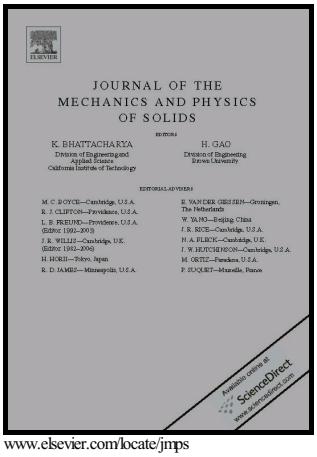

Dislocation-density function dynamics – an all-dislocation, full-dynamics approach for modeling intensive dislocation structures

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Dislocation-density function dynamics – an all-dislocation, full-dynamics approach for modeling intensive dislocation structures

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Abstract

It has long been recognized that a successful strategy for computational plasticity will have to bridge across the meso scale in which the interactions of high quantities of dislocations dominate. In this work, a new meso-scale scheme based on the full dynamics of dislocation-density functions is proposed. In this scheme, the evolution of the dislocation-density functions is derived from a coarse-graining procedure which clearly defines the relationship between the discrete-line and density representations of the dislocation microstructure. Full dynamics of the dislocation-density functions are considered based on an "all-dislocation" concept in which statistically stored dislocations are preserved and treated in the same way as geometrically necessary dislocations. Elastic interactions between dislocations in a 3D space are treated in accordance with Mura's formula for eigen stress. Dislocation generation is considered as a consequence of dislocations to maintain their connectivity, and a special scheme is devised for this purpose. The model is applied to simulate a number of intensive microstructures involving discrete dislocation events, including loop expansion and shrinkage under applied and self stress, dipole annihilation, and Orowan looping. The scheme can also handle high densities of dislocations present in extensive microstructures.

Keywords: Dislocation; plastic deformation; dislocation density; meso-scale simulation; precipitation strengthening

1. Introduction

In recent years, there has been considerable interest in the development of computational methods for crystal plasticity based on density representations of dislocations (Acharya 2001; Arsenlis et al. 2004; Yefimov and Van der Giessen 2005; Hochrainer, Zaiser and Gumbsch 2007; Alankar, Eisenlohr and Raabe 2011; Hirschberger et al. 2011; Puri, Das and Acharya 2011,