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Hydrogen and Helium Trapping in Small Tungsten Vacancy Clusters: Insights into Fusion-Relevant Structural Damage from Molecular Dynamics

Intense irradiation in tungsten generates structural defects capable of trapping external gases, leading to macroscopic degradation. To predict this damage, an understanding of gas-defect interactions at the atomic scale is essential. In this study, we investigate the physical mechanisms governing hydrogen (H) and helium (He) trapping in small vacancy clusters, comprising 3 to 8 vacancies, within a body-centered cubic (BCC) tungsten lattice. The investigation is conducted using classical molecular dynamics simulations with an EAM/He interatomic potential. First, the geometries of vacancy clusters in the absence of gas atoms are analyzed to identify the most compact and energetically stable configurations at 0 K. Subsequently, gas atoms are introduced into the available octahedral and tetrahedral interstitial sites, and the systems are thermally equilibrated at 300 K. Based on these equilibrium configurations, average trapping energies are calculated to identify the preferred binding sites for each gas species and to assess their thermodynamic stability

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