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 ABAQUUS 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.

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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), self-consistent models (Lebensohn et al., 2004, 2007; Lebensohn and Tomé, 1993; Molinari et al., 1987), and crystal plasticity finite element model (Bachu and Kalidindi, 1998; Kalidindi and Anand, 1994; Kalidindi et al., 1992; Kalidindi and Schoenfeld, 2000; Needelman 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 stress gradient tensor at the microlayer 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 fault 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; Needelman 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; Erjeau 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 a 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 by 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
polycrystalline metals that deform by crystallographic slip. This approach was found to be able to speed up the crystal plasticity computations by two orders of magnitude compared to the conventional crystal plasticity model. Another special advantage of the spectral database is that trade-offs can be made by the user in terms of the desired accuracy and computation speed in any simulation through the selection of the truncation levels in the number of dominant DFTs used.

The spectral database described above has been demonstrated only for rigid–viscoplastic deformation, and has not been incorporated into FE simulation tools. The aim of the present work is to expound the advantages of the spectral crystal plasticity database in addressing the high computational cost associated with implementing the classical crystal plasticity theories into FE simulation tools for CPFEM simulations. More specifically, the spectral database approach is extended from rigid–viscoplastic into elastic–viscoplastic and successfully integrated with the commercial FE package ABAQUS through a user material subroutine, UMAT (ABAQUS, 2010). The new spectral database CPFEM described here is validated by comparing the predicted material mechanical response and texture evolution with the corresponding predictions from the conventional CPFEM for selected deformation processes. Application of this approach to large-scale applications such as metal forming operations will be explored in future work. It should be noted that the spectral database CPFEM described in this paper is applied here only to cubic metals that deform solely by slip without any twinning or phase transformation. Extensions to include other deformation modes will also be pursued in future work.

This paper is organized as follows. We briefly summarize in Section 2 the classical crystal plasticity framework used in this paper. We then summarize briefly the spectral database crystal plasticity computational scheme in Section 3. We proceed to demonstrate the necessary steps to integrate the DFT database approach for crystal plasticity computations with the FE package ABAQUS in Section 4. In particular, we illustrate how the crystal plasticity calculations using spectral databases are extended from rigid–viscoplastic behavior into elastic–viscoplastic deformation, and the details of the computation of the Jacobian required for implementing the spectral databases with any implicit FE tool. In Section 5, we validate the predictions from new spectral database CPFEM tools developed in this paper against the corresponding predictions from the classical CPFEM tools using a few selected case studies. We present conclusions of this work in Section 6.

2. Crystal plasticity framework

Crystal plasticity models are used in many applications because of their ability to relate the anisotropic behavior of polycrystalline materials to their microstructures (Asaro and Needleman, 1985b; Bridier et al., 2009; Bronkhorst et al., 1992a; Delannay et al., 2002; Garmestani et al., 2002; Goh et al., 2003; Hosford and Caddell, 1993; Kalidindi et al., 1992, 2004; Mayeur and McDowell, 2007; Mayeur et al., 2008; McDowell, 2010; Raabe et al., 2005; Raabe et al., 2001; Van Houtte et al., 2002). These physics-based constitutive equations not only provide better predictions of the anisotropic material response but can also capture the texture evolution in a polycrystalline sample subjected to finite plastic deformation. Some of the main details of crystal plasticity constitutive equations used in this work (Kalidindi et al., 1992) are summarized below.

For finite deformations, the total deformation gradient tensor $\mathbf{F}$ on a crystalline region can be decomposed into elastic and plastic components as $(\text{Asaro and Needleman, 1985a})$

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$$

(1)

where $\mathbf{F}^e$ contains deformation gradients due to elastic stretching and lattice rotation, while $\mathbf{F}^p$ denotes the deformation gradient due to plastic deformation. The constitutive equation in the crystal can be expressed as

$$\mathbf{T}^e = \mathcal{L}\mathbf{E}^e$$

(2)

where $\mathcal{L}$ is the fourth-order elasticity tensor, $\mathbf{T}^e$ and $\mathbf{E}^e$ are a pair of work conjugate stress and strain measures defined using the elastic deformation gradient tensor as

$$\mathbf{T}^e = \mathbf{F}^{-1}[(\det \mathbf{F})\mathbf{T}\mathbf{F}^{-T}], \quad \mathbf{E}^e = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I})$$

(3)

where $\mathbf{T}$ is the Cauchy stress in the crystal and $\mathbf{I}$ is the second-order identity tensor. The evolution of $\mathbf{F}^p$ can be expressed as

$$\dot{\mathbf{F}}^p = \mathbf{L}^p \mathbf{F}^p$$

(4)

where $\mathbf{L}^p$ is the plastic velocity gradient tensor given by

$$\mathbf{L}^p = \sum_\alpha \dot{s}^\alpha \mathbf{m}^\alpha_0 \otimes \mathbf{n}^\alpha_0$$

(5)

where $\dot{s}^\alpha$ is the shearing rate on the slip system $\alpha$, and $\mathbf{m}^\alpha_0$ and $\mathbf{n}^\alpha_0$ denote the slip direction and the slip plane normal of the slip system $\alpha$, respectively in the initial configuration. In the rate dependent formulation, the shearing rate on each slip system depends on the resolved shear stress $\tau^\alpha$ and the slip resistance $s^\alpha$ of that slip system. It can be expressed in a power-law relationship as $(\text{Hutchinson, 1976; Kalidindi et al., 1992; Needleman et al., 1985; Pan and Rice, 1983})$

$$\dot{s}^\alpha = \frac{s^\alpha}{\tau^\alpha}$$

(6)
where \( \dot{\gamma}_0 \) is the reference value of the shearing rate, and \( m \) is the strain rate sensitivity parameter. For most metals at room temperature, the value of \( m \) is usually taken to be very small (~0.01). The evolution of the slip resistance can be described phenomenologically by a saturation-type law as (Brown et al., 1989)

\[
\dot{s}^a = \dot{h}_a \left( 1 - \frac{s^a}{a} \right)^\alpha \sum_p |\gamma^p| \tag{7}
\]

where \( \dot{h}_a, s, \) and \( a \) denote the slip hardening parameters. It should be noted that Eq. (7) implies that slip on one system hardens all other systems equally. Finally, the lattice spin tensor \( \mathbf{W}^* \) (and the related lattice rotation tensor, \( \mathbf{R}^* \)) in the crystalline region is given by

\[
\mathbf{W}^* = \mathbf{R}^* \mathbf{R}^{T*} = \mathbf{W} - \mathbf{W}^p, \quad \mathbf{W}^p = \frac{1}{2} (\mathbf{L}^p - \mathbf{L}^{pT}) \tag{8}
\]

where \( \mathbf{W} \) is the applied spin tensor, and \( \mathbf{W}^p \) is the plastic spin tensor.

A detailed description of the implementation of the above crystal plasticity constitutive equations with the implicit version of the FE package ABAQUS is described by Kalidindi et al. (Kalidindi et al., 1992). This classical CPFEM is used to validate the spectral CPFEM introduced in this paper.

3. Crystal plasticity computations using DFTs

The crystal plasticity framework described earlier demands significant computational resources. This is a direct consequence of the fact that most metals have a very weak dependence on strain rate at room temperature which demands the use of a small value for the strain rate sensitivity parameter in the flow rule used in the rate-dependent crystal plasticity formulations (see Eq. (6)) (Hutchinson, 1976; Needleman et al., 1985; Pan and Rice, 1983). Knezevic et al. (Al-Harbi et al., 2010; Kalidindi et al., 2009; Knezevic et al., 2009) have developed a new database approach to obtain the solutions involved in these computations at dramatically reduced computational cost. In this approach, a DFT-based database is used to reconstruct directly the solutions for the main functions of the conventional crystal plasticity theory for any given crystal orientation under any applied deformation mode. In this method, spectral representations are established for the following three main functions: (i) the deviatoric stress tensor \( \mathbf{\sigma}(g, \mathbf{L}) \), (ii) the lattice spin tensor \( \mathbf{W}^*(g, \mathbf{L}) \), and (iii) the total shear rate \( \sum_p |\gamma^p|(g, \mathbf{L}) \). In these functions, the independent variable, \( g \), denotes the crystal lattice orientation defined using the Bunge–Euler angles \( (\phi_1, \phi, \phi_2) \) (Bunge, 1993), and \( \mathbf{L} \) represents the velocity gradient tensor applied at the crystal level. In any time step in the simulation of the deformation process, the stress function gives the values of the deviatoric stress components at the crystal level, the spin tensor predicts the crystal rotation, and the total shear rate determines the slip hardening rates as defined in Eq. (7).

The domain of these functions is the product space of the orientation space and the deformation mode space. The deformation mode space includes the complete set of all velocity gradient tensors which can be efficiently described as (Van Houtte, 1994)

\[
\mathbf{L} = \dot{\mathbf{e}} \mathbf{D}_o + \mathbf{W}, \quad \mathbf{D}_o = \sum_{j=1}^3 \mathbf{D}_j \mathbf{e}_j^o \otimes \mathbf{e}_j^o, \quad \dot{\mathbf{e}} = \frac{1}{2} [\mathbf{L} + \mathbf{L}^T]
\]

\[
D_1 = \sqrt{\frac{2}{3}} \cos \left( \theta - \frac{\pi}{3} \right), \quad D_2 = \sqrt{\frac{2}{3}} \cos \left( \theta + \frac{\pi}{3} \right), \quad D_3 = -\sqrt{\frac{2}{3}} \cos(\theta) \tag{9}
\]

where \( \{\mathbf{e}_i^o, i = 1, 2, 3\} \) denotes the principal frame of the unit, traceless, \( \mathbf{D}_o \), and the range of angular variable \( \theta \) that defines all possible diagonal matrices is \( [0, \frac{2\pi}{3}] \). The spectral databases are built in the \( \{\mathbf{e}_i^o\} \) reference frame using two primary variables, \( g^o \) and \( \theta \), where \( g^o \) denotes the crystal lattice orientation with respect to the \( \{\mathbf{e}_i^o\} \) reference frame. The spectral representations of the functions of interest are then expressed as (Knezevic et al., 2009)

\[
\mathbf{W}_{rq}^* = \frac{\dot{\mathbf{e}}}{N_{g^o}N_o} \sum_k \sum_n B_{nkr} e^{ikg^o} e^{\frac{2\pi}{N_o} n} + \mathbf{W} \tag{10}
\]

\[
\mathbf{\sigma}_{rq}^* = \frac{s^m}{N_{g^o}N_o} \sum_k \sum_n C_{nkr} e^{ikg^o} e^{\frac{2\pi}{N_o} n} \tag{11}
\]

\[
\left( \sum_p |\gamma^p| \right)_{rq} = \frac{1}{N_{g^o}N_o} \sum_k \sum_n G_{nkr} e^{ikg^o} e^{\frac{2\pi}{N_o} n} \tag{12}
\]

where \( r \) and \( q \) enumerate the grid points in the orientation space \( g^o \) and the deformation mode space \( \theta \), respectively. The corresponding total numbers of grid points in the periodic orientation and deformation mode spaces are denoted by \( N_{g^o} \) and \( N_o \), respectively. The spectral databases for the function of interest described above are stored in the form of Fourier
coefficients $B_{mn}$, $C_{nn}$, and $G_{mn}$ (referred to as the DFTs), where $k$ and $n$ represent frequencies in the DFT space, $B$ and $C$ denote second-rank tensors, and $G$ is a scalar. It is found that only a small number of the DFTs (hereafter called dominant DFTs) are needed to reconstruct the values of the functions of interest with a small error compared to the direct crystal plasticity computations (Knezevic et al., 2009). For example, the error between the spectral predictions and the direct computations was less than 5% when using 300 DFTs. The use of a small number of dominant DFTs speeds up the crystal plasticity calculations by about two orders of magnitude.

4. Integrating the spectral databases into FE simulation tools

The remarkable savings in the computational time involved in solving the crystal plasticity constitutive equations using the new spectral database scheme described in the previous section provides a significant incentive for incorporating it with a finite element package. This will allow the user to conduct more efficient CPFEM simulations at dramatically reduced computational cost. This section explains how the crystal plasticity DFT databases could be integrated with the commercial finite element package ABAQUS through a user materials subroutine (UMAT); this approach will be hereafter referred to as spectral database CPFEM or simply SD-CPFEM. To use the new spectral database scheme in the FE analysis, two tasks must be accomplished. First, the crystal plasticity computations using spectral databases should be extended from rigid–viscoplastic behavior to elastic–viscoplastic deformation. Second, the fourth-rank Jacobian matrix (defined as the derivative of the stress tensor with respect to the increment in strain tensor) needs to be computed efficiently to facilitate integration of the spectral databases with any implicit finite element code. Both of these developments are discussed in more detail next.

4.1. Including elastic deformation in the DFT database approach

The crystal plasticity calculations using spectral databases need to be extended from rigid–viscoplastic behavior to elastic–viscoplastic deformation. Although the elastic deformation in most metals subjected to finite plastic deformation is indeed very small and can be neglected, it is essential to include elasticity for implementing crystal plasticity computations with most commercial FE codes. This is mainly because most FE simulation tools, such as ABAQUS (ABAQUS, 2010), provide the total deformation gradient at each integration point as an input to the user-defined material constitutive response (through subroutines such as UMAT in ABAQUS), and expect to be returned the full stress tensor (not just the deviatoric stress tensor). Furthermore, elasticity plays an important role in phenomena such as the springback effect, which is an elasticity driven change in the shape of a part upon unloading.

The following constitutive relations are used to include the elastic deformation with the spectral crystal plasticity approach described in the previous section:

$$
\tau^{\nu_i} = \tilde{\mathbf{C}} \mathbf{D}^{\nu_i}
$$

where $\mathbf{D}^{\nu_i}$ is the elastic stretching tensor, $\tilde{\mathbf{C}}$ is the 4th-rank elasticity tensor, and $\tau^{\nu_i}$ is the Jaumann rate of the Kirchoff stress seen by an observer who rotates with the lattice and is defined as

$$
\tau^{\nu_i} = \dot{\mathbf{W}}^\nu \tau + \tau \mathbf{W}^\nu
$$

The Jaumann rate of the Kirchoff stress can be related to the Jaumann rate of the Cauchy stress $\sigma^{\nu_i}$ as follow:

$$
\tau^{\nu_i} = \sigma^{\nu_i} + \text{tr} (\mathbf{D}^{\nu_i}) \sigma
$$

where $\sigma^{\nu_i}$ is the Jaumann rate of the Cauchy stress based on the axes that spin together with the lattice and is defined as

$$
\sigma^{\nu_i} = \dot{\mathbf{W}}^\nu \sigma + \sigma \mathbf{W}^\nu
$$

In order to use the above relations, the total stretching tensor $\mathbf{D}^{\nu}$ (symmetric part of the velocity gradient tensor) needs to be decomposed into elastic and plastic parts. This decomposition must be accomplished such that the deviatoric stresses computed from both the crystal plasticity DFT databases (see Eq. (11), denoted here as $\sigma^{\text{DFT}}(\mathbf{D}^p)$) and the above Jaumann rate relations (denoted as $\sigma^{\text{DFT}}(\mathbf{D}^p, \mathbf{W}^\nu, \Delta t)$) are equal to each other within an acceptable tolerance. It should be noted that the trace of the stretching tensor contributes exclusively to the elastic deformation (assuming that the plastic deformation in metals is isochoric). In other words, only the five independent components of the deviatoric stretching tensor need to be decomposed into elastic and plastic parts. The following modified Newton–Raphson scheme has been developed to accomplish this decomposition:

$$
[D^{\nu}]_{n+1} = [D^{\nu}]_n - \lambda [J^{-1}]_n \text{[Err]}_n
$$

where

$$
\text{Err} = \sigma^{\text{DFT}}(\mathbf{D}^p) - \sigma^{\text{DFT}}(\mathbf{D}^p, \mathbf{W}^\nu, \Delta t)
$$

$$
J = \frac{\partial \text{Err}}{\partial \mathbf{D}^{\nu}} = - \frac{\partial \sigma^{\text{DFT}}(\mathbf{D}^p)}{\partial \mathbf{D}^p} - \frac{\partial \sigma^{\text{DFT}}(\mathbf{D}^p, \mathbf{W}^\nu, \Delta t)}{\partial \mathbf{D}^{\nu}}
$$
In Eq. (17), the subscripts \( n \) and \( n+1 \) refer to the estimates of \( \mathbf{D}^n \) at \( n \) and \( n+1 \) iterations, respectively. The value of the scalar parameter \( \lambda \) in Eq. (17) is selected such that the magnitude of the step correction \( \|\Delta \mathbf{D}^n\| = \|\mathbf{D}^{n+1} - \mathbf{D}^n\| \leq \eta \varepsilon_{\text{yield}} \), where \( \varepsilon_{\text{yield}} \) denotes the magnitude of the total strain at yielding and \( \eta \) is a numerical constant taken as 0.1.

It was observed that the initial guess of \( \mathbf{D}^n \) strongly affected the number of iterations required to reach convergence in the iterative procedure presented in this paper. The following strategy was found to give good results for the initial guess of \( \mathbf{D}^n \). First, the values of the deviatoric stress components and the lattice spin tensor are calculated using the spectral crystal plasticity approach assuming rigid–viscoplastic behavior, i.e. \( \mathbf{D}^n = \mathbf{D}^\text{p} \). These values are then used in (Eqs. (13)–(16)) to calculate the deviatoric elastic stretching tensor, \( \mathbf{D}^\text{e} \). If \( \|\mathbf{D}^\text{e}\| < 0.1\|\mathbf{D}\| \), use the computed \( \mathbf{D}^\text{e} \) as the initial guess to start the iterations. Else, the deviatoric stretching tensor, \( \mathbf{D}^\text{e} \), is used as an initial guess for \( \mathbf{D}^n \). The iterations are carried out until the maximum of the absolute difference in all components of \( \mathbf{D}^n \) between two successive iterations is less than \( 10^{-4}\|\mathbf{D}\| \). Convergence is typically obtained within two iterations; a higher number of iterations are generally required near the elastic–plastic transition zone or during any loading path change.

To verify the stability and accuracy of the above iteration scheme, we have simulated a reverse shearing process using both the SD-CPFEM approach described in this work and compared the results with those obtained from the classical CPFEM approach (Kalidindi et al., 1992). The FE model is a single cuboid-shaped three-dimensional eight-noded solid element (C3D8) in ABAQUS (ABAQUS, 2010) with the same initial crystal orientation assigned to all eight integration points. The single element is sheared up to a shear strain of \( \gamma = 0.5 \) followed by shearing in the opposite direction. The elastic and plastic property parameters in this model are listed in Table 1 (these correspond to OFHC copper reported in literature (Kalidindi et al., 1992)). The single crystal is assumed to exhibit the twelve \{111\} (110) slip systems characteristic of fcc metals. Fig. 1 shows the predicted stress–strain responses from both the SD-CPFEM (using 500 dominant DFTs for the stress, the shearing rate, and the lattice spin components) and the classical CPFEM for a selected crystal lattice orientation. Several other similar results are obtained for other random crystal orientations. It is clear that the new iteration algorithm described above can accurately capture the elastic response during loading and unloading cycles, and the predictions from both approaches are in excellent agreement with each other.

4.2. Computation of the Jacobian

The implementation of UMAT in ABAQUS (ABAQUS, 2010) requires the computation of the Jacobian defined as

\[
\mathbf{J} = \frac{\partial \Delta \mathbf{\sigma}}{\partial \Delta \mathbf{e}} = \frac{\partial \mathbf{\sigma}}{\partial \mathbf{E}_t}
\]  

(20)

where \( \Delta \mathbf{\sigma} \) and \( \Delta \mathbf{e} \) are the increments in the stress and strain tensors in a given time increment, respectively, and \( \mathbf{E}_t \) is the relative strain tensor in the same time increment. The Jacobian matrix of Eq. (20) is used in the Newton–Raphson iterative method for revising the estimated displacements such that the corresponding stresses are likely to better satisfy the principal of virtual work at the end of the increment. It should be noted that the Jacobian matrix plays an important role in

| Elastic and plastic parameters of the OFHC copper used in this work (Kalidindi et al., 1992). |
|---------------------------------|---------------------------------|---------------------------------|----------------|----------------|----------------|----------------|
| \( C_{11} \) (MPa) | \( C_{12} \) (MPa) | \( C_{44} \) (MPa) | \( m \) | \( S_h \) (MPa) | \( h_o \) (MPa) | \( s_o \) (MPa) | \( \alpha \) |
| 168,400 | 121,400 | 75,400 | 0.01 | 16 | 180 | 148 | 2.25 |

Fig. 1. Stress–strain curves of reverse shearing process using both the SD-CPFEM and the classical CPFEM of copper single element.
the rate of convergence of the solution to the global equilibrium equations, but has no effect on the accuracy of the solution. For the present work, the following analytical expression for the Jacobian is developed

\[ \mathcal{J} = \frac{\partial \mathbf{\sigma}}{\partial \mathbf{E}_t} = \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{E}_t} + \mathbf{I} \otimes \frac{\partial \mathbf{p}}{\partial \mathbf{E}_t} = \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{D}} \frac{\partial \mathbf{D}}{\partial \mathbf{E}_t} + \mathbf{I} \otimes \frac{\partial \mathbf{p}}{\partial \mathbf{E}_t} \]  

(21)

with

\[ \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{D}} = \left[ \frac{1}{2 + \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{D}_t}} \right]^{-1} \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{D}_t} \]  

(22)

where \( \mathbf{p} \) denotes the pressure, and \( \mathbf{I} \) and \( \mathbf{1} \) are the second-rank and fourth-rank identity tensors, respectively. The term in Eq. (22) that requires long computations is \( \frac{\partial \mathbf{\sigma}}{\partial \mathbf{D}} \). This term is evaluated analytically using the chain rule as follow:

\[ \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{D}} = \left( \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{\varphi}_1^{(0)}, \varphi_1^{(0)}, \varphi_2^{(0)} \frac{\partial \mathbf{\varphi}}{\partial \mathbf{D}} \right) + \left( \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{\varphi}_1^{(1)}, \varphi_2^{(1)}, \varphi_2^{(1)} \frac{\partial \mathbf{\varphi}}{\partial \mathbf{D}} \right) + \left( \frac{\partial \mathbf{\sigma}^r}{\partial \mathbf{\varphi}_1^{(2)}, \varphi_2^{(2)}, \varphi_2^{(2)} \frac{\partial \mathbf{\varphi}}{\partial \mathbf{D}} \right) \]  

(23)

where \( \langle \varphi_1^{(0)}, \varphi_1^{(1)}, \varphi_1^{(2)} \rangle \) denotes the set of three Bunge–Euler angles that describe the orientation matrix \( \mathbf{Q}^U \) used to transform the deviatoric stress tensor from the principle frame of \( \mathbf{D}^s \) \( \{ e_s \} \) into the sample frame \( \{ e_s \} \):

\[ e_s^i = \sum_j Q_{ij}^U e_s^j \]  

(24)

Analytical expressions for each of the terms in Eq. (23) have been derived and validated by comparing the values produced from these expressions with the corresponding values computed numerically by slightly perturbing the independent variable in each expression. Details of the computation of these terms are presented in Appendix A. It should be noted that, in any time step in the simulation, the term \( \frac{\partial \mathbf{\sigma}}{\partial \mathbf{D}} \) will be already calculated as a part of the iteration scheme to decompose the deviatoric stress tensor from the principle frame of \( \mathbf{D}^s \) \( \{ e_s \} \) into the sample frame \( \{ e_s \} \).

### 5. Case studies

In order to demonstrate the viability and computational advantages of the new spectral CPFEM developed in this work, we compare the stress–strain responses and the evolution of crystallographic texture in polycrystalline aggregates of OFHC copper and interstitial-free (IF) steel predicted from the new spectral approach with the corresponding results from the classical CPFEM for selected deformation processes, including non-monotonic loading histories. The predictions from the two approaches reported here are produced using the commercial FE package ABAQUS (ABAQUS, 2010) and specially developed user material subroutines (described in this paper and those in Kalidindi et al. (Kalidindi et al., 1992)).

#### 5.1. Plane strain compression of copper

We first simulated plane strain compression of a polycrystalline aggregate of OFHC copper. For fcc metals, the family of twelve \( \{ \{111\} \} \) \{110\} slip systems are assumed to be the potential slip systems for plastic deformation. The three-dimensional FE model consisted of 500 C3D8 elements. In this model, the top surface was subjected to a displacement boundary condition, which resulted in a 65% reduction in height corresponding to an axial true strain of about 1.0. The displacements of nodes on the two lateral faces are constrained such that these nodes remain on their respective planes. The initial texture was assumed to be random consisting of 4000 different crystal orientations. Each integration point inside each element was assigned a single crystal orientation chosen randomly from the set of 4000 crystal orientations. The elastic and plastic parameters of the OFHC copper used in this case study are shown in Table 1.

We compared in Fig. 2 the stress–strain responses and deformed texture produced from the SD-CPFEM (for clarity, only few points are shown in the plot), based on 500 dominant DFTs for the stress, the shearing rate, and the lattice spin components, against the corresponding predictions from the conventional CPFEM (Kalidindi et al., 1992). It is clear that the SD-CPFEM approach produced excellent predictions but at a significantly faster computational speed. In this case study, the simulation took 8964 s (~2.5 h) using the classical CPFEM, and only 602 s (~10 min) for the spectral CPFEM based on 500 dominant DFTs. It is underlined that the simulation speed of the spectral CPFEM can be controlled through the selection of the appropriate number of dominant DFTs. The user can select a small number of DFTs to increase the computational speed of the simulation at the expense of accuracy. For example, in this case study the same simulation required only 231 s (~4 min) when using 150 DFTs. The predictions from the SD-CPFEM based on 150 dominants DFTs are compared against those obtained from the classical CPFEM in Fig. 3. It is clear that the predictions from the SD-CPFEM using a small number of dominant DFTs are still in reasonable agreement with the predictions from the conventional CPFEM.

To better quantify the computational efficiency of the SD-CPFEM, we repeated the simulations described above for different number of elements including 500, 4000, and 10,976 C3D8 elements. We again assigned a single crystal orientation...
chosen randomly from a set of large crystal orientations to each integration point inside each element. It should be noted that the random texture is selected because it produces the most heterogeneous microscale stress and strain fields in the sample. The sample is subjected to plane strain compression up to an axial strain of 1.0 (~65% reduction in height). Table 2 compares the simulation time between the classical CPFEM and the SD-CPFEM based on 500 DFTs and 150 DFTs for different number of elements. It is seen that the SD-CPFEM can speed up the computation time by about 40 times compared to the classical CPFEM when using a small set of dominant DFTs.

5.2. Simple shear of IF steel

In the next case study, we compared the stress–strain curves and texture evolution produced from the SD-CPFEM against the corresponding results from the conventional CPFEM for a simple shear deformation of a polycrystalline interstitial free (IF) steel. For bcc metals, the families of 48 potential slip systems are assumed to include \( \{110\}\{111\}, \{112\}\{111\}, \text{ and } \{123\}\{111\} \). For the SD-CPFEM simulations discussed in this case study, we used the spectral database developed for bcc metals and validated in our prior work (Al-Harbi et al., 2010). It was reported earlier that because of the availability of higher number of slip systems in the bcc metals (48 slip system in bcc compared to 12 in fcc metals), the spectral database for bcc metals was more compact compared to the one obtained for fcc metals. In other words, a smaller number of dominant DFTs can be used for bcc metals to achieve the desired accuracy.

The FE model is discretized into 500 three-dimensional solid elements (C3D8). A simple shear deformation is applied up to a shear strain \( \gamma = 1.0 \). To produce the most heterogeneous stress and strain fields in the model and therefore allow better opportunity to validate the spectral database approach described in this work, each integration point is assigned a single crystal orientation chosen randomly from a set of 4000 crystal orientations that produce a random texture. The values of the elastic and plastic parameters of the IF steel used in this case study are shown in Table 3 (Al-Harbi et al., 2010).

Fig. 4 shows a comparison of the stress–strain responses and final texture predicted by both the spectral database and conventional CPFEM codes. It is seen that the two predictions are in excellent agreement with each other. It should be noted that the predictions from SD-CPFEM are obtained with significantly less computational cost compared to the classical CPFEM. For this case study, the classical CPFEM required 4380 s, whereas the SD-CPFEM took only 336 s when using 500 DFTs for the stress, the shearing rate, and the lattice spin components.
5.3. Plane strain compression followed by simple shear

To validate the SD-CPFEM for the case of non-proportional loading, we simulated a plane strain compression followed by simple shear of a polycrystalline OFHC copper. The FE model consisted of 500 C3D8 elements with one crystal orientation per integration point. The initial texture is assumed to be random. The first step in this simulation involved an imposed displacement boundary condition on the top surface of the model, which resulted in a 35% reduction in height corresponding to an axial true strain of about 0.4. All faces of the sample are constrained to remain planar in this step. In the second step, an imposed simple shear deformation is applied up to a shear strain of $\gamma = 0.5$ as shown in Fig. 5(a and b). The elastic and plastic parameters of the OFHC copper used in this case study are similar to the one shown in Table 1. The stress–strain response
from the SD-CPFEM is compared against the corresponding predictions from the classical CPFEM in Fig. 5(c). The predicted textures from the two approaches after each deformation step are shown in Fig. 6. It was seen once again that the predictions from the spectral database approach matched very well with the corresponding predictions from the conventional CPFEM at a dramatically reduced computation cost. This prediction took 6380 s for the classical CPFEM and only 527 s for the SD-CPFEM when using 500 DFTs for the stress, the shearing rate, and the lattice spin components.
6. Conclusions

In this paper, we have demonstrated the first integration of our recently developed spectral database approach to crystal plasticity calculations for face centered and body centered cubic polycrystalline metals that deform by crystallographic slip with the implicit version of the finite element package, ABAQUS, accomplished through the development of a user material subroutine, UMAT. For this purpose, we have developed a Newton-type iteration scheme to extend the spectral crystal plasticity computations using spectral databases from rigid–viscoplastic to elastic–viscoplastic deformation. We have also established an efficient analytical expression for the Jacobian required to implement the spectral databases with any implicit finite element code. The case studies showed that the new spectral crystal plasticity FE approach produces excellent predictions similar to the classical crystal plasticity FE method but at a significantly faster computational speed. It was seen that the spectral databases implemented in the FE package ABAQUS can speed up the computational time by about 40 times compared to the classical CPFEM.

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Appendix A

We have derived analytical expressions for the Jacobian matrix required for implementing the spectral approach to crystal plasticity computations with the FE package ABAQUS. Below is a brief description of the derivation of the term $\frac{\partial}{\partial D_p}$ using the chain rule:
\[
\frac{\partial \boldsymbol{\sigma}}{\partial \mathbf{D}'} = \begin{pmatrix}
\frac{\partial \sigma_1'}{\partial \mathbf{e}_1} & \frac{\partial \sigma_2'}{\partial \mathbf{e}_1} \\
\frac{\partial \sigma_1'}{\partial \mathbf{e}_2} & \frac{\partial \sigma_2'}{\partial \mathbf{e}_2}
\end{pmatrix}
\]

(A1)

For simplicity of notation, the above relation will be expressed in a condensed form as

\[
\frac{\partial \sigma'}{\partial \mathbf{D}'} = \begin{pmatrix}
\frac{\partial \sigma'}{\partial \mathbf{e}_1} & \frac{\partial \sigma'}{\partial \mathbf{e}_2} \\
\frac{\partial \sigma'}{\partial \mathbf{e}_3} & \frac{\partial \sigma'}{\partial \mathbf{e}_4}
\end{pmatrix}
\]

(A2)

where \( \mathbf{g} = (\varphi_1', \varphi_2', \varphi_3', \varphi_4') \) denotes the set of three Bunge–Euler angles that describe the orientation matrix \( \{ \mathbf{Q}' \} \) used to transform the deviatoric stress tensor from the principle frame of \( \mathbf{D}' \) (\( \{ \mathbf{e}' \} \)) into the sample frame (\( \{ \mathbf{e} \} \)).

Recall that the deviatoric stress tensor is calculated using the spectral approach (see Eq. (11)) as

\[
\sigma'_{\text{eq}}(\theta, \phi, \mathbf{g}) = s \dot{\epsilon}_m \frac{1}{N_g N_0} \sum_k \sum_n \mathbf{C}_{kn} e^{i \frac{2 \pi k}{N_g} \varphi} e^{i \frac{2 \pi n}{N_0} \theta}
\]

(A3)

where the superscript (Pr) indicates that the stress values are defined in the principal frame of \( \mathbf{D}' \). This stress tensor can be transformed to the sample frame using the second-rank transformation

\[
\sigma'_{\text{eq}} = [\mathbf{Q}']^T [\sigma'_{\text{eq}}(\theta, \phi, \mathbf{g})] [\mathbf{Q}']^T
\]

(A4)

where \( \mathbf{g} \) denotes the crystal lattice orientation defined using the Bunge–Euler angles (\( \varphi_1, \varphi_2 \)) (Bunge, 1993). It should be noted that the Bunge–Euler angles \( \mathbf{g} \) and \( \mathbf{g}' \) are not independent of each other. In fact, one can readily show

\[
[\mathbf{Q}] = [\mathbf{Q}]^T [\mathbf{Q}]
\]

(A5)

where \( [\mathbf{Q}] \) is the orientation matrix that brings the crystal frame \( \{ \mathbf{e}' \} \) into coincidence with the principal frame of \( \mathbf{D}' \), i.e. \( \{ \mathbf{e}' \} \) and \( \{ \mathbf{e} \} \) is the rotation matrix that relates the crystal frame \( \{ \mathbf{e}' \} \) to the sample frame \( \{ \mathbf{e} \} \). These orientation matrices can be calculated using their respective three Bunge–Euler angles. For example, the rotation matrix \( [\mathbf{Q}] \) is given by

\[
[\mathbf{Q}] = \begin{bmatrix}
\cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi & - \cos \varphi_1 \sin \varphi_2 - \sin \varphi_1 \cos \varphi_2 \cos \Phi & \sin \varphi_1 \sin \Phi \\
\sin \varphi_1 \cos \varphi_2 + \cos \varphi_1 \sin \varphi_2 \cos \Phi & - \sin \varphi_1 \sin \varphi_2 + \cos \varphi_1 \cos \varphi_2 \cos \Phi & - \cos \varphi_1 \sin \Phi \\
\sin \varphi_2 \sin \Phi & \cos \varphi_1 \sin \Phi & \cos \Phi
\end{bmatrix}
\]

(A6)

Using the above relations, the analytical expressions for each of the term in Eq. (A2) can be derived as follows (for simplicity, assume that there is no strain hardening, i.e. \( s \) is constant in Eq. (A3)):

\[
(1) \quad \frac{\partial \sigma'}{\partial \mathbf{e}_1} \Big|_{\mathbf{e}, \mathbf{g}} = \frac{m s}{\mathbf{e}} [\mathbf{Q}'] [\sigma'_{\text{eq}}(\theta, \phi, \mathbf{g})] [\mathbf{Q}']^T
\]

(A7)

\[
(2) \quad \frac{\partial \sigma'}{\partial \mathbf{e}_2} \Big|_{\mathbf{e}, \mathbf{g}} = [\mathbf{Q}'] \left[ \frac{\partial \sigma'_{\text{eq}}}{\partial \theta} \right] [\mathbf{Q}']^T
\]

(A8)

where

\[
\frac{\partial \sigma'_{\text{eq}}}{\partial \theta} = s \dot{\epsilon}_m \frac{1}{N_g N_0} \sum_k \sum_n \mathbf{C}_{kn} e^{i \frac{2 \pi k}{N_g} \varphi} e^{i \frac{2 \pi n}{N_0} \theta}, \quad \mathbf{C}_{kn} = 2\pi \text{ in } \mathbf{C}_{kn}
\]

(A9)

It is clear that the spectral representation presented in this work allows efficient calculation of the term \( \frac{\partial \sigma'_{\text{eq}}}{\partial \theta} \).

\[
(3) \quad \frac{\partial \theta}{\partial \mathbf{D}'} = \frac{\partial \theta}{\partial \mathbf{D}_1} \frac{\partial \mathbf{D}_1}{\partial \mathbf{D}'}
\]

(A10)

where \( \mathbf{D}_1 \) is the first eigenvalue of \( \mathbf{D}_0 \) (see Eq. (9)). The term \( \frac{\partial \theta}{\partial \mathbf{D}_1} \) is calculated directly from Eq. (9) and an analytical expression of \( \frac{\partial \theta}{\partial \mathbf{D}_1} \) is derived using the determinant of \( \mathbf{D}_0 \) defined as

\[
\det(\mathbf{D}_0) = \det \left( \frac{1}{\mathbf{e}} \mathbf{D}' \right) = \mathbf{D}_1 \mathbf{D}_2 \mathbf{D}_3 = \mathbf{D}_0^3 - \frac{1}{2} \mathbf{D}_1
\]

(A11)

(4) The computation of the term \( \frac{\partial \sigma'}{\partial \mathbf{g}} \Big|_{\mathbf{e}, \theta} \) involves the calculations of the derivatives \( \frac{\partial \sigma'_{\text{eq}}}{\partial \mathbf{g}} \) and \( \frac{\partial \sigma'_{\text{eq}}}{\partial \theta} \) (see Eq. (A4)):

\[
\frac{\partial \sigma'}{\partial \mathbf{g}} \Big|_{\mathbf{e}, \theta} = \frac{\partial \left( \frac{\partial \sigma'_{\text{eq}}}{\partial \mathbf{g}} \right)}{\partial \theta} - \frac{\partial \left( \frac{\partial \sigma'_{\text{eq}}}{\partial \theta} \right)}{\partial \mathbf{g}}
\]

(A12)
where

\[ \frac{\partial \sigma^{(pr)}}{\partial \rho} = \frac{\partial \sigma^{(pr)}}{\partial \rho} = 0 \]  

(A13)

The term \( \frac{\partial \sigma^{(pr)}}{\partial \rho} \) is calculated using an expression similar to Eq. (A9) and \( \frac{\partial \sigma^{(pr)}}{\partial \rho} \) is derived using Eq. (A5). Furthermore, the term \( \frac{\partial \sigma^{(pr)}}{\partial \rho} \) in Eq. (A12) is calculated using Eq. (A6).

(5) The term \( \frac{\partial \sigma^{(pr)}}{\partial \rho} \) is calculated using the relation

\[ \mathbf{D}^{(pr)} \mathbf{N}^{(0)} = \mathbf{N}^{(0)} \]  

(A14)

where \( \mathbf{N}^{(0)} \) denotes the column \( i \) of \( \{\mathbf{Q}^{(i)}\} \), which represents the eigenvector of \( \mathbf{D}^{(pr)} \) corresponding to the eigenvalue \( \lambda \). To avoid the additional calculations of evaluating the derivative of the eigenvalues with respect to \( \mathbf{D}^{(pr)} \), we use the orthogonality property of the eigenvectors and rewrite Eq. (A14) as

\[ \mathbf{D}^{(pr)} \mathbf{N}^{(0)} \cdot \mathbf{N}^{(0)} = \mathbf{N}^{(0)} \cdot \mathbf{N}^{(0)} = 0 \quad \text{for } i \neq j \]  

(A15)

Then, the term \( \frac{\partial \sigma^{(pr)}}{\partial \rho} \) can be readily calculated using Eqs. (A15) and (A6).

To validate the methods described above for deriving each of the term, we compared the values produced from the final expressions of these terms with the corresponding values computed numerically by slightly perturbing the independent variable in each expression.

References

ABAQUS, 2010. © Dassault Systèmes Simulia Corp., Providence, RI, USA.


