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Quantifying the effect of hydrogen on dislocation dynamics: A three-dimensional discrete dislocation dynamics framework

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Abstract

We present a new framework to quantify the effect of hydrogen on dislocations using large scale three-dimensional (3D) discrete dislocation dynamics (DDD) simulations. In this model, the first order elastic interaction energy associated with the hydrogen-induced volume change is accounted for. The three-dimensional stress tensor induced by hydrogen concentration, which is in equilibrium with respect to the dislocation stress field, is derived using the Eshelby inclusion model, while the hydrogen bulk diffusion is treated as a continuum process. This newly developed framework is utilized to quantify the effect of different hydrogen concentrations on the dynamics of a glide dislocation in the absence of an applied stress field as well as on the spacing between dislocations in an array of parallel edge dislocations. A shielding effect is observed for materials having a large hydrogen diffusion coefficient, with the shield effect leading to the homogenization of the shrinkage process leading to the glide loop maintaining its circular shape, as well as resulting in a decrease in dislocation separation distances in the array of parallel edge dislocations. On the other hand, for materials having a small hydrogen diffusion coefficient, the high hydrogen concentrations around the edge characters of the dislocations act to pin them. Higher stresses are required to be able to unpin the dislocations from the hydrogen clouds surrounding them. Finally, this new framework can open the door for further large scale studies on the effect of hydrogen on the different aspects of dislocation-mediated plasticity in metals. With minor modifications of the current formulations, the framework can also be extended to account for general inclusion-induced stress field in discrete dislocation dynamics simulations.

Keywords: Discrete dislocation dynamics; Hydrogen; Diffusion; Embrittlement

1. Introduction

Hydrogen (H) embrittlement is one of the most common types of environmentally induced damage that affects the reliable performance of structural materials in many applications [1, 2] [3] [4] [5, 6]. One of

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