Molecular dynamics simulations of H/He interaction with W

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Tungsten (W) and W alloys are regarded as the most promising candidates for plasma facing materials (PFMs), which will be widely used in the next generation of fusion reactors. However, blistering in W-PFM induced by extremely high fluxes of low-energy hydrogen (H) and helium (He) ions irradiation will seriously influences the plasma stability and limits the lifetime of PFM.

Based on the W-H-He potential developed by ourselves, we systematically investigate the interaction between H/He and different kinds of defects in W using molecular dynamics (MD) calculations. We have demonstrated the physical origin of H-H repulsion and He-He attraction in W, and given the binding energy dependence of H/He, vacancy and self-interstitial atom to the H/He-vacancy cluster on H/He-vacancy ratio. The formation and growing process of H-vacancy clusters and He-vacancy clusters have been demonstrated, respectively. However, higher H concentration is needed to form the H-vacancy clusters, while the He-vacancy clusters tend to form spontaneously.

In addition, the diffusion behaviour of small He clusters was also investigated by means of mean squared displacements (MSDs). The diffusivities of He clusters generally decrease with the cluster size increasing, and generally rise with the temperature increasing. When the size of the clusters is greater than 5, the clusters hardly diffuse in W. However, it is possible for He atoms to separate from the clusters under high temperatures. He atoms can form several small clusters at low temperatures, but large clusters at higher temperatures. Thus, the He bubble formation will be greatly influenced by the temperature, which is due to the fact that the small clusters hardly diffuse at low temperatures, and become mobile at high temperatures.

MD simulations have been performed to investigate the H-He interaction in W. We firstly studied the H-He binding energies in small vacancy cluster with different vacancy cluster size and different H/He ratio, which will give us the basic information of H-He interaction behavior in W, the results show that the binding energies between H and He-vacancy cluster are positive value, which means He-vacancy cluster could trap several H atoms. Even if the He/vacancy ratio is higher, the H binding energy is still positive, but with a small value. Thereafter, MD simulations were performed to investigate the dynamical effects of H-He interaction with different vacancy concentration and different H/He ratio at different temperatures. The present simulation will benefit the understanding of H-He interaction in W, especially for the understanding of experiments.