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P4.114 Simulation study of evolution of helium bubbles in bulk W with vacancies

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Tungsten (W) is considered as a primary candidate material for plasma facing components, which endures high fluence plasma in future fusion reactor. Extremely insoluble helium(He) introduced into W exposed to high fluence He plasma tend to agglomerate into bubbles, which play a significant role in the radiation-induced micro-structural evolution and properties degradation. Therefore, to understand the relevant underlying physics, especially the micro-structural evolution process dominated by He defects interactions, is of fundamental importance to the development of plasma facing materials and components. Because in-situ observation is difficult by present experimental techniques, molecular dynamics (MD) simulations have been widely employed to study the atomic-level evolution process of He bubbles in W.
Atomistic simulations have been employed to investigate the atomic-level evolution process of He bubbles in bulk W. In this paper MD simulations were used to study the effects on the early stage of He bubbles formation with the He concentration up to 1at% and temperature (300-2100 K). The results show that the size of He-V clusters increases with increasing in the irradiation temperature and He concentration.The sizes of He bubbles obey the normal distribution. He defects interactions result in W interstitial atoms and vacancies with diferent types and sizes. The effects of He-induced and preexisting vacancies in W on the He bubbles evolution are compared. Furthermore, molecular statics(MS) simulations were firstly performed to study the growth of nano-sized He bubbles from energetic perspective. It is revealed that the formation energy of He bubbles is strongly related with its size and He/V ratio. These results also provide input parameters to larger scale simulations methods, such as in kinetic Monte Carlo methods and rate theory.

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