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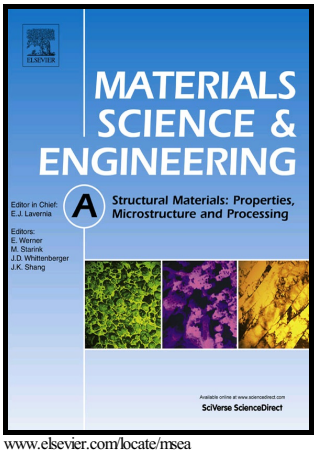

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Strain Rate Effect on Dislocation Climb Mechanism via Self-interstitials

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Abstract

The climb mechanism of an edge-dislocation is investigated by combining Transition State Theory and potential energy surface searching technique (an atomistic modeling framework named as ABC-T). As common point defects, self-interstitial-atoms (SIAs) and their agglomeration around dislocations in 'clouds' have complex and significant impact on the onset of metal plasticity. Reproducing atomic details of the interactions between SIAs and dislocations in a dynamic scenario is crucial for understanding the dynamic strain aging, and also the irradiation hardening. In order to describe the kinetics of SIA clouds in the vicinity of an edge dislocation, we choose a single SIA bi-dumbbell in body-centered-cubic (BCC) Fe in this study. The bi-dumbbell is absorbed completely to form a jog pair in our simulations at realistic laboratory strain rate. While at higher strain rate dislocation pinning with a stop-and-go manner is induced by incomplete absorption. As a transition state before the jog pair, a defect attaches to dislocation line and requires much higher activation energy than the thermal energy at room temperature to further evolve. Although more realistic picture of this interaction needs free energy calculation and dynamics trajectory to confirm different evolution pathways, our results offer a direct qualitative comparison between strain rates revealing the intrinsic difficulty of dislocation climb.

Keywords: Dislocation climb, Strain rate, Transition state theory, Effective activation barrier

1. Introduction