IAEA FEC 2014

Contribution ID: **299** Type: **Poster**

Super-Saturated Hydrogen Effects on Radiation Damages in Tungsten under High-Flux Divertor Plasma Irradiation

Friday 17 October 2014 08:30 (4 hours)

Tungsten is a prime candidate as divertor material of ITER and DEMO reactors which would be exposed to unprecedentedly high-flux plasmas as well as neutrons. Radiation defects such as vacancies and impurities inherent in the divertor plasmas will play primary roles in enhancement of tritium retention in the tungsten. In this paper, for a better characterization of the radiation damages in the tungsten under the divertor condition, we examine influences of super-saturated hydrogen on vacancies in the tungsten. The present first-principle calculations based on density functional theories (DFT) reveal unusual phenomena predicted at super-saturated hydrogen concentration as follows.

1) Strongly enhanced vacancy concentration with the super-saturated hydrogen is predicted by a thermodynamics model assuming multiple-hydrogen trapping in the vacancies. This is ascribed to strong lowering of vacancy formation energies by trapping many hydrogen atoms.

2) The hydrogen trapping enhances vacancy clustering, also. Formation energies of di-vacancies are significantly lowered by trapping single hydrogen atoms. The calculated formation energies for the first nearest neighbor and the second nearest neighbor configurations almost coincide with an experimental value deduced from field ion microscopy.

3) DFT molecular dynamics revealed that hydrogen clusters can prevent a vacancy from recombining with the neighboring crowdion-type self-interstitial-atom. This suggests that neutron damage effects will be increased in the presence of the hydrogen clusters.

Country or International Organisation

Japan

Paper Number

MPT/P7-36

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Session Classification: Poster 7