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Emersion Project (AO2015): Nanoscale assembly of non-miscible metals by numerical engineering of their interfaces.

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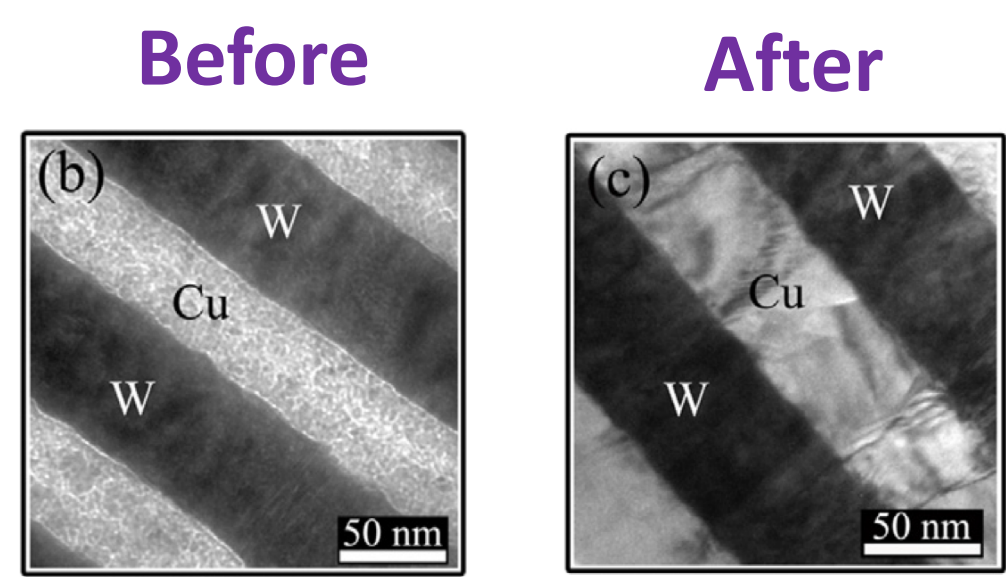
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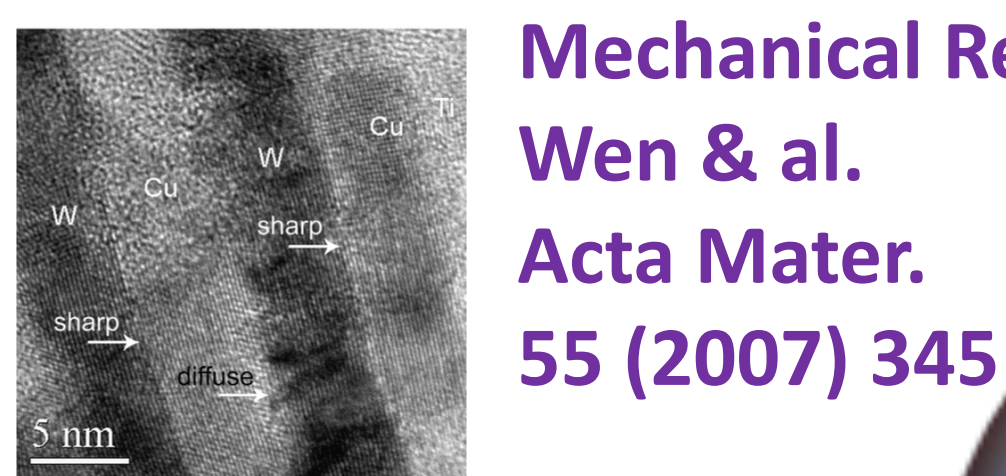
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Emersion Project (AO2015): Nanoscale assembly of non-miscible metals by numerical engineering of their interfaces.

Binary alloy systems undergo non-equilibrium phase separation in which domains of two stable phases grow from a thermodynamically unstable homogeneous phase as a result of quenching below a critical temperature.

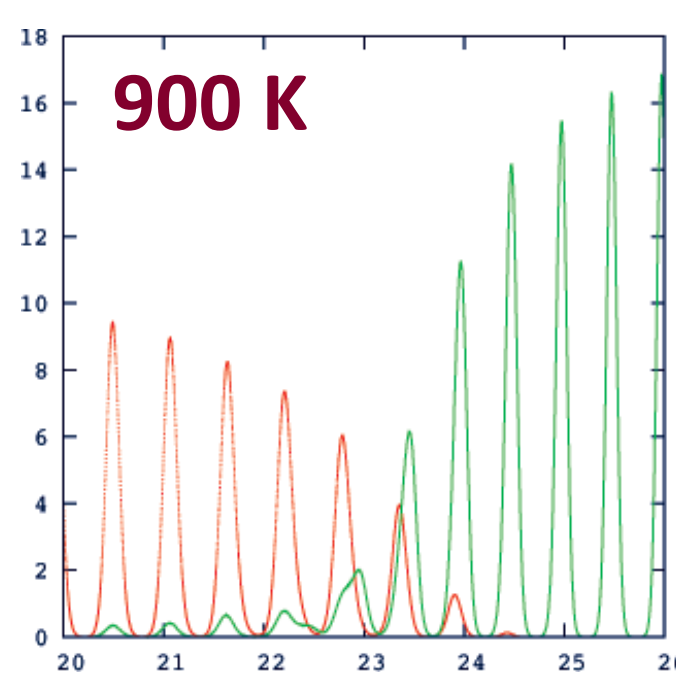
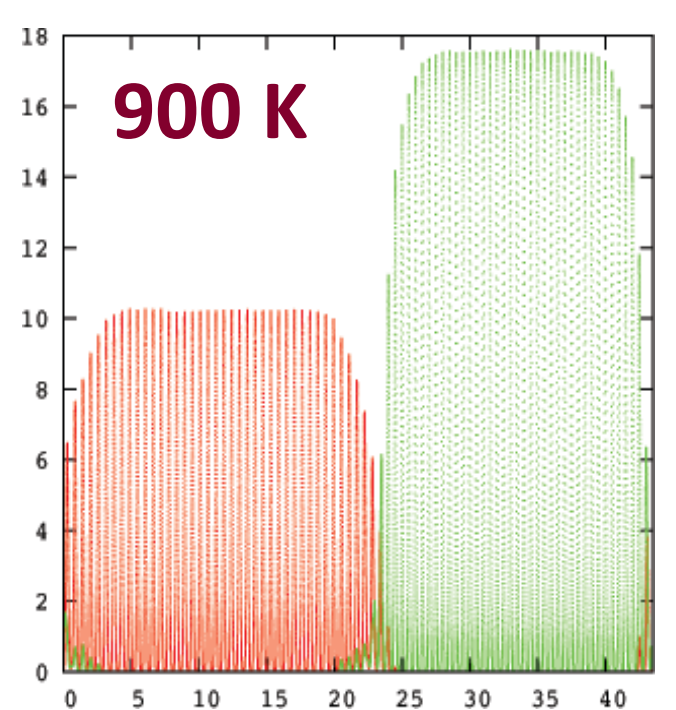


Radiation Resistance
Gao et al. JNM 413 (2011) 11



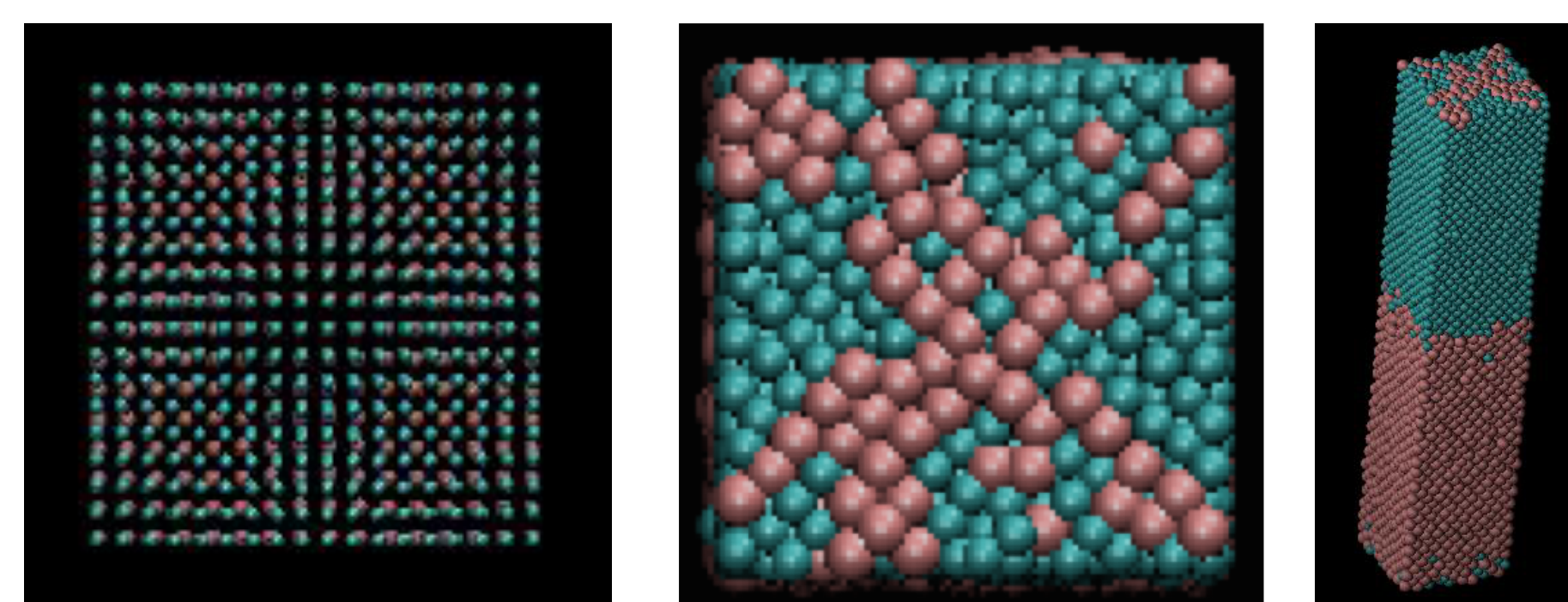
Mechanical Resistance
Wen & al. Acta Mater. 55 (2007) 345

Coupling between thermodynamic and defect kinetic of out-of-equilibrium systems affects the interface design and the final microstructural response of the system

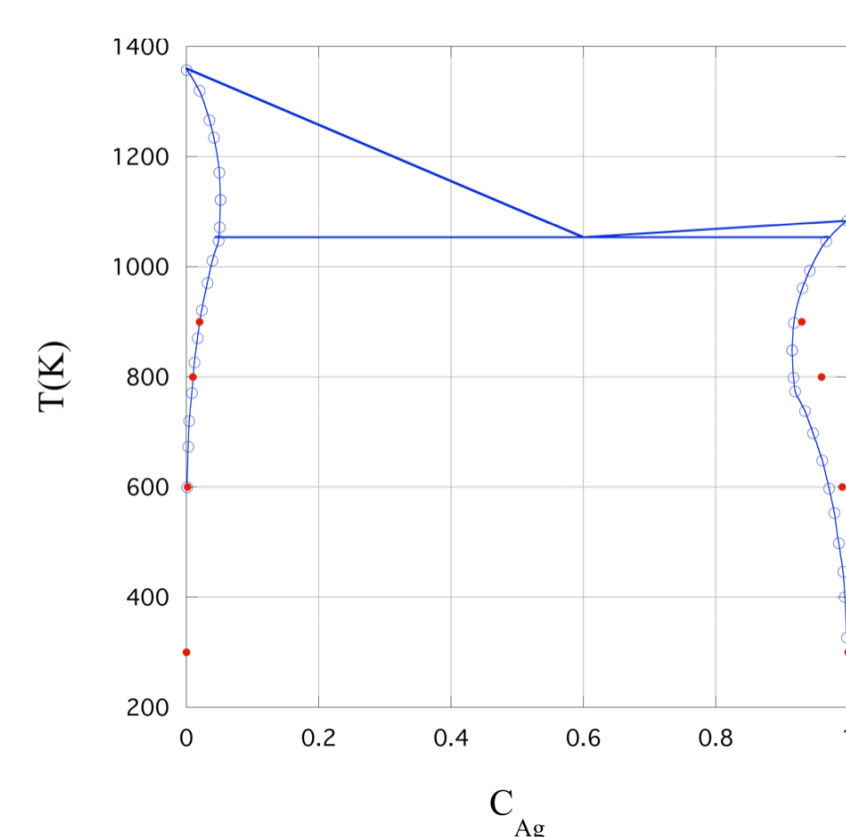


Energy minimization at $T > 0$ K

- Mixing occurs over several atomic layers at the interface
- Segregation proceeds in the absence of bulk diffusion (no vacancies) and is favored near the misfit dislocations
- The composition at the interface is asymmetric



Relaxed interfaces at $T = 0$ K & MD at $T = 900$ K



The GCMC model (dots) predicts consistently the asymmetry of the miscibility gap

Application & Motivation:

- Design of bulk layered systems with enhanced mechanical properties.
- Atomic scale welding between immiscible metals

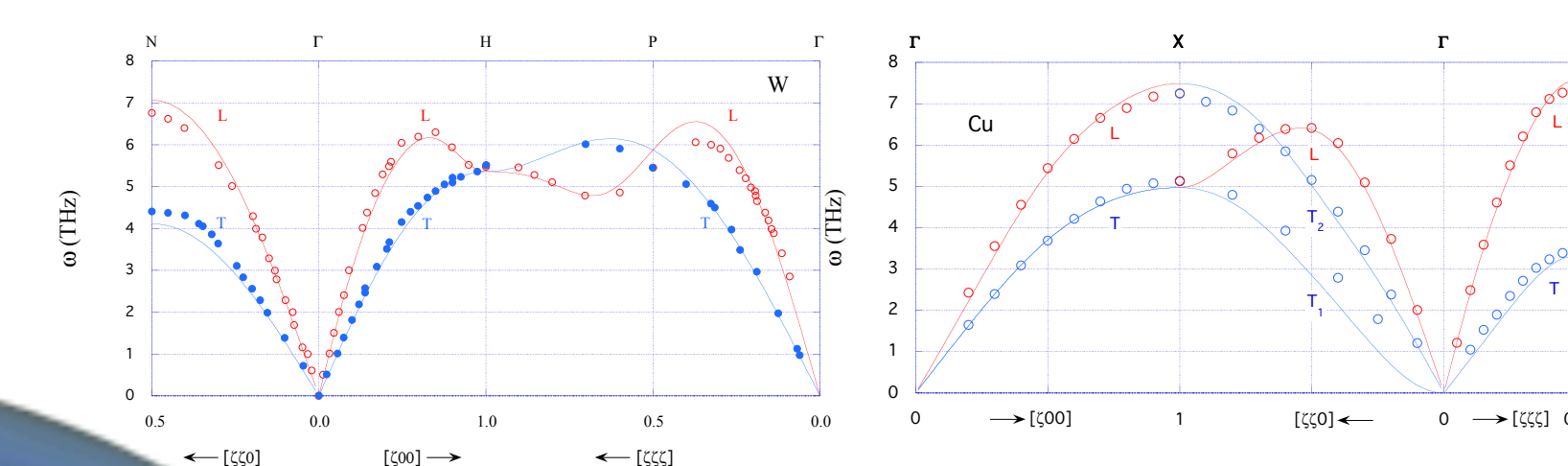
Tight-binding 2nd moment approximation

$$U_i^R = \sum_{\substack{j \neq i \\ \alpha \neq \beta}} A_{\alpha\beta} \exp \left[-p_{\alpha\beta} \left(\frac{r_{ij}}{d_{\alpha\beta}} - 1 \right) \right] \quad \alpha, \beta = Ag, Cu$$

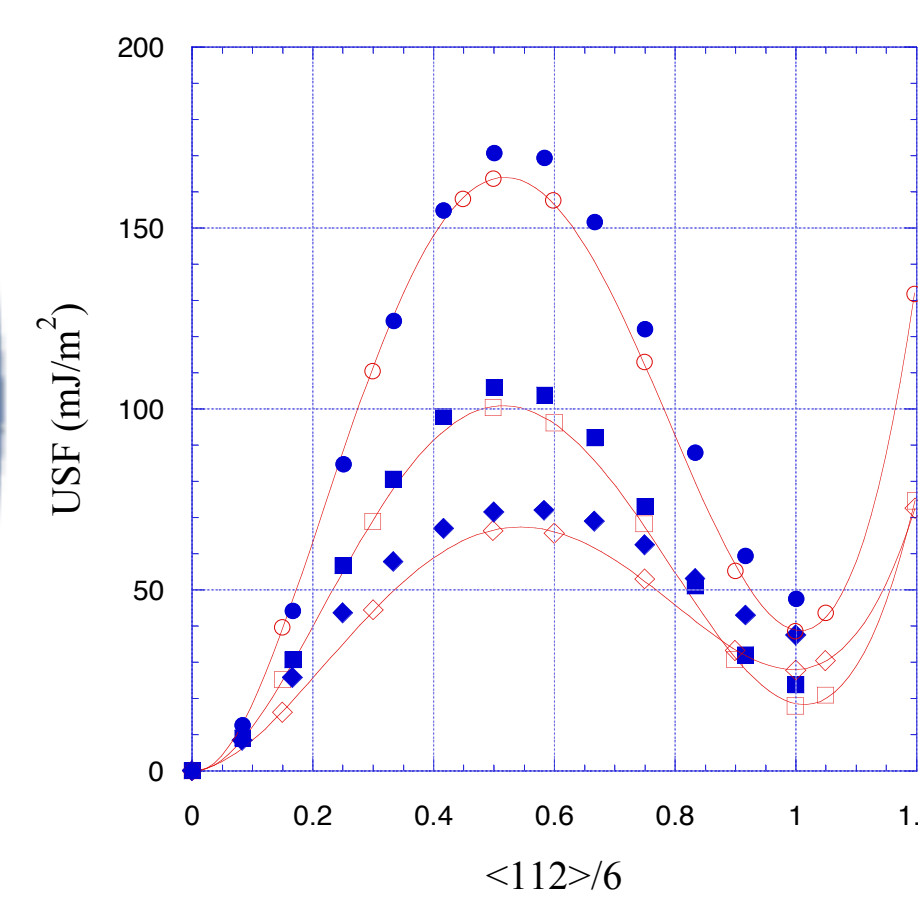
$$U_i^B = \sqrt{\sum_{\substack{j \neq i \\ \alpha \neq \beta}} \xi_{\alpha\beta}^2 \exp \left[-2q_{\alpha\beta} \left(\frac{r_{ij}}{d_{\alpha\beta}} - 1 \right) \right]}$$

	E_{coh}	a	B	C_{44}	C'
Cu	-3,50 (-3,50)	3,62 (3,62)	10,44 (10,44)	5,95 (6,03)	1,97 (1,91)
Ag	-2,95 (-2,95)	4,09 (4,09)	11,55 (11,55)	4,71 (5,45)	1,86 (1,85)

	A	p	q	ξ	ΔH_{dis} Cu(Ag)	ΔH_{dis} Ag(Cu)
Cu-Ag	0,11876	10,3615	3,02855	1,2996	0,40 (0,40)	0,28 (0,28)



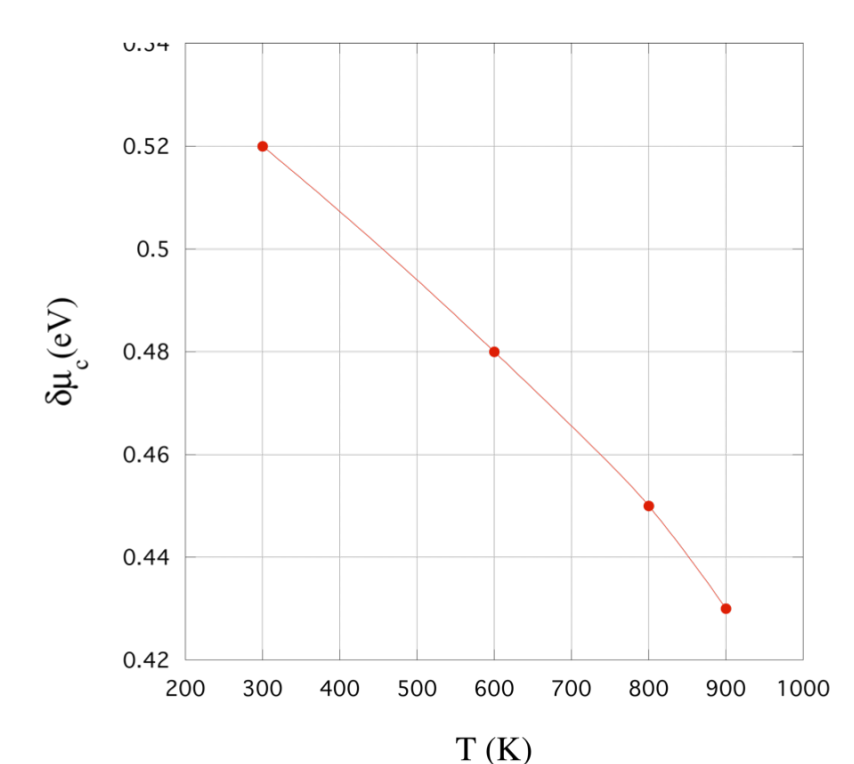
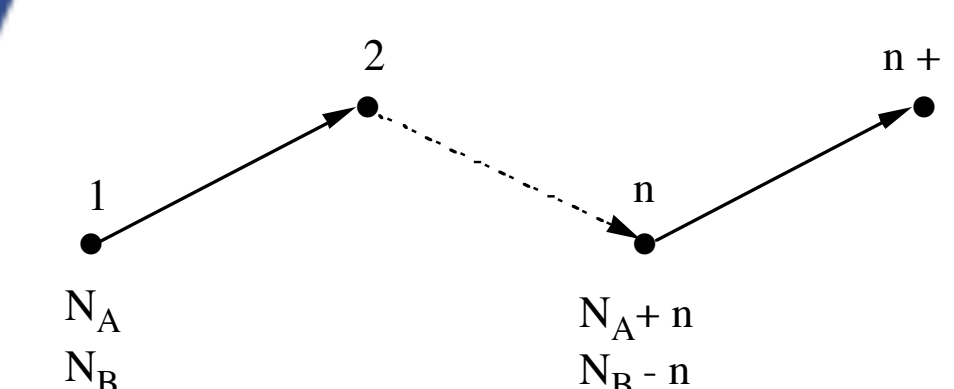
Assessment of the potential of the chemical elements of the binary systems



Benchmark the interatomic potentials against DFT and experiments.

Description of unstable defect configurations (NEB) to assess the transferability of the potential to out of equilibrium states

Step 2n	$\vec{r}_i = \vec{r}_i + \delta\vec{r}_i$
Step 2n+1	$\delta N = 0; \delta N_A = -\delta N_B = \delta n$ $P = \min[1, \exp(-\beta(\delta U - \mu_A \delta n))]$



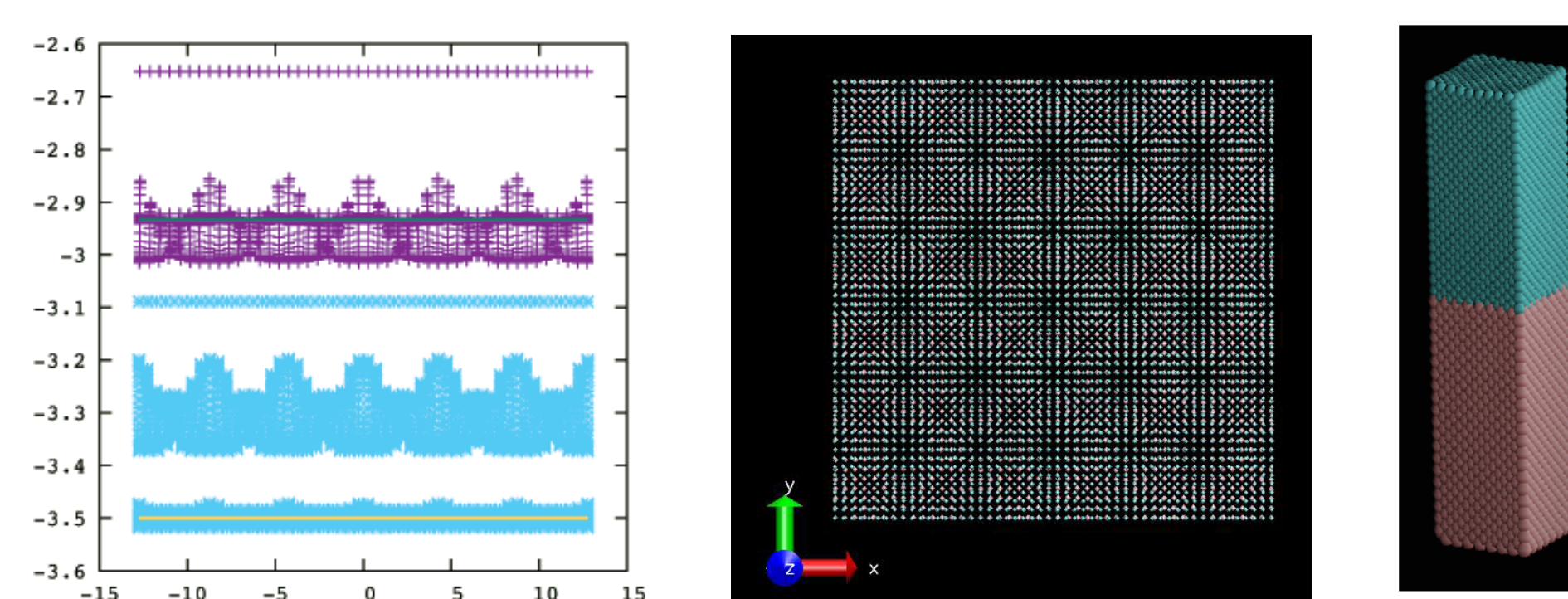
Semi-coherent interfaces

Teaming up thermodynamic and kinetics in immiscible metals to describe interfaces at the nanoscale.

Atomistic modelling of the interface.

Cohesion model using semi-empirical potentials.

Energy minimization (100) interface => Misfit dislocations at $T = 0$ K



$$\sigma_{zz} = 0 \quad \begin{array}{l} Ag : 23 \times 23 \times 5 (100) \text{ cells} - N_{Ag} = 10580 \text{ atoms} \\ Cu : 26 \times 26 \times 5 (100) \text{ cells} - N_{Cu} = 13520 \text{ atoms} \end{array}$$

GCMC: assessment of the potential in mixture systems at any T in their solid-state range.

The modeling of the effects related to the existing interactions between defects and interfaces of ultra-thin heterophase layers composed of two metals with positive enthalpy of mixing is the key to improve the understanding of the fundamental mechanisms that modify the physics of these systems in the region surrounding the interface. The objective of the project is to capitalize this knowledge to eventually develop systems with well defined interface characteristics, exceeding the performance of current materials (thermal barriers, coatings, ...). We team up theoretical models, numerical and experimental approaches to solve this problem, to accelerate the discovery of the most promising metal couples, to predict their behavior in deployment conditions (these conditions are intrinsically out-of-equilibrium), and to develop and validate predictive models that ultimately help us designing advanced materials that exploit the metastability of particular architectures and microstructures.