§10. Super-saturated Hydrogen Effects on Radiation Damages in Tungsten

Kato, D., Muroga, T.,
Iwakiri, H. (Univ. Ryukyus),
Watanabe, Y. (JAEA),
Morishita, K. (Kyoto Univ.),
Ferro, Y. (Aix-Marseille Univ.)

Tungsten is a prime candidate as the divertor material of the ITER and DEMO reactors, which would be exposed to unprecedentedly high-flux plasmas as well as neutrons. For a better characterization of radiation damages in the tungsten under the divertor condition, we examine influences of super-saturated hydrogen on vacancies in the tungsten [1]. The present calculations based on density functional theories (DFT) reveal unusual phenomena predicted at super-saturated hydrogen concentration: 1) Strongly enhanced vacancy concentration with the super-saturated hydrogen concentration is predicted by a thermodynamics model assuming multiple-hydrogen trapping, i.e., hydrogen clusters formation, in the vacancies; and 2) DFT molecular statics analysis revealed that hydrogen clusters can prevent a vacancy from recombining with the neighboring crowdion-type self-interstitial-atom (SIA). This suggests that neutron damage effects will be increased in the presence of the hydrogen clusters.

The present DFT calculations were performed with VASP (Vienna Ab-initio Simulation Package) code. For the exchange-correlation energy functional in the DFT, Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) was used. Six valence electrons (6s and 5d) assigned to each tungsten atom and one electron of each hydrogen atom are explicitly treated in a field of residual ions, while core electrons of each tungsten atom are represented by a generalized pseudo-potential of the projector augmented wave method. The electron wave functions are expanded in terms of plane-wave basis. Reference bcc super-cells containing 54 and 128 tungsten atoms are used with the periodic boundary condition. The Monkhorst-Pack scheme was adopted for k-point sampling in the Brillouin-zone. Ionic configurations were relaxed by using a combination of the quasi-Newton method and conjugate-gradient method to the equilibrium configuration. Equilibrium volumes and bulk moduli as well as the total energy are determined by fitting computed energy-volume curves to Birch-Murnaghan's equation of state.

DFT results give fairly large binding energies between H and vacancies in tungsten indicating that the multiple-H trap by the vacancies forming VH_j complexes is energetically favourable. Figure 1 shows the H-trapping effect on the mono-vacancy concentration in tungsten calculated by using a statistical model based on the thermodynamics [2, 3]. Fractional abundance curves assuming the multiple trapping up to six H atoms are plotted. An extraordinary abundance of the vacancies is predicted in the equilibrium state due to the multiple hydrogen trapping. This is ascribed to strong lowering of the vacancy formation energy by trapping many hydrogen atoms.

The most stable SIA in tungsten is predicted by DFT calculations to be of 111-crowdion configuration. A mono-vacancy and a SIA in the 111-crowdion are automatically recombined, if the vacancy falls into a recombination radius around the major radius of the crowdion (5.4 Å for tungsten). We investigated the recombination in a case that the vacancy is occupied by an octahedron of six hydrogen atoms forming the VH_6 complex by DFT molecular statics. The present results reveal that there is a meta-stable state of the 111-crowdion with the VH_6 complex inside the recombination radius. The formation energy of the meta-stable state is 0.6 eV smaller than sum of the individual formation energies for the VH_6 complex and the 111-crowdion, indicating that the VH_6 complexes can trap the 111-crowdion. This effect of the hydrogen cluster implies that the radiation damage remaining after collision cascades by energetic primary knock-on atoms will be increased in the presence of the hydrogen clusters.

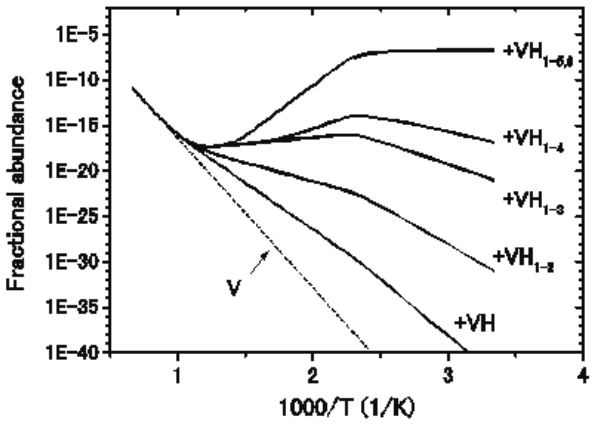

Fig. 1. Fractional abundance of VH_j complexes in tungsten as a function of inverse temperature. A fractional abundance of hydrogen atoms is assumed as 10^{-6}. The dashed line stands for the thermal vacancy.

1) Kato, D. et al.: FEC 2015 (Hotel Park Inn Pribaltiyskaya, St. Petersburg, Russia, 13-18 October, 2014) MPT/P7-36.
2) Kato, D. et al.: J. Plasma Fusion Res. Ser. **8** (2009) 404.
3) Fernandez, N., Ferro, Y., Kato, D.: Acta Materialia **94** (2015) 307.