Poster Session | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[PO-B2]Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-08]Diffusion of Point Defects on Tungsten Surface

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Hydrogen (H) / helium (He) retention in tungsten (W) and can significantly reduce the thermal conductivity and sputtering threshold of W, and at the same time, continuous bombardment with 14.1 MeV neutron can introduce Frenkel defects (composed of self-interstitial atoms (SIAs) and vacancies), which lead to a high concentration of W impurity. The surface deformation and blisters are observed experimentally in W, in which the surface morphology is relevant to the plasma fluence and surface directions [1-2]. The near-surface atomistic configuration is changed via diffusion of frenkel defects which is driven by heat and/or bubble loop punching process. Therefore, revealing the evolution mechanism of point defects on the W surfaces under H/He irradiation is crucial for W application in future fusion reactors.

We employ the first-principles and molecular dynamics simulation to calculate the energy barriers of single adatom (AD) and vacancy (VA) diffusion on the W (100), (110) and (111) surface. The diffusion paths of defects is determined by the dimmer method built in the SEAKMC code [3]. At least three diffusion paths with high energy barriers are found for both AD and VA on the (100) surface. However, only one path with low energy barrier of both AD and VA on the (110) surface are dominated throughout the diffusion process. Moreover, the diffusion of AD and VA on the (111) surface is investigated, in which the formation energies of different surface defects are biased. Nonetheless, the symmetry of the (111) surface will break spontaneously at the certain temperature and concentration of impurity through the thermodynamic calculation, and the morphology is in good agreement with the SEM images [1]. The work will help to understand the early stage of surface morphology evolution under irradiations or in the annealing process.

Keywords: tungsten, point defects, diffusion, surface

References

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