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PROCEEDINGS

Formation of Stacking Fault Pyramid in Zirconium

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ABSTRACT

Zirconium alloys were widely used as fuel cladding in nuclear reactors. Stacking fault pyramid (SFP) is an irradiation-induced defect in zirconium. In this work, the formation process of SFP from a hexagonal vacancy plate on basal plane is studied by molecular dynamics (MD) simulations. The results show that, during the SFP formation from a basal vacancy plate, the $\frac{1}{2}[0001]$ (<*c*>/2) dislocation is firstly dissociated into two partial dislocations $\frac{1}{18}\langle 20\bar{2}3\rangle$ and $\frac{1}{9}\langle\bar{1}013\rangle$. The former one resides on the basal plane, while the latter one glides on the first-order pyramidal plane. The partials on adjacent pyramidal planes react further and form a partial dislocation on the pyramidal edge, i.e. $\frac{1}{9}[10\bar{1}\bar{3}]+\frac{1}{9}[0\bar{1}13]\rightarrow\frac{1}{9}[1\bar{1}00]$. A critical edge length of the initial vacancy plate is observed, below which perfect SFP is formed while above which truncated SFP is formed. The critical edge length increases with the increasing temperature. Under a compressive stress, the SFP collapses into an <*c*>/2 dislocation loop and then becomes a faulted loop. Under shear stress, the formation of SFP is facilitated, i.e. the critical edge length increases with the increasing shear stress. The current work is useful for understanding the irradiation effects in zirconium alloys.

KEYWORDS

Molecular dynamics simulations; stacking fault pyramid; zirconium

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