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Crystal plasticity finite element simulations using a database of discrete Fourier transforms

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ABSTRACT

In recent work, we have demonstrated the viability and computational advantages of using a compact database of discrete Fourier transforms (DFTs) for facilitating crystal plasticity solutions in cubic polycrystalline materials subjected to arbitrary deformation paths. This new DFT database approach allows for compact representation and fast retrieval of crystal plasticity solutions, which is found to be able to speed up the calculations by about two orders of magnitude. In this paper, we present the first successful implementation of this spectral database approach in a commercial finite element code to permit computationally efficient simulations of heterogeneous deformations using crystal plasticity theories. More specifically, the spectral database approach to crystal plasticity solutions was successfully integrated with the commercial finite element package ABAQUS through a user material subroutine, UMAT. Details of this new crystal plasticity spectral database-FE approach are demonstrated and validated through a few example case studies for selected deformation processes on face centered and body centered cubic metals. The evolution of the underlying crystallographic texture and its associated macroscale anisotropic properties predicted from this new approach are compared against the corresponding results from the conventional crystal plasticity finite element method. It is observed that implementing the crystal plasticity spectral database in a FE code produced excellent predictions similar to the classical crystal plasticity FE method, but at a significantly faster computational speed and much lower computational cost.

1. Introduction

Crystallographic texture and its evolution are known to be major sources of anisotropy in polycrystalline metals. Highly simplified phenomenological models cannot usually provide reliable predictions of the materials anisotropy under complex deformation paths, and lack the fidelity needed to optimize the microstructure and mechanical properties during the production process. On the other hand, physics-based models such as crystal plasticity theories have demonstrated remarkable success in predicting the anisotropic mechanical response in polycrystalline metals and the evolution of underlying texture in finite plastic deformation. However, the use of crystal plasticity models is extremely computationally expensive, and has not been adopted broadly by the advanced materials development community.

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Crystal plasticity theories aim to predict the plastic anisotropy of polycrystalline materials by accounting for the fundamental mechanism of plastic deformation at the scale of the constituent single crystals by taking into account the details of slip system geometry in each individual crystal. To predict the response of the overall polycrystalline aggregate, one needs to use one of the homogenization models that can be classified based on the assumptions made with regard to the local interactions between grains, such as Taylor-type (also known as full constraints) Taylor (1938), relaxed constraints (Kocks and Mecking, 2003), LAMEL (Van Houtte et al., 2005), self-consistent (Lebensohn et al., 2004, 2007; Lebensohn and Tomé, 1993; Molinari et al., 1987), and crystal plasticity finite element (Bachu and Kalidindi, 1998; Kalidindi and Anand, 1994; Kalidindi et al., 1992; Kalidindi and Schoenfeld, 2000; Needleman et al., 1985; Peirce et al., 1982, 1983) models. The simplest and the most widely used approach is the Taylor-type model. In this method, the applied velocity gradient tensor at the microscale is assumed to be the same as the one applied at the macroscale (on the polycrystal). The macroscopic stress for the polycrystal is obtained by volume averaging the stresses inside the polycrystal. The Taylor-type model usually provides good predictions of the overall anisotropic stress–strain response and the averaged texture evolution for single-phase, high stacking faulty energy, cubic metals (Bronkhorst et al., 1992b). However, it usually lacks good predictions at the scale of individual crystals and it fails to show the development of heterogeneities within the grains (Bhattacharyya et al., 2001; Kalidindi et al., 2004; Van Houtte et al., 2005).

The most sophisticated and successful model that takes into account the local interactions between all grains in the sample is the crystal plasticity finite element method (called CPFEM) (Bachu and Kalidindi, 1998; Kalidindi and Anand, 1994; Kalidindi et al., 1992; Kalidindi and Schoenfeld, 2000; Needleman et al., 1985; Peirce et al., 1982, 1983). This approach uses the finite element method to find the response of the polycrystal by placing a finite element mesh over the grains such that each element represents one grain or a part of the grain. The crystal lattice orientations and material state variables are updated at every integration point in the finite element mesh by solving the crystal plasticity constitutive equations. In this approach, the equilibrium and compatibility conditions are satisfied using a weak form of the principle of virtual work. This model not only provides excellent predictions of the texture and anisotropic stress–strain response, but also predicts the local lattice rotations and heterogeneity of plastic deformation at the crystal level (Choi et al., 2011; Delaire et al., 2000; Erieau and Rey, 2004; Héripré et al., 2007; Kalidindi et al., 2004; Kanjarla et al., 2010; Musienko et al., 2007; Raabe et al., 2002; Sachtleber et al., 2002; St-Pierre et al., 2008; Zhao et al., 2008). This approach, however, requires very large computational resources because of the high computational time required to solve the highly nonlinear, numerically stiff, crystal plasticity constitutive equations at every integration point. This makes the use of CPFEM impractical when the size of the polycrystalline aggregate is very large. It should be noted that when using CPFEM for large-scale applications such as metal forming operations, a representative polycrystalline microstructure needs to be assigned to each integration point in the FE model. In this case, a suitable homogenization approach needs to be employed to obtain the mechanical behavior of the polycrystalline aggregate at each material point. The execution of such simulations becomes computationally prohibitive if the model consists of a large number of elements. Several approaches have been developed to improve the computational efficiency of these simulations (see, e.g., (Luo and Rousselier, 2014; Raabe and Roters, 2004; Raabe et al., 2004; Rousselier et al., 2012; Tikhovskiy et al., 2007; Zhao et al., 2008)). The recently developed crystal plasticity fast Fourier transform (CPFFT) method offers a promising alternative approach to CPFEM with periodic boundary conditions (Lebensohn, 2001; Lebensohn et al., 2008; Suquet et al., 2012). This approach has been shown to offer significant computational advantages through the use of an efficient FFT-based algorithm (Liu et al., 2010; Prakash and Lebensohn, 2009).

Several higher-order homogenization models have also been proposed to obtain the response of the polycrystal from the responses of constituent single crystals. The most widely used approach is the viscoplastic self-consistent model (Lebensohn et al., 2004, 2007; Lebensohn and Tomé, 1993; Molinari et al., 1987). The self-consistent approach assumes that each crystal acts as an ellipsoidal inclusion embedded in a homogenous effective medium that has the average behavior of the polycrystal. Therefore, the local interaction between each crystal and the neighboring crystals is taken in an average sense over the complete polycrystal. On the other hand, the LAMEL model considers the local interactions between immediate neighboring grains by careful examination of the stress equilibrium at the grain boundaries (Kanjarla et al., 2010; Liu et al., 2002; Van Houtte et al., 2002, 2006, 2005). Numerous studies have been published to compare the predictions from the different homogenization methods (see for example (Lebensohn et al., 2003; Van Houtte et al., 2002, 2005)). Van Houtte et al. (2002, 2005) provided quantitative comparisons between different homogenization methods including full-constraints, relaxed constrains, LAMEL, visco-plastic self-consistent, and CPFEM models. The CPFEM is usually used to validate any other homogenization model because it accounts for both stress equilibrium and strain compatibility (although in a weak numerical sense). However, one should note that the predictions from the CPFEM depend on the mesh density of the FE model. It is believed that for higher anisotropic materials and/or complex deformation processes, higher mesh resolution would be necessary in order to describe the microstructure and capture the intergranular heterogeneous strain and stress fields. However, this would incur much higher computational cost.

There is a critical need to speed up solutions to the crystal plasticity constitutive equations in order to use CPFEM within reasonable computation cost in a number of advanced metals development efforts (including various hexagonal metals such as Mg, Ti, and Zr alloys). Recently, our research group has established a new strategy to speed up the crystal plasticity computations at the crystal level through the use of a compact database of discrete Fourier transforms (DFTs) (Al-Harbi et al., 2010; Kalidindi et al., 2006; Knezevic et al., 2009, 2008). This spectral database is used to efficiently reproduce the solutions for the main functions of the crystal plasticity theory for any given crystal orientation subjected to arbitrary deformation mode. The spectral database approach has been successfully applied in both face-centered and body-centered cubic