Phase field modeling of He precipitate networks on solid-state interfaces

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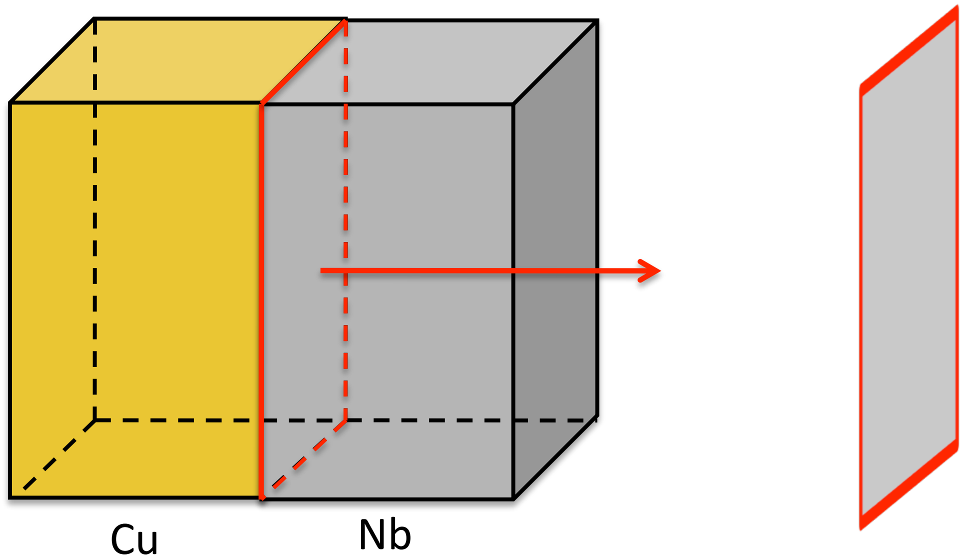
Wetting of solid state interfaces

Water droplets wetting the surface of a leaf and a glass pane



A solid state interface forms between blocks of Cu and Nb

Preferential He precipitation at high energy regions of the interface

1. A. Kashinath, A. Misra, and M. J. Demkowicz, "Stable Storage of Helium in Nanoscale Platelets at Semicoherent Interfaces," *Phys. Rev. Let.*, vol. 110, Feb 19 2013.
2. A. Kashinath, *(Unpublished)*

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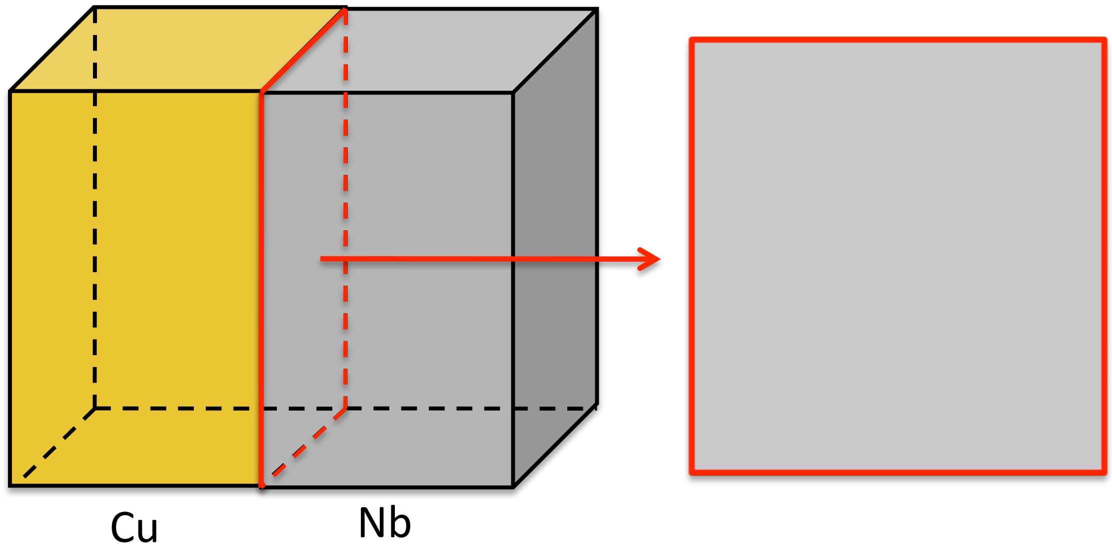

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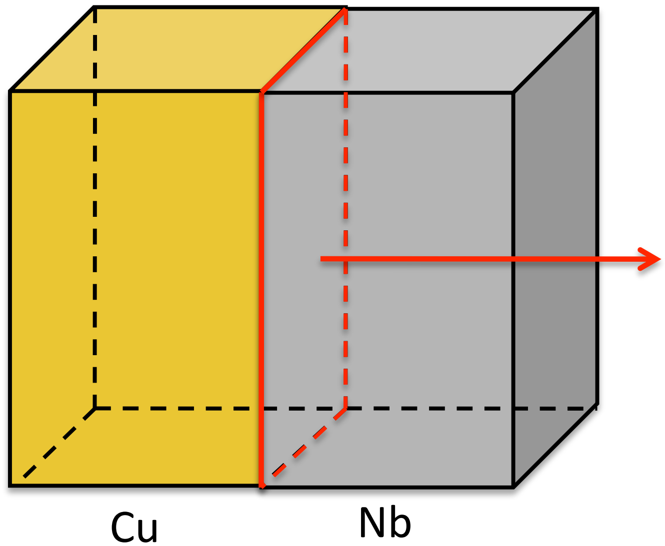

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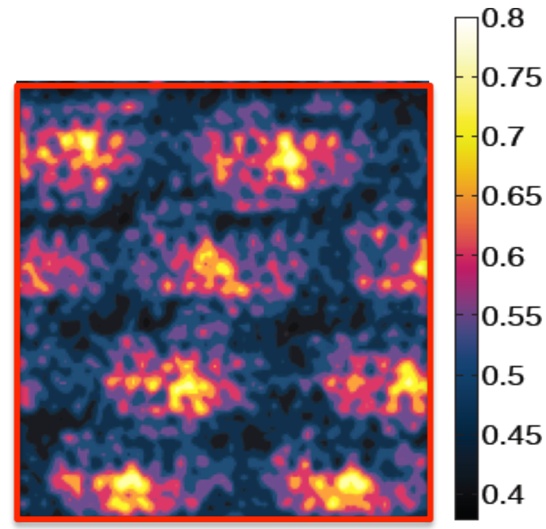

Location dependence of Υ_{CuNb}(J/m^2) at the interface plane [1]

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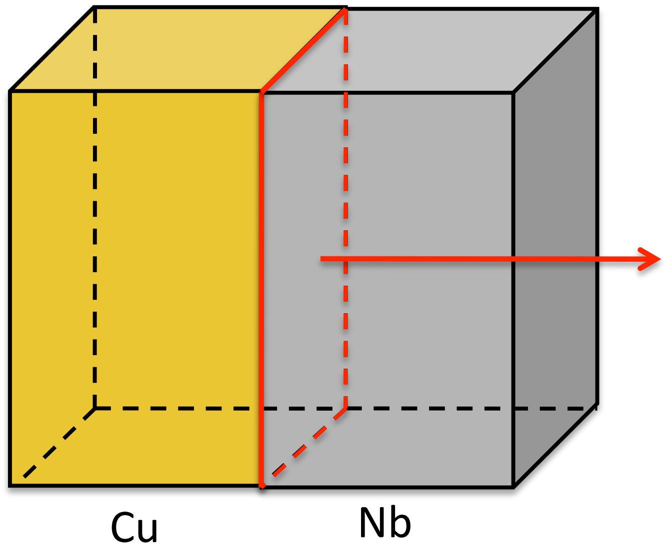

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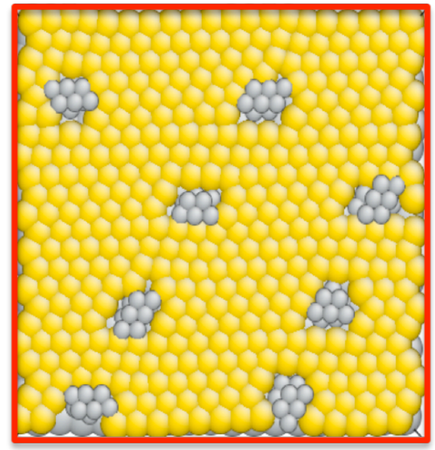

Atomistic simulation of precipitation of He in the Cu-Nb interface[2]

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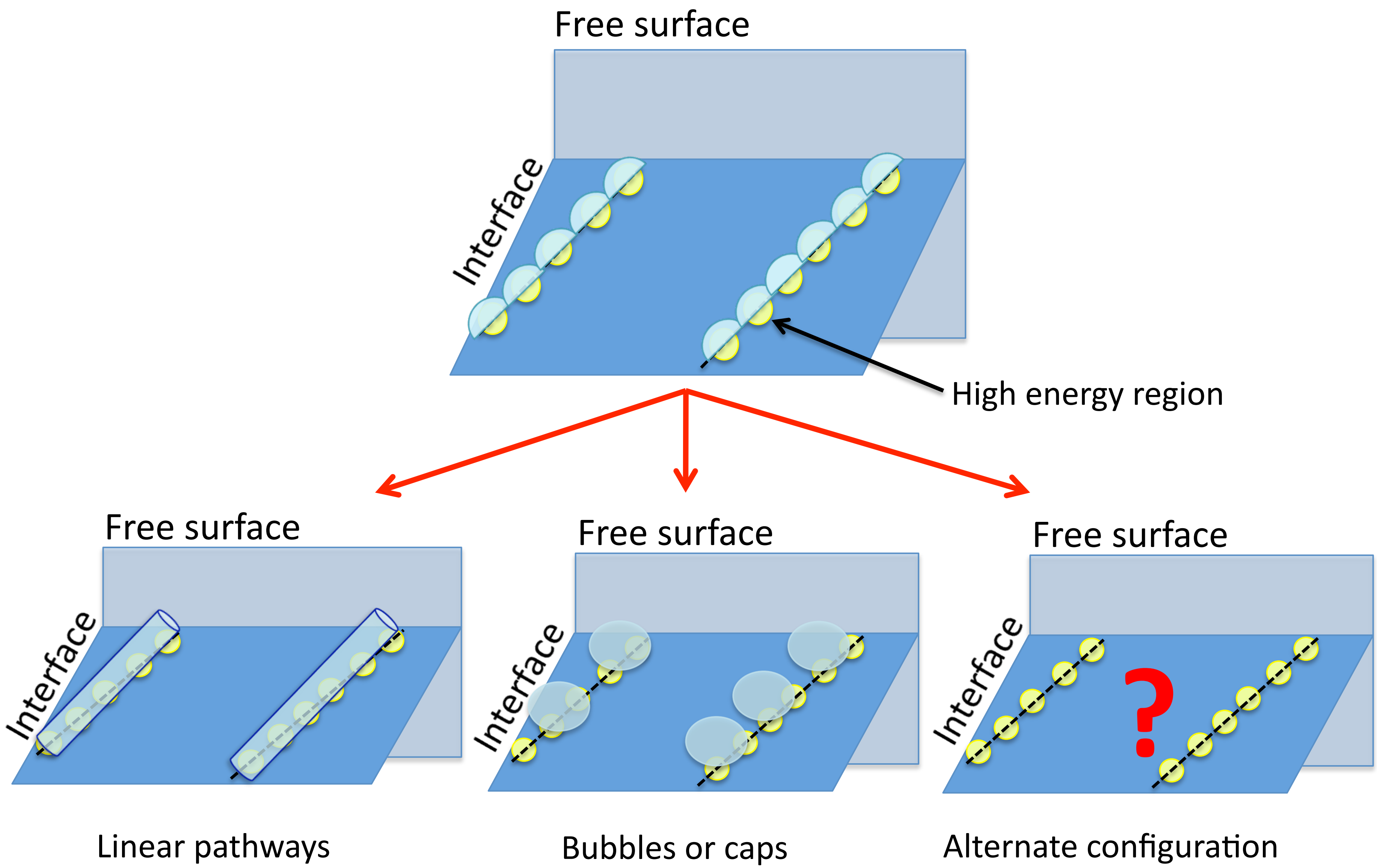
How do He networks behave?



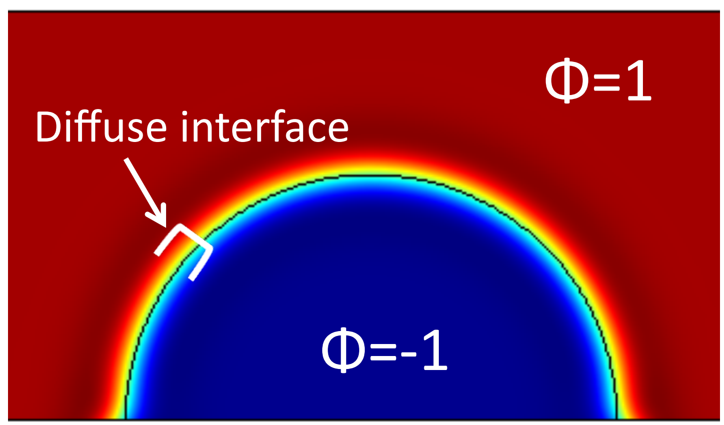
Phase field method

- Describes microstructures using continuum field variables (Φ) by solving Cahn-Hilliard Equation

$$\boxed{\frac{\partial \varphi_g}{\partial t} = \nabla \bullet M_g \nabla \frac{\delta F}{\delta \varphi_g}}$$

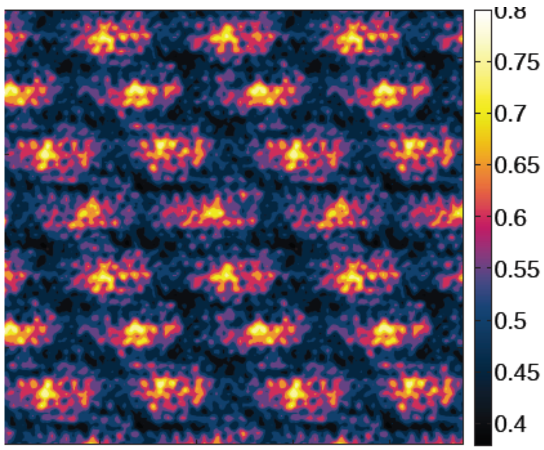
$$F = \int_V [\underbrace{f(\varphi_g)}_{\text{Bulk energy}} + \underbrace{\frac{\kappa}{2}\left|\nabla \varphi_g\right|^2}_{\text{Interface energy}}]$$

- Tracks evolution of complicated, arbitrary morphologies without explicitly tracking surfaces

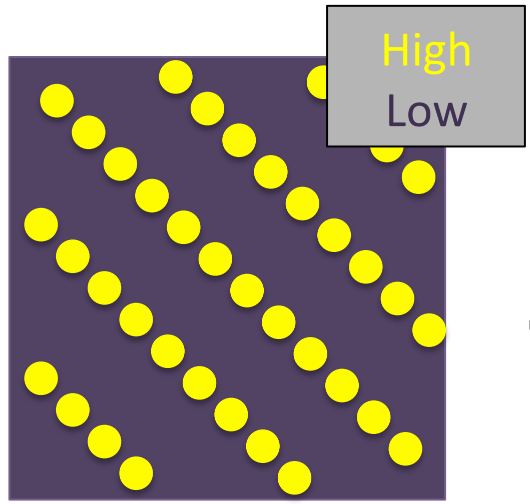


3. Millett, P.C. *et al.*, *Journal of Nuclear Materials,* **425,** 1-3, p. 130 (2012)

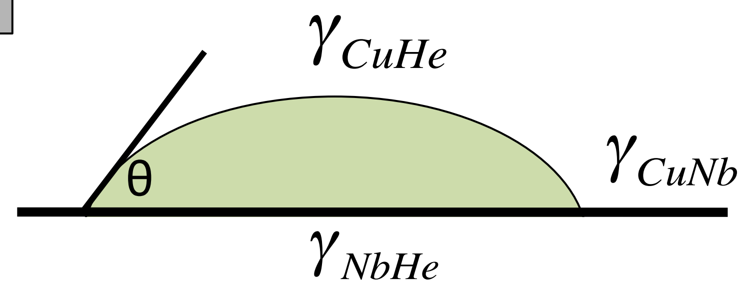
Building a COMSOL Model



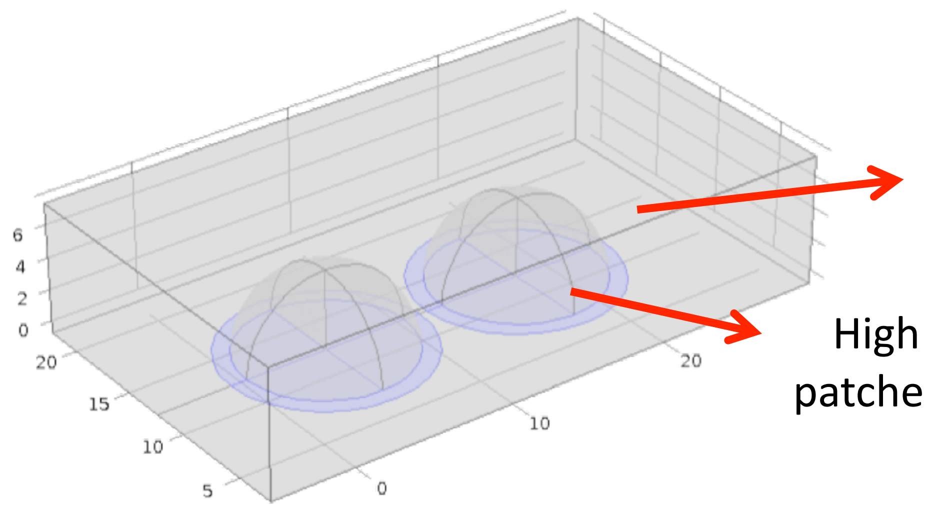
Location dependant interface energy



Simplified model of interface energy



$$\theta = \cos^{-1}\left(\frac{\gamma_{CuNb} - \gamma_{NbHe}}{\gamma_{CuHe}}\right)$$

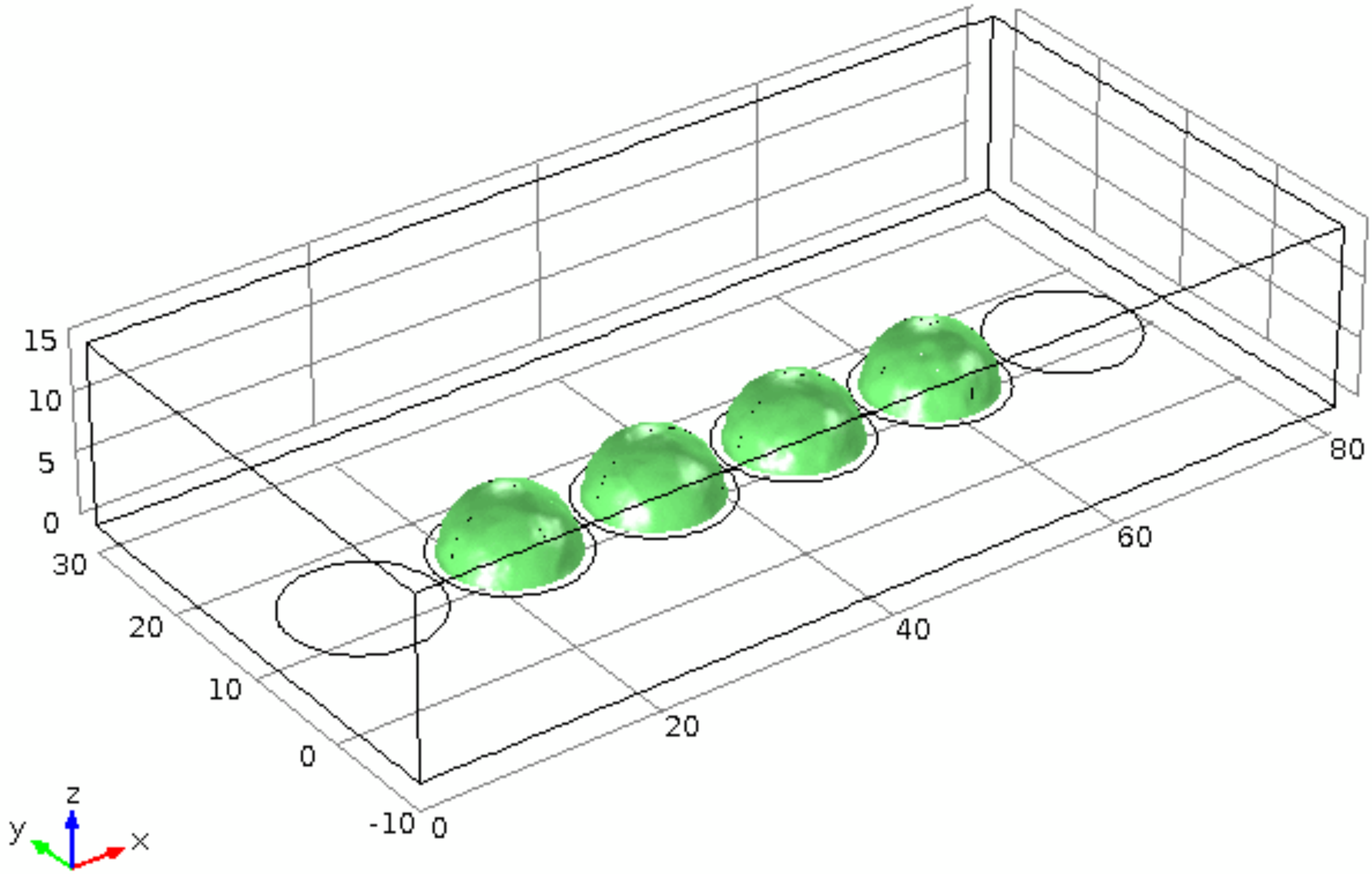


Low energy surface, large θ

High energy patches, small θ

4. Rosen, M. *Surfactants and Interfacial Phenomena.* pp. 243-276, (2004)

He network behavior at a single interface



Conclusions

- Constructed a phase field model in COMSOL for wetting of solid state interfaces by He

- Single line of high energy patches results in cap configuration

- Other geometries of high energy patches (i.e. multiple rows) need to be examined to achieve other He network geometries