

Reduction of interstitial mobility by multicomponent alloying with transition metal elements in bcc W

We present the first-principles calculations of the defect energetics in W ternary alloys. Two different kinds of solute atoms make a pair and tend to strongly attract a W self-interstitial atoms, forming a solute-interstitial triple complex. The attractive interaction between a solute atom and a self-interstitial atom in W-based binary systems has been reported over the years, however, the calculation results presented here suggest that it can be even stronger in ternary systems. The attractive interaction works as the primary dissociation barrier for the triple defect complex, reducing the interstitial mobility. The dissociation energy needed to break the triple complex can be higher than the mono vacancy migration energy, and it changes the irradiated damage mechanism under the fusion environment where a number of point defects are created due to cascade collisions.