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PROCEEDINGS

Theoretical Study on Hydrogen Diffusion Influenced Screw Dislocation Motion in Body-Centered Cubic Iron

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ABSTRACT

Hydrogen has the potential to be the clean energy solution to achieve the sustainable development goals (SDGs). However, from preparation to utilization, the hydrogen embrittlement can not be neglected. Hydrogen embrittlement occurs as a result of hydrogen affecting dislocations motion and cracks opening. Dislocation motion in hydrogen environment has not been clarified although several mechanisms have been proposed, including the hydrogen enhanced decohesion (HEDE), the hydrogen enhanced macroscopic ductility (HEMP), the hydrogen enhanced local plastic model (HELP), etc. It is essential to comprehend the underlying hydrogen-dislocation interactions that cause embrittlement. Also, dynamics of dislocation motion influenced by hydrogen in metals should be well understood.

Molecular dynamics (MD) simulations are performed in this study to reveal mechanism of the screw dislocation motion in body-centered cubic iron. An advanced neural network potential is used which describe iron-H binary system [1]. The simulation results suggest that hydrogen atoms instead of restricting screw dislocation, accelerate dislocation motion by reducing the activation barrier of kink formation. Moreover, a sophisticated numerical model describing coupled dynamics between hydrogen diffusion and screw dislocation motion as the function of applied stresses, temperatures and hydrogen concentrations is presented. The numerical computation results support the observations from MD results and more detailed information are obtained that the acceleration effect of hydrogen on dislocation motion is stronger when hydrogen concentrations increase. The results of MD simulations and numerical calculations are expected to illustrate the screw dislocation dynamics in hydrogen environment, providing core data for hydrogen embrittlement investigation.

KEYWORDS

Dislocation motion; hydrogen diffusion; iron; molecular dynamics simulation; numerical simulation

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