Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Coupling discrete dislocation dynamics with polycrystal plasticity

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ABSTRACT

Lebensohn et al. [1] recently introduced an alternative description of crystal plasticity based on a fast-Fourier transform (FFT) algorithm. The FFT approach solves for the equilibrium stress and strains under the constraint of strain compatibility for systems with periodic microstructures. As currently developed, the FFT model describes plasticity with a set of elasto-viscoplastic constitutive relations for deformation at the single-grain level. The EVP constitutive relation represents an average deformation and cannot describe the details of the dislocation microstructures, such as pileups near boundaries that can serve as stress concentrators or the development of correlations between dislocation structures and local grain orientations. To include such details, we are developing an approach to directly include dislocation evolution (as modeled with discrete dislocation dynamics simulations) within the FFT formulation of polycrystal plasticity. This discussion will focus on the linkage of the FFT formulation to dislocation dynamics simulations. In the FFT method, the local behavior of a heterogeneous medium is calculated from a convolution of the solution of an equivalent homogeneous problem and a polarization field that reflects the actual heterogeneity. One first calculates the Green's functions for the micromechanical fields of an equivalent linear homogeneous medium with eigenstrains. The eigenstrains represent any additional strains in an elasticity problem, e.g., plastic strains from the presence of dislocations [2]. The polarization field describes the heterogeneity of the medium, including any possible nonlinearity of the local mechanical behavior. The convolution integrals of the Green's function and the polarization field in real space can be reduced to simple products in Fourier space of the transform of the polarization field and the transform of the Green's function. The FFT algorithm is used to efficiently transform the polarization field to Fourier space and then to back-transform the product to real space. We will present a different formalism of dislocation dynamics in which the dislocations are represented by steps in the deformation tensor. The deformation tensor is a direct measure of the slip in the lattice caused by the dislocations and can be considered as an eigenstrain. Given the eigenstrains, the stresses are calculated via the FFT method, which has two advantages, the first being the computational efficiency of the FFT method. The second advantage is that the stress fields are based on anisotropic elasticity. Use of the FFT method introduces some uncertainties into the calculations arising from the FFT grid. In this discussion, we will review the method and discuss limitations and applications. This study is supported by the National Science Foundation at Iowa State University under Contract DMR-1308430. The authors acknowledge many beneficial discussions with Ricardo Lebensohn of the Los Alamos National Laboratory.

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