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Ab Initio Investigation of He Bubbles at the $Y_2Ti_2O_7$-Fe Interface in Nanostructured Ferritic Alloys THOMAS DANIELSON, ERIC TEA, CELINE HIN, Virginia Tech — Nanostructured ferritic alloys are promising materials candidates for the next generation of nuclear reactors due to their ability to withstand high temperatures, high pressures, high neutron flux and especially, the presence of high concentrations of transmutation product helium. As helium diffuses through the matrix, large number densities of complex oxide nanoclusters, namely $Y_2Ti_2O_7$, Y_2O_3 and Y_2TiO_5, act as trapping sites for individual helium atoms and helium clusters. Consequently, there is a significant decrease in the amount of helium that reaches grain boundaries, mitigating the threat of pressurized bubble formation and embrittlement. In order to understand the helium trapping mechanisms of the oxides at a fundamental level, the interface between the nanoclusters and the iron matrix must be modeled. We present results obtained using density functional theory on the $Y_2Ti_2O_7$-Fe interface where the structure has been modeled based on experimental observations. Helium has been added along the interface in order to investigate the influence of helium on the structure and to obtain thermodynamic and kinetic parameters of helium along the interface.

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