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Atomistic modeling of Helium effects on H retention in Fe

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Understanding the interaction between hydrogen (H) isotopes and helium bubbles in reduced activation ferritic-martensitic (RAFM) steels is vitally important to assess the potential for tritium retention in fusion blanket structures. Here, we report results from density functional theory calculations and molecular dynamics (MD) simulations of the interaction and diffusion of H near body-centered cubic (bcc) Fe - He planar interfaces, as well as near embedded nanometer scale helium bubbles as a function of helium to vacancy ratio (values between 0.5 and 1.5) for temperatures between 300 and 723 K. The density functional theory calculations indicate a strong trapping interaction for H at the Fe-He interface, with an average de-trapping energy of 0.9±0.1 eV. Likewise the MD simulations indicate that H prefers to reside at the interface between nanometer sized helium bubbles and the bcc Fe matrix, with only a small fraction of trapped H inside the bubble. Molecular statics simulations reveal that the de-trapping energy of hydrogen from a 2 nm He bubble at a density of 1.0 He/vacancy was 0.8 eV. The results of this modeling can inform a quantitative estimation of He trapping by helium bubbles needed to assess tritium retention in Fe-based fusion structural and breeding blanket materials.

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