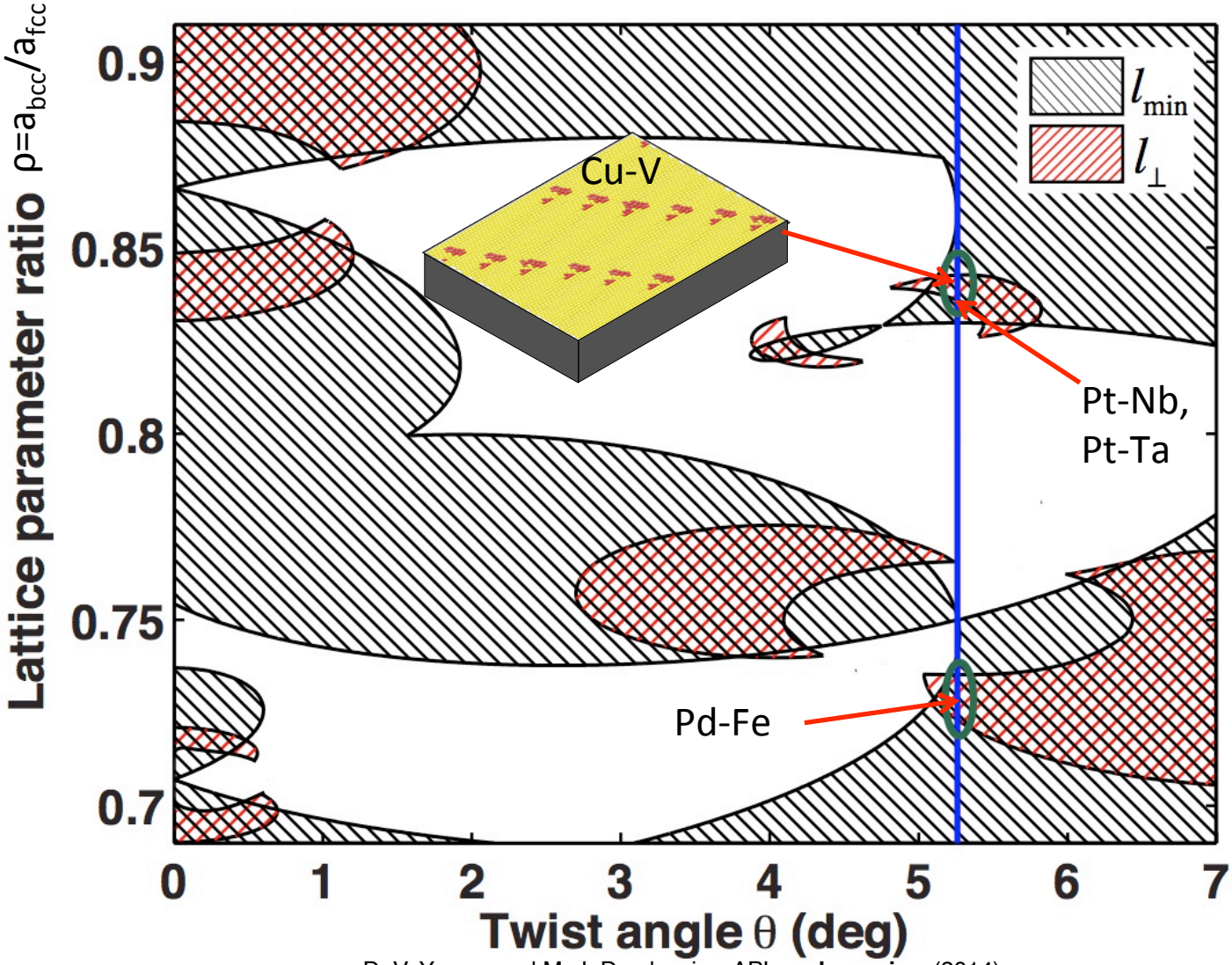
$$f_{bind} = \frac{R}{K_i} = l_{\perp}^4 \frac{K_i a_{fcc}^5}{6 D_{He}} < f_{bind}^{\max} = 10^{-2}$$

T-t_l envelopes where $f_{bind} < 10^{-2}$ for $K_0=10^{32}/m^2s$ and different values of $l_{\perp}$



We chose: $l_{\perp}^{upper} = 30$

Solution space

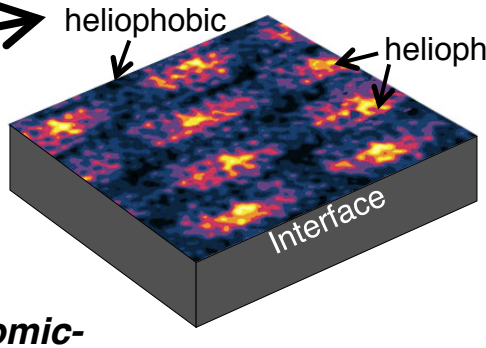


D. V. Yuryev and M. J. Demkowicz, APL **under review** (2014)

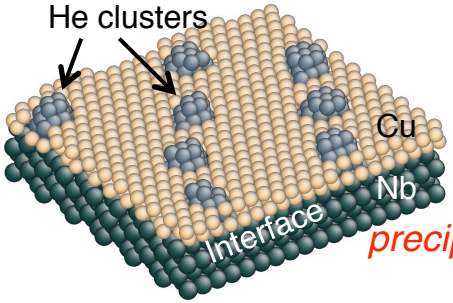
Sputter deposited CuV interfaces are good candidates for He outgassing

Designing interfaces that outgas He

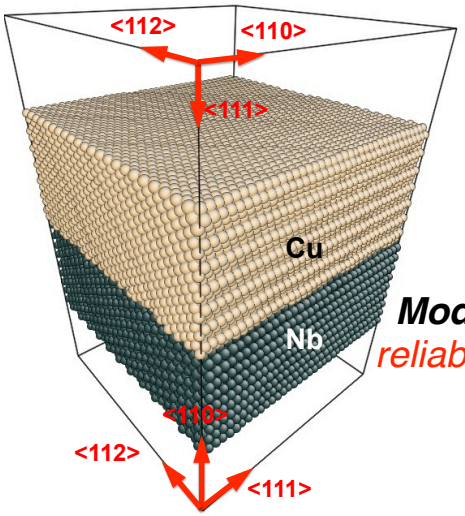
Forward problem: **multiscale modeling**



ROM1:
interface wetting

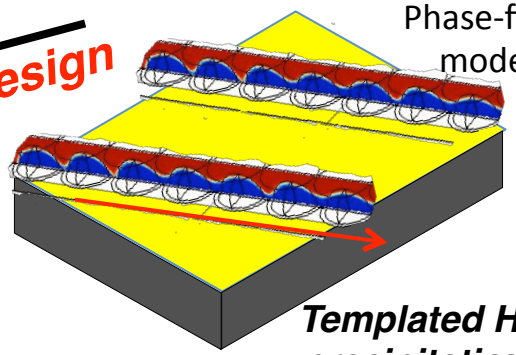


Atomic-level insight:
precipitation mechanism

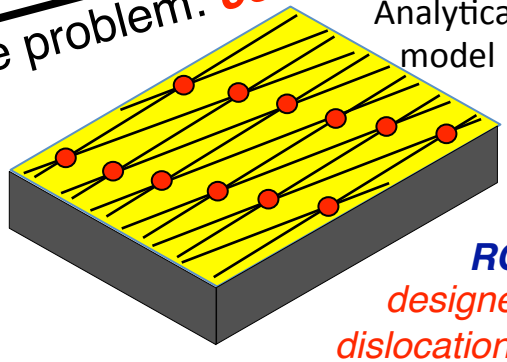


Model system:
reliable simulation

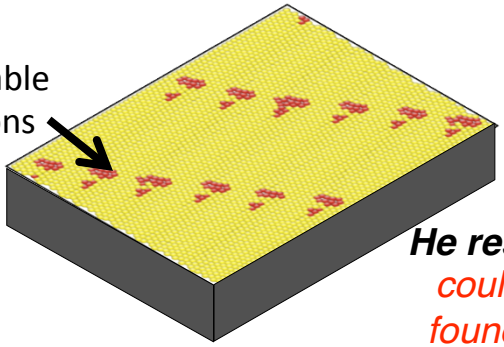
Inverse problem: **computational design**



Templated He precipitation:
enables outgassing



ROM 2:
designer interface
dislocation arrangement



He resistant interface:
could not have been found by "hit-or-miss"

We are here

Conclusions

- He precipitates on misfit dislocation intersections (MDIs) at interfaces in fcc/bcc metal layered composites
- Precipitation occurs by wetting of high energy regions of the interface, which are located at MDIs
- Layered composites containing interfaces that template He precipitation into continuous channels have been designed and are now being synthesized and tested
- Such composites may mitigate He-induced surface damage by providing paths for He outgassing while maintaining cohesion across the interface