ID: P1.24

Title: Grain-Boundary Diffusion and Segregation of Hydrogen in Iron: A Path-Integral Molecular Dynamics Study

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Understanding the H diffusion and transport in Fe and Fe alloys is extremely important because H severely degrades ductility and causes H embrittlement, which has been a serious materials problem. Interstitial atom migration in crystalline metals is widely believed to be more rapid along the grain boundary (plane defect) than through the regular lattice, since the free volume of the grain-boundary regions is greater than that of the lattice. Such a transport phenomenon is known as ``grain-boundary diffusion." In this study, we investigated the H diffusivity and the H-trapping effect at the several different grain boundaries (GBs) in body-centered cubic α-Fe, by performing path-integral molecular dynamics (PIMD) modeling and adopting an {\em ab-initio}-based potential. To characterize the {\em apparent} activation free energies for H diffusion across and along the GB plane at finite temperatures, we evaluated the differences between the free energies of the system for H at the interstitial or binding sites using the PIMD method. For example, from the obtained PIMD-based free-energy profiles for H diffusion at a Σ3{112} symmetric tilt GB, we confirmed that the H atom is strongly trapped in the vicinity of the GB; the PIMD-based values of the maximum binding free energy for H around a GB are 0.15 eV at 1000 K and 0.20 eV at 300 K, while its classical limit is 0.10 eV. Thus, the quantum nature of H is found to enhance the H-trapping effect in the vicinity of the GB as temperature decreases. Through the similar calculations, we found that the H atom is strongly trapped in the vicinity of the GB, and there is a high barrier for H diffusion both across and along the GB. Our results indicate that the GB planes do not act as fast pathways for H diffusion in α-Fe.