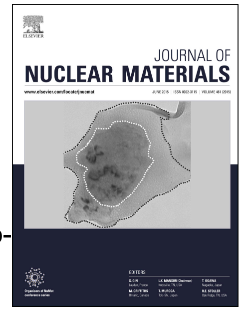

Atomistic study of hydrogen behavior around dislocations in α iron

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Abstract

Atomic-level studies have been performed to investigate the hydrogen behavior near a 1/2<111>{110} edge dislocation and a 1/2<111> screw dislocation in α iron. Molecular statics analysis has been carried out to determine the stress distributions and hydrogen binding energy around the dislocation cores. The results reveal that the hydrogen binding is more sensitive to the hydrostatics stress than the shear stress around the edge dislocation, while the shear stress plays a leading role on the hydrogen binding around the screw dislocation. In addition, nudged elastic band (NEB) calculations have been applied to explore different migration paths and the corresponding migration energy barriers of a single hydrogen atom at the dislocation cores. It is of interest to note that both edge and screw dislocations are not able to offer fast pipe diffusion of hydrogen atoms along the dislocation line, as normally considered. Instead, hydrogen atoms prefer to diffuse slowly along oblique paths crossing the edge dislocation line on the slip plane and spiral paths surrounding the screw dislocation line. Furthermore, molecular dynamics simulations have been performed to study the diffusion behavior of hydrogen at the dislocation cores, which verifies the results of NEB calculations.

Keywords: molecular dynamics, hydrogen, iron, dislocation, diffusion

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