Available online at www.sciencedirect.com
ScienceDirect
International Journal of Plasticity 24 (2008) 1264–1276
INTERNATIONAL JOURNAL OF Plasticity
www.elsevier.com/locate/ijplas

Computationally efficient database and spectral interpolation for fully plastic Taylor-type crystal plasticity calculations of face-centered cubic polycrystals

Marko Knezevic [a], Surya R. Kalidindi [a,*], David Fullwood [b]

[a] Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA
[b] Department of Mechanical Engineering, Brigham Young University, Provo, UT 84602, USA

Received 16 September 2007; received in final revised form 5 December 2007
Available online 23 December 2007

Abstract

A new computationally efficient database approach to fully plastic Taylor-type crystal plasticity calculations is presented in this paper. In particular, we explore strategies that circumvent the need to repeatedly solve sets of highly non-linear, extremely stiff, algebraic equations with poor convergence characteristics that are inherent to these calculations. The suggested strategies consist of computing only once all of the needed variables in crystal plasticity calculations, storing them, and retrieving the values of interest according to the need in any specific simulation. An algorithm is presented here that facilitates this approach, and involves local spectral interpolation using discrete fourier transform (DFT) methods. The approach described here results in major improvements in the computational time over both the conventional crystal plasticity calculations and our previously developed spectral approach using generalized spherical harmonics (GSH). Details of this new approach are described and validated in this paper through a few example case studies.

Keywords: A. Microstructures; B. Crystal plasticity; B. Viscoplastic material; C. Numerical algorithms; Spectral methods

* Corresponding author. Tel.: +1 215 895 1311; fax: +1 215 895 6760.
E-mail address: skalidin@coe.drexel.edu (S.R. Kalidindi).

0749-6419/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijplas.2007.12.002

1. Introduction

Crystal plasticity theories aim to predict the anisotropic stress–strain response and the concomitant evolution of the underlying texture in polycrystalline metals at finite plastic strains. These theories have enjoyed tremendous successes in single phase high-stacking faulty energy cubic metals where the dominant mechanism of plastic deformation is crystallographic slip on specific slip systems (e.g. Asaro and Needleman, 1985; Beaudoin et al., 1995; Beaudoin et al., 1993; e.g. Bronkhorst et al., 1992; Delannay et al., 2002; Kalidindi et al., 1992; Mathur and Dawson, 1989; Van Houtte et al., 2002). However, even the implementation of the simplest of these theories in the simulation of bulk deformation processing operations on polycrystalline metallic samples demands major computational resources. Consequently, these theories are not yet widely employed by the broader metal working industry. There is a critical need to develop a highly efficient computational framework that can compete favorably, in both computational speed and resources, with the tools currently used by this industry. The added benefit, of course, is that these physics-based models will provide better insights into the evolution of the underlying microstructure in the work-piece and its associated macroscale anisotropic properties.

In recent years, a number of strategies have been explored to speed up the crystal plasticity calculations. These have included the Bunge–Esling approach (Bunge and Esling, 1984; Kalidindi and Duvvuru, 2005; Li et al., 2003), and the use of generalized spherical harmonics (GSH) for developing efficient spectral representations for functions involved in the crystal plasticity calculations (Kalidindi et al., 2006). While these techniques demonstrated tremendous potential, our recent work has revealed that the computation of the generalized spherical harmonics itself was the speed limiting factor with these approaches. One of the main advantages of using the generalized spherical harmonics (as opposed to other Fourier bases) was that they are already symmetrized to reflect the appropriate crystal and sample symmetries, and therefore provide a compact representation of the orientation dependence of any variable of interest in the crystal plasticity computations (Bunge, 1993).

In this paper, we report a completely new approach that has been observed to speed up tremendously the crystal plasticity calculations. In prior efforts (Kalidindi et al., 2006), our approach centered on seeking efficient spectral representations for the orientation dependence of various important variables in the crystal plasticity calculations (i.e. stresses, lattice spins, and total shearing rates in individual crystals). In this work, we observed that it is much more efficient computationally to simply store all of the important variables of interest on a uniform grid in the orientation space and subsequently employ a local spectral interpolation using Discrete Fourier Transform (DFT; also called Fast Fourier Transform or FFT) methods to recover the values of any of these variables for any orientation and deformation mode of interest. Details of this new approach are described and validated in this paper through a few example case studies involving crystal plasticity calculations. In the present study, we have confined our attention to fully plastic Taylor-type (full constraints) model calculations for fcc polycrystals with equal hardening of all slip systems. Application of this approach to more sophisticated constitutive models (such as elastic–viscoplastic models with latent hardening) and higher-order homogenization theories (such as self-consistent models or crystal plasticity finite element models) will be explored in future work.