8P58 低放射化フェライト鋼中の炭化析出物中における空孔と水素同位体との相互作用に関する第一原理計算

Ab-initio Study of the Interaction between Vacancies and Hydrogen Isotopes in Primary Precipitates in Carbonized Precipitates of Reduced Activation Ferritic Steel F82H.

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A recent experiment for hydrogen retention in F82H steel by thermal desorption spectroscopy after deuterium-ion irradiation shows the primary precipitates of metal carbide such as $M_{23}C_6$ and MX might play a role of remarkable trap site for hydrogen isotopes. However, the trapping and diffusion behaviour of hydrogen isotopes is not understood well. Since it is well known that vacancies in crystals are major trapping sites for hydrogen, the purpose of this study was to theoretically understand fundamental feature of the interaction between vacancies and hydrogen in carbides by density functional theory (DFT) calculations.

The interstitial sites of the H atom in the VC crystal are situated near the center of the triangle formed by the V atoms and are strongly covalently bonded to the neighboring C atoms. Such chemical bonding states could explain the increased hydrogen solution energy in the VC crystal. The method of determining the saddle point directly by structural optimization with appropriate selection of the initial positions of hydrogen atoms is an effective method to derive the diffusion path and migration energy.

The H atoms in the C vacancy in the VC crystal are bound to the surrounding Cr atoms by relatively weak covalent forces and Coulombic attraction, and up to four H atoms are trapped. In the case of the Cr vacancy, H atoms are strongly covalently bonded to neighboring C atoms as well as the interstitial H atom, trapping up to six H atoms.

Four types of Cr vacancies in addition to the C vacancy can exist in $Cr_{23}C_6$ subjected to displacement damage under irradiation. On the whole, the H atoms in the vacancies in $Cr_{23}C_6$ have a weak bonding force with the Cr atom but a strong repulsive force with the C atom. As a result, no H atom is trapped in the Cr(4a) vacancy, and H atoms are trapped only at a distance from the C atom in the Cr(48H) and Cr(32f) vacancies. The Cr(8c) and C vacancies are relatively far from the C atoms and have higher hydrogen trapping energies. Especially, the Cr(8C) vacancy traps up to four hydrogens owing to its large volume.