Ab Initio Study of Helium Cluster Formation at the Vacancy in Palladium

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Helium generated from the tritium decay is one of the main reasons for macroscopic radiation damage in the structural componets of nuclear devices such as fission reactors and tritium storage media. In contrast to the hydrogen isotopes, helium with its closed electron shell is inert inside metals and tends to accumulate into bubbles which can cause deterioration of material properties and influence the lifetime of reactor components[1]. We perform *ab initio* calculations of helium atoms inside palladium using the density functional theory (DFT) and the projector augmented wave (PAW) method within the generalized gradient approximation (GGA). Electronic and structural properties including the binding energy, site preference, possible diffusion path and migration energy are analyzed based on the potential energy surface. We find a deep trapping energy for helium atoms at vacancies. We further study the helium-tritium interaction and the helium-helium interaction at the vacancy site. The results shed light on the early step in the formation of helium bubbles in the material.

[1] H. Trinkaus, and B.N. Singh, J. Nucl. Mater. **323**, 229 (2003).