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

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10/10/13

Funding: This work was supported by Center for Materials at Irradiation and Mechanical Extremes, an EFRC, funded by the DOE Office of Basic Energy Sciences
Wetting of solid state interfaces

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

A solid state interface forms between blocks of Cu and Nb

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

Preferential He precipitation at high energy regions of the interface

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

Preferential He precipitation at high energy regions of the interface

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How do He networks behave?

- Linear pathways
- Bubbles or caps
- Alternate configuration

Free surface

High energy region
Phase field method

- Describes microstructures using continuum field variables ($\Phi$) by solving Cahn-Hilliard Equation

\[
\frac{\partial \varphi_g}{\partial t} = \nabla \cdot M_g \nabla \frac{\delta F}{\delta \varphi_g}
\]

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

\[
F = \int_V \left[ f(\varphi_g) + \frac{K}{2} \left| \nabla \varphi_g \right|^2 \right] dV
\]

Bulk energy

Interface energy

Diffuse interface

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 \( \theta \)

High energy patches, small \( \theta \)

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