Interatomic potentials and displacement cascade simulations for W and W-based alloys

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Abstract: Tungsten (W) and W-based alloys are considered as the most promising plasma-facing materials for future fusion reactors due to their excellent performance. In this presentation, we will talk about some recent work in our group as following. First of all, a series of interatomic potentials for W, W-based alloys (such as W-Mo/Re/Ta/V) and W-V/Mo/Ta-He systems were developed for the displacement cascade simulations; then we performed systematic investigations on the displacement cascades in bulk W and W-base alloys with molecular dynamics simulations. Based on our potentials and molecular dynamics simulations, the displacement cascade database for W has been constructed, including seven typical PKA directions with 11 PKA energies ranging from 1 keV to 300 keV, totally 1700+ cascade events. The nucleation of C15 clusters has been observed in W bulk, and a new formation mechanism of <111> interstitial loops via the collapse of C15 clusters will be discussed. We also found that temperature gradient field will result in the directional diffusion of <111> dumbbell and 1/2<111> interstitial loop in W from the cold to the hot region, while stress gradient field will let the <111> dumbbell and 1/2<111> interstitial loop move toward the region where the stress is concentrated. The effects of transmutation elements, such as Re and Ta, on the generation and evolution of defects were analyzed. It was found that both the presence of Re and Ta atoms do not significantly affect the number of surviving defects, while the Re atom segregation has pinning effect on the mobility of defect clusters, and the presence of Ta inhibits the transition from <100> dislocation loops to 1/2<111> ones at high temperature. These results can provide important acknowledge for predicting the microstructural evolutions of W-based materials under radiation.

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