Direct Transformation of Stacking Fault Tetrahedrons to Voids under Irradiation in Pure Ni and NiCoCr Medium-Entropy Alloys

It is well known that vacancy clusters tend to agglomerate to stacking fault tetrahedrons (SFTs) rather than voids in most face-centered-cubic (fcc) metals. However, void swelling becomes one of the dominant effects of irradiation for materials when temperature is increasing. Recent researches observed that the SFTs coexisted with voids under irradiation in many fcc metals, which indicates an extraordinary relationship between SFTs and voids. In present study, molecular dynamics simulations have been performed to model void creation in pure Ni and NiCoCr Medium-Entropy Alloys (MEAs) with preexisting SFTs. It is observed that the void can be directly transformed from SFT under a single cascade simulation in pure Ni. However, in the NiCoCr MEA, the inhibited void transformation and the coexistence of SFTs and voids are both observed, as observed in experiments. The supersaturated vacancy atmosphere deriving from the collapse of SFTs, induced by displacement cascade simulations, could be the physical origin for void nucleation. The much lower stacking fault energy in NiCoCr MEA than that in pure Ni indicates that the SFT in NiCoCr MEA is more stable, which might be one of the major reasons for the inhibited transformation of SFT into voids in NiCoCr MEA.