Phase Field Modeling of Helium Precipitate Networks on Solid-state Interfaces

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Abstract

Abstract: We describe simulations performed in COMSOL Multiphysics® of the precipitation of helium (He) on solid-state interfaces. The non-uniform precipitation of He at certain interfaces is a result of a heterogeneous energy distribution in the interface plane: He wets high interface energy ("heliophilic") regions but does not wet low interface energy ("heliophobic") ones [1]. Using a phase-field model, which we implement in the PDE mathematics solver in COMSOL, we simulate the growth, coalescence, and stability of He networks on planar interfaces with patterned energy distributions. Our work leads to interface design criteria that predict whether stable linear pathways of He precipitates may form at a given interface. These criteria may be used in the design of structural materials with increased resistance to He damage, which is a major concern in nuclear energy applications.

Results: In this study, a layer of a metal nanocomposite containing helium bubbles is modeled using a phase-field method. Figure 1 depicts the model. The top and bottom surfaces of the simulation cell are the interfaces that contain high energy patches (represented by circles) corresponding to a lower wetting angle than the rest of the interface, which has a higher wetting angle (and thus is of lower energy). On the high energy patches, a small amount of He is placed.

Two illustrative results are presented in Figures 2 and 3. In Figure 2, the high-energy areas have a wetting angle of 40°, while the low energy areas have a wetting angle of 150°. The He bubbles are grown through multiple study steps and the resulting He network is allowed to relax between growth steps. The final configuration is a stable He pathway that spans the entirety of the high energy patches initially wetted by He. Similar results are found for patches of "high wettability", i.e. wetting angles less than 70°. Figure 3 depicts an identical system to that of Figure 2, except the high energy patches have a wetting angle of 110°. In this system, a stable pathway does not form, but rather the He coalesces into one large bubble that spans just two high energy patches. Similar results are found for high energy patches of "lower wettability", i.e. wetting angles greater than 70°.

Conclusion: These preliminary simulations indicate that high energy patches that correspond to low wettability regions result in stable linear channels of He, while high energy patches that correspond to high wettability regions result in the coalescence of the He into a large He bubble. Additional factors that may influence He network morphology includes spacing between high energy patches and interactions between additional parallel lines of high energy patches.

These factors are currently under study.

Reference

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Figures used in the abstract

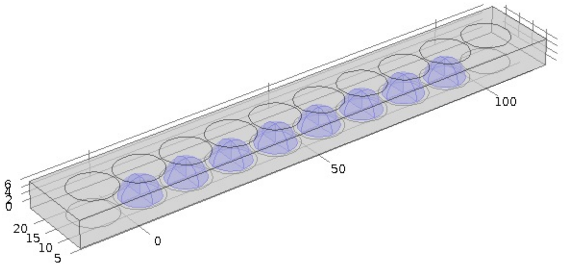

Figure 1: Initial system model. A small He bubble is placed on high energy patches.

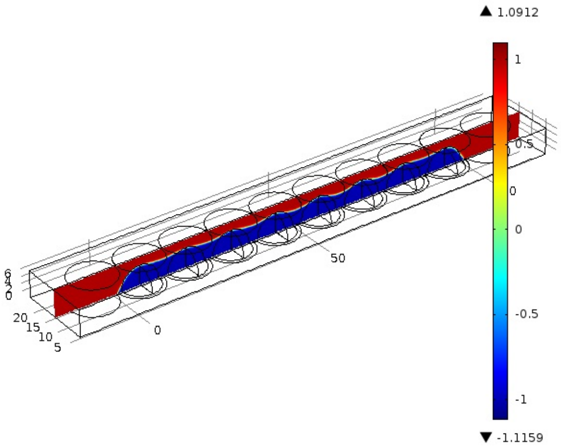

Figure 2: Final He network after He bubbles are grown and relaxed. The high energy regions have a wetting angle of 40d° and the rest of the interface has a wetting angle of 150°.

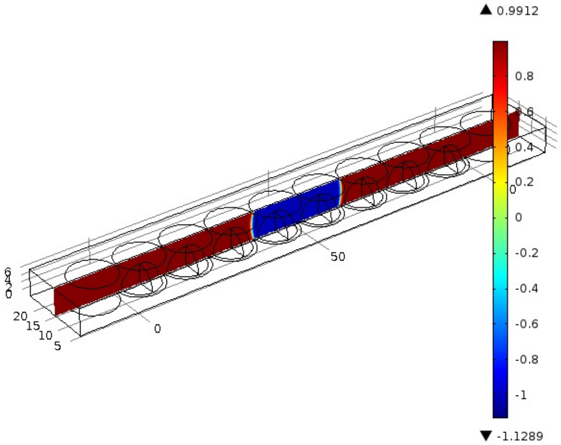

Figure 3