Fast Fourier Transform-based Modeling for the Determination of Micromechanical Fields in Polycrystals

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Emerging characterization methods in experimental mechanics pose a challenge to modelers to devise efficient formulations that permit interpretation and exploitation of the massive amount of data generated by these novel methods. In this overview we report on a numerical formulation based on fast Fourier transforms, developed over the last 15 years, which can use the voxelized microstructural images of heterogeneous materials as input to predict their micromechanical and effective response. The focus of this presentation is on applications of the method to plastically-deforming polycrystalline materials.

INTRODUCTION

Polycrystalline metals play a key role as structural materials in vast sectors of the economy, like energy, car-making, aerospace, and defense. In nature, geological materials also appear as aggregates of single crystal grains whose microstructures are used to infer the deformation history of rocks, for example. Relevant properties like the in-service performance of metallic components, or the mechanical response of Earth materials in natural conditions, emerge from microscopic and nanoscopic features, such as the structure and dynamics of crystalline defects (vacancies and interstitials, dislocations, grain boundaries, voids), as well as the size, morphology, spatial distribution, and orientation of the constituent single crystal grains. The latter represents, in a broad sense, the texture of a polycrystal, including under this definition the crystallographic, morphologic, and topologic distributions of the single crystal grains in the aggregate. Until recently, due to a lack of appropriate experimental probes, no technique was able to fully characterize the texture of polycrystalline structures in three dimensions (3-D), let alone follow its in-situ evolution during a thermo-mechanical process. This limitation is rapidly disappearing. Serial-sectioning by focused-ion-beam (FIB) combined with electron back-scatter diffraction (EBSD) now provides a way (although destructive) to characterize local orientations in 3-D (e.g., Reference 1) with nanometric spatial resolution. Moreover, novel synchrotron-based x-ray diffraction techniques can be used for in-situ measurement of the positions, shapes, and crystallographic orientations (e.g., Reference 2), and even local strains of bulk grains in an aggregate,[3,4] with micrometric and sub-micrometric resolution.

From a modeling and simulation perspective, one of the challenges arising from the aforementioned advances is to keep up with the pace of these emerging characterization techniques. New, robust, and very efficient numerical formulations are needed for interpretation and exploitation of the massive amount of data generated by these measurements. It is also noteworthy that most of the techniques provide images of microstructure in which the orientation (or phase identification) is defined on a regular grid of points.

This overview reports on a technique originally developed by Moulinec and Suquet[5,6] as an efficient method to compute the micromechanical fields and effective response of heterogeneous materials, directly from an image of their microstructure. This image can be a two-dimensional (2-D) phase contrast image obtained by optical or scanning electron microscopy, a 3-D tomographic image, a 2-D or 3-D orientation image obtained by EBSD, or a numeri-

How would you…

…describe the overall significance of this paper?

This paper presents some recent applications to plastically deforming polycrystals of an efficient numerical formulation based on fast Fourier transforms, which can use direct input from voxelized microstructural images for the prediction of the micromechanical fields and the effective response of heterogenous materials.

…describe this work to a materials science and engineering professional with no experience in your technical specialty?

Interpretation of the massive amount of data (i.e,. microstructure images comprising millions of voxels) produced by emerging three-dimensional (3-D) characterization methods of polycrystalline materials, require very efficient models. Such models should be able to use direct input from those images to predict mechanical response. In this work we present a formulation based on fast Fourier transforms for an efficient solution of the micromechanical problem.

…describe this work to a layperson?

Polycrystalline materials play a key role in vast sectors of the economy. Their mechanical response depends on their microscopic properties, which are heterogenous, as they in turn depend on the orientation of the constituent crystals. New experimental methods permit nowadays to characterize the orientation and distribution of these crystals in 3-D. Further applications of these measurements require the use of models. Here we report on a very efficient model with which we can predict the mechanical response of a polycrystal directly based on a 3-D image of its microstructure.

cally generated phase and/or orientation image. At the core of the proposed method, the input image is manipulated using the fast Fourier transform (FFT) algorithm, a numerical tool extensively used in signal and image processing, extended in the present approach to solve a micromechanical problem.

While other numerical schemes (based on the finite element method, FEM) have been extensively used to deal with problems involving crystal plasticity (CP) (for an excellent and up-to-date review on CP-FEM, see Reference 7), the large number of degrees of freedom (DOF) required by such FEM calculations using direct input from microstructural images limits the size of the polycrystalline microstructures that can be investigated by these methods, within reasonable computing times. Considering, for example, a typical size of a 3-D experimental dataset to be 10^7 voxels, and assuming that the number of DOF required in an FEM calculation is roughly of the same order as the total number of voxels in the image, gives an idea of the daunting task that use of such image-based CP-FEM calculation may become.

Conceived as an alternative to CP-FEM, the methodology presented here, based on CP and FFT, is endowed with some unique features. In the first place, owing to the intensive use of FFTs (and the lack of any large matrix inversion), it is very efficient, making it an excellent candidate to incorporate fine-scale microstructural information in plastic deformation simulations with a level of fidelity unreachable with CP-FEM. Moreover, the CP-FFT formulation is meshless, and, as such, can use direct input from (and/or its results can be validated against) 3-D images of the material's microstructure mapped onto a regular grid (voxelized data), thereby providing a one-to-one mapping between the simulation grid and the data generated by 3-D experimental techniques. On the disadvantage side, the requirement of periodic boundary conditions makes the CP-FFT formulation less general than CP-FEM.

FORMULATION

The FFT-based method was originally developed[5,6,8,9] as a fast algorithm to compute the local and effective mechanical response directly from an image of a composite material (in which the source of heterogeneity is related to the spatial distribution of phases with different mechanical properties), and was later adapted[10–12] to deal with plastically deforming 3-D polycrystals (in which the heterogeneity is related to the spatial distribution of crystals with directional mechanical properties).

The FFT-based formulation is conceived for periodic unit cells and provides an "exact" solution (within the limitations imposed by the unavoidable discretization of the problem and the iterative character of the numerical algorithm, see below) of the governing equations (equilibrium and compatibility). It shares some common characteristics with the phase-field method (PFM), although it is limited to what, in the context of PFM, is known as long-range interactions, since no heterogeneous chemical energy term is involved in the mechanical response and/or microstructure evolution of a single-phase polycrystal. A similar phase-field analysis was proposed[13] to obtain the local fields in elastically heterogeneous polycrystals. The FFT-based approach, however, is not restricted to linear behaviors. Problems involving materials deforming in non-linear regimes are treated similarly to a linear problem by using the concept of linear reference material.[5,6]

The FFT-based formulation iteratively adjusts a compatible strain (or strain-rate) field, related with an equilibrated stress field through a constitutive potential, such that the average of local work (or power) is minimized. The method is based on the fact that the local mechanical response of a heterogeneous medium can be calculated as a convolution integral between the Green function associated with appropriate fields of a linear reference homogeneous medium and a polarization field, which is obtained as the product of the difference between the local (fluctuating) and the linear reference (constant) stiffness and (a current guess of) the strain field. For periodic media, use can be made of the Fourier transform to reduce convolution integrals in real space to simple products in Fourier space. Thus, the FFT algorithm can be utilized to transform the polarization field (obtained directly from the input microstructure's image) into Fourier space and, in turn, to obtain the mechanical fields by transforming back into Cartesian space. However, since the polarization field depends precisely on the a priori unknown strain field, an iterative scheme has to be implemented to obtain, upon convergence, a compatible strain field and a stress field in equilibrium. Details of the formulation are presented in original papers on composites[5,6,8,9] and polycrystals.[10–12]

Regarding the specific iterative procedure required to solve a given micromechanical problem, several versions of the FFT-based method are presently

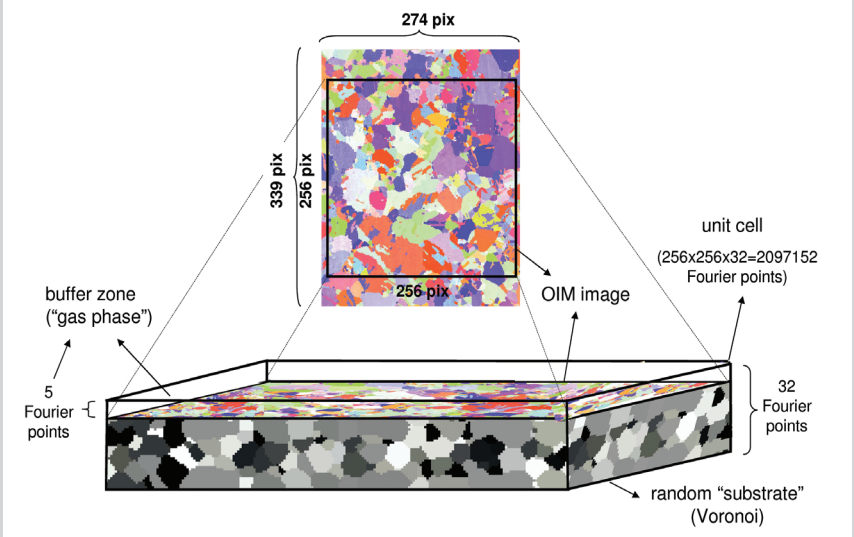


Figure 1. Schematic representation of the Cu 3-D unit cell used in the FFT-based simulations of local orientation and misorientation evolution, with direct input from EBSD images.[12]

available. The original formulation of Moulinec and Suquet,[5,6] now known as the "basic" scheme, has been proven to converge for linear materials at a rate (number of iterations at convergence) that is proportional to local contrast in mechanical properties. To improve the convergence of this basic scheme, which is slow for heterogeneous materials with very high contrast, accelerated schemes have been proposed by different authors (a non-exhaustive list of such propositions includes Eyre and Milton,[14] Brisard and Dormieux,[15] Zeman et al.[16]). When the mechanical contrast is infinite, convergence is not ensured and, to overcome this limitation, Michel et al.[8] proposed the so-called "augmented Lagrangians" scheme (see also Willot and Pellegrini[17] for a modified version of the algorithm), which conceptually consists of iteratively adjusting two strain (or strain-rate) and two stress fields. By construction, one of the strain fields is compatible and one of the stress fields is in equilibrium, while the other strain and stress fields are related through the constitutive potential. The iterative procedure is designed to make the pairs of strain and stress fields to converge to each other. At convergence, the method delivers a compatible strain field related with an equilibrated stress field through the local constitutive equation.

Regarding the use of the FFT-based methodology for the prediction of the micromechanical response of plastically-deforming polycrystals, several applications to date were based on the popular rigid-viscoplastic (VP) approximation to crystal plasticity,[18] under which the elastic strains are considered negligible compared with the plastic strains and the (viscoplastic) strain-rate $\dot{\varepsilon}(\mathbf{x})$ is constitutively related with the stress $\sigma(\mathbf{x})$ at a single-crystal material point $\mathbf{x}$ (belonging to the regular Fourier grid) through a sum over the N active slip systems, of the form:

$$\dot{\varepsilon}(\mathbf{x}) = \dot{\gamma}_o \sum_{k=1}^{N} m^k(\mathbf{x}) \left(\frac{\left| m^k(\mathbf{x}) : \sigma(\mathbf{x}) \right|}{\tau_o^k(\mathbf{x})} \right)^n \times \mathrm{sgn}\left(m^k(\mathbf{x}) : \sigma(\mathbf{x}) \right) \quad (1)$$

where $\tau_o^k(\mathbf{x})$ and $m^k(\mathbf{x})$ are the critical resolved shear stress (CRSS) and the Schmid tensor associated with slip system k at point, $\mathbf{x}$, $\dot{\gamma}_o$ is a normalization factor and n is the rate-sensitivity exponent. This power-law constitutive description leads to a problem of a heterogeneous medium with high contrast in local properties, which in general needs to be solved with Michel et al.'s[8] augmented Lagrangian method.[11,12]

APPLICATIONS TO VISCOPLASTIC POLYCRYSTALS

The FFT-based formulation for viscoplastic polycrystals, based on the constitutive representation given by Equation 1 has been applied to both numerically generated and measured orientation images.

Periodic microstructures (as required by the method) can be numerically generated by a variety of methods, of which we highlight the Voronoi tessellation as an example. Since an FFT-based calculation requires a discrete description of the microstructure on a regularly spaced grid over a periodic unit cell, the generation is simpler than in the case of having to determine Voronoi cells in a continuum. The procedure consists in distributing N points of a random sequence in a unit cell, and, to ensure periodicity, periodically duplicating these points immediately outside the unit cell. This Poisson distribution constitutes the nuclei of the random grains. Next, the sides of the unit cell are partitioned into regularly spaced points, determining a 2-D or 3-D regular Fourier grid, and each of these Fourier points is assigned to its nearest nucleus (including those that are across the unit cell limits), determining N different domains (grains). Crystallographic orientations (either randomly or preferentially distributed) can then be assigned to these domains.

Periodic polycrystalline unit cells generated as described above and solved with the VP-FFT method have been utilized for a variety of studies, including: the efficient determination of ensemble averages over a large number of configurations, for comparison of the latter with the effective response and field fluctuations statistics obtained from homogenization approaches (e.g., Reference 19), and the orientation dependence of strain localization in strongly heterogeneous polycrystals (e.g., Reference 20). Among these applications, it is worth mentioning a recent study on dilatational plasticity of porous polycrystalline materials,[21] in which the effect of the crystallinity (and heterogeneity) of the material surrounding intergranular voids on the growth of such voids was for the first time assessed and quantified, and compared with homogenization approaches.

Pixelized or voxelized orientation images measured by EBSD can also be used as input for a VP-FFT calculation, but, unlike numerically generated microstructures, in which periodic boundary conditions can be imposed, a unit cell constructed from an experimental orientation image will exhibit, in general, abrupt changes from grains located inside the unit cell to other, completely uncorrelated grains located across the unit cell limits when periodic boundary conditions are imposed. This could adversely affect the model predictions, especially for grains close to the unit cell boundaries. However, the inaccuracies associated with the presence of these spurious "grain boundaries" appear to be of minor importance, at least for linear materials.[19]

Figure 1[12] illustrates the use of the VP-FFT formulation for a quantitative study of the average orientations and intragranular misorientations developed in a copper polycrystal deformed in tension. 2-D EBSD was used to characterize the local orientations measured in an area of about 500×500 μm, located on one of the flat surfaces of a recrystallized copper sample, with a spatial resolution of 2 μm, before and after 11% deformation. Since in this case the actual 3-D microstructure of the bulk of the sample was not known,

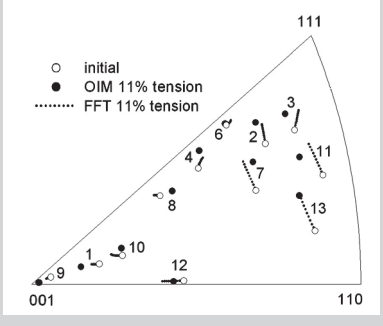


Figure 2. Inverse pole figure of the measured initial orientation and the final average orientation and trajectories predicted with the FFT-based approach for the 13 largest Cu grains in the image.[12]

a 3-D unit cell was built assuming a randomly generated distribution of bulk grains underneath the measured surface grains (i.e., a 3-D substrate), having the same average grain size and overall crystallographic orientation distribution as the surface grains. For this, a 3-D Voronoi microstructure was generated as described above and in turn the experimental 2-D and the numerically generated 3-D images were merged and "relaxed," following the procedure described in Reference 12. Such an approximation of the actual 3-D microstructure can of course be avoided if experimental data obtained with 3-D techniques is available. While, by construction, the first layer of the resulting configuration has the same topology as the experimental 2-D image, without any further manipulation, the measured surface grains would become bulk grains, upon the imposition of periodic boundary conditions across the unit cell. Therefore, to reproduce the actual free surface condition of the measured grains, several layers of Fourier points were replaced by a "buffer zone," or "gas phase," with infinite compliance (i.e., identically zero local stress).

Figure 2 shows in an inverse pole figure representation of the actual initial orientations and final average orientations of the 13 largest grains in the measured image, and the predicted trajectories of the mean orientations. The small crosses defining these trajectories were calculated by VP-FFT in increments of 1% overall plastic strain,

Table I. Average Misorientation of the 13 Largest Cu Grains after 11% Tensile Strain, Measured by EBSD and Predicted with the FFT-based Approach[12]

Grain #	EBSD (deg.)	FFT (deg.)
1	2.89	2.18
2	2.52	2.05
3	2.92	2.97
4	2.86	2.33
5	2.26	2.35
6	3.14	2.70
7	3.37	3.06
8	3.21	2.62
9	2.65	2.80
10	2.92	2.37
11	2.22	2.79
12	4.33	3.36
13	3.09	3.26

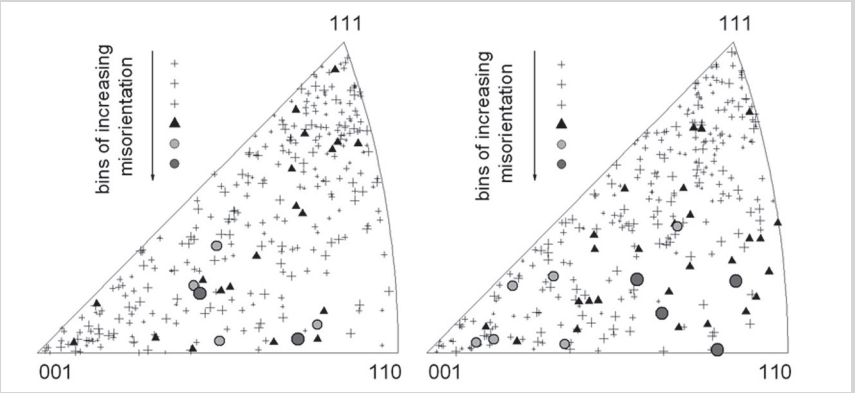


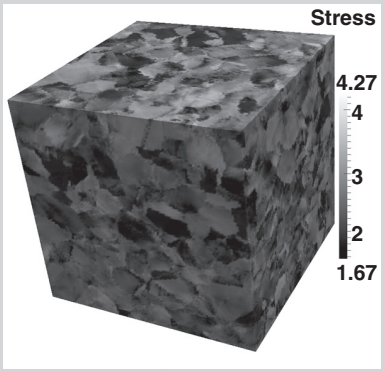
Figure 3. Inverse pole figures of the average orientations and misorientations of the 306 largest Cu grains after 11% tensile strain, (a) measured by EBSD, and (b) predicted with the FFT-based approach. The misorientations were grouped in bins of equal size, and different symbols were assigned to each bin.[12]

using an explicit microstructure update scheme, rigorous for the crystallographic orientations and the CRSS, and including a uniform stretching approximation for the grain morphology that maintains the required regularity of the Fourier grid as deformation proceeds (see Reference 12 for details).

Grains in the region close to the <001>-corner rotate toward the stable orientation <001>. Grains with initial orientations close to the upper half of the <001>-<111>-line exhibit rotations along this line toward the other stable orientation (i.e., <111>). The grains starting near the <110>-corner, or in intermediate orientations between <110> and the mid-section of the <001>-<111>-line rotate toward this line, before going to the stable orientation <111>. The total rotations of these grains are the largest. These features are acceptably reproduced by our simulations, except for the reorientation of grains #8 and #10.

A much less investigated aspect of the local texture evolution is the orientation dependence of the average misorientations. Table I reports the predicted values (in degrees) of the average misorientations (defined as the average over every pixel belonging to a given grain with respect to the average orientation of that grain) inside the 13 largest grains, which are in good agreement with the corresponding experimental values.

To elucidate whether an orientation dependence of the average misorientations exists (and if our model is capable of reproducing it), we investigated the behavior of a larger number of representative grains. Figure 3 shows the average orientations (given by each pole projected in the inverse pole figure) and the average misorientations (given by the different symbols used) of the largest 306 grains (roughly 70% of the measured area), as measured by EBSD and predicted with the FFT-based approach, after 11% tensile strain. The misorientation values of the grains were grouped into six bins of equal size, and different symbols were assigned to each bin. As expected, after 11% tension there is already a mild but noticeable trend of large grains to rotate toward one of the stable <001> and <111> orientations (the region near <110> is mildly depleted of orientations). Moreover, it is evident from both the experiments and the simulations that most of the grains with the highest average misorientation are grains transitioning from their initial orientation near <110> toward the stable orientations. This observation can be explained in the following terms: depending on their initial orientation, the grains of a face-centered cubic (fcc) polycrystal in tension are attracted toward one of the two stable orientations (i.e., <001> or <111>). Grains with orientations in a region of the orientation space, spanning from near <110> toward the mid-section of the <001>-<111>-line, can be pulled simultaneously toward both stable orientations. In this case, the instability of the initial grain orientation and the contribution of interactions with neighbor grains may define the preference of different portions of these "indecisive" grains to rotate toward different stable



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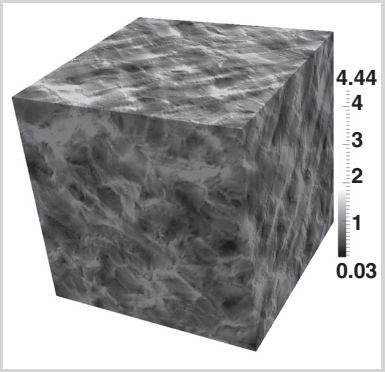

b

Figure 4. Von Mises equivalent (a) stress and (b) strain-rate on the surface of the simulation volume for the measured nickel alloy polycrystal.[23]

orientations. This conflicting attraction toward two different orientations may be accommodated by the development of relatively higher misorientations between different grains' sub-domains, which corresponds to the concept of transition bands[22] in fcc metals.

Only full-field models that account for topological information and grain interaction in the determination of the local micromechanical fields can capture the above described effects. Only image-based models like the VP-FFT formulation can directly use input and be validated with voxelized data. Moreover, the efficient VP-FFT scheme is able to compute this problem (involving more than 2 million DOF) in only a few CPU hours, using standard computational resources.

The final example to be shown here concerns the use of the VP-FFT approach to compute and perform a statistical analysis of the predicted micromechanical fields that develop in a real polycrystal (an IN100 nickel alloy sample) measured by serial-sectioning.[23] From the original image of dimensions 389×146×184 voxels, a subset of 128×128×128 voxels was extracted for input of the VP-FFT model.

Figure 4 shows the predicted von Mises equivalent stress and strain-rate fields on the boundary of the measured microstructure, for an axisymmetric strain-rate of value 1 imposed along the z-axis, and a CRSS of the {111}<110> slip systems of value 1. In what follows we quantify the spatial relationship between high stress regions and microstructural features such as grain boundaries, triple lines, and quadruple points. Euclidean distance maps (see, e.g., Reference 24) for each feature were computed. For this, it was first necessary to classify each voxel based on its neighborhood as being adjacent to a boundary, a triple line, or a quadruple point (otherwise the voxel belongs to the bulk of a grain), in order to calculate a global average distance to each feature. Next, to analyze the relationship between stress and microstructure, the Fourier points were binned according to their predicted von Mises stress, and the distances to each feature type were averaged over the points in each stress class. Figure 5 shows the resulting plot of average distance to boundaries, triple lines, or quadruple points as a function of stress level. Each point represents the averaged distance, normalized by the global average distance to the nearest feature, for points over a certain range of stress, normalized by the global average stress. For grid points with stresses close to the average, the averaged distances are also close to the average values. As the stress increases, the averaged distance decreases, which means that the highest stress points lie close to microstructural features, as one might expect. It is also the case, however, that points with low stresses also lie close to boundaries, triple lines and quadruple points, suggesting that not only do grain boundaries give rise to stress concentrations but that shielding can also occur. See Reference 23 for further extreme value statistics of the predicted micromechanical fields and its correlation with other microstructural features, like crystallographic orientation.

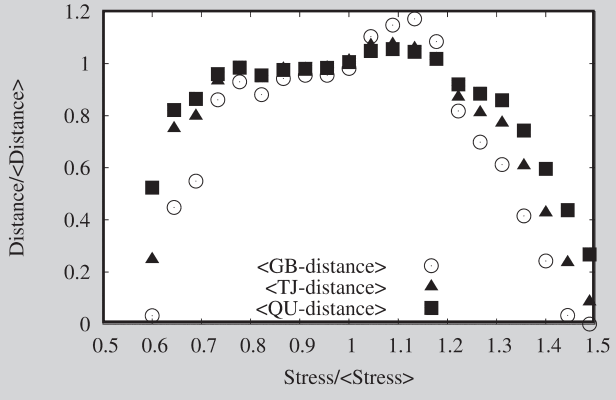

Figure 5. Average normalized distances for the three different microstructural features: grain boundaries (GB), triple lines (TJ), and quadruple point (QU) for each stress class.[23]

CONCLUSION

This study shows that the FFT-based formulation is a viable alternative for performing micromechanical analyses of large sets of microstructural data, such as those produced by emerging methods in 3-D microstructural characterization. In particular, the viscoplastic approximation to crystal plasticity is a useful tool for solving problems involving plastically deforming polycrystals. The existing numerical implementation of the model is being improved via parallelization, incorporating better schemes for microstructural update, and accounting for elasticity in conjunction with viscoplasticity, for a more widely applicable and powerful elasto-viscoplastic (EVP) formulation. Experiments are underway to nondestructively map grain orientations in 3-D using synchrotron radiation[25] before and during a tensile test. These measurements will provide the datasets required for direct validation of the FFT method, as well as other methods that incorporate crystal plasticity.

Besides the rigorous updating of the local crystallographic orientations (due to plastic rotations), and critical resolved shear stresses (due to strain-hardening) presently implemented as part of the VP-FFT formulation, an

accurate prediction of microstructure evolution with a FFT-based approach also requires an appropriate update scheme for the grain morphology due to material convection in a heterogeneous strain field. This problem was first addressed by Lahellec et al.[26] who proposed two ways of dealing with the issue, in the context of the FFT formulation for composite materials. The first approach consists of a Lagrangian large-strain implementation of the FFT-based model for hyperelastic materials and the application of FFT in the initial configuration, in which the grid of Fourier points (simultaneously considered as computational grid and material point grid) remains regular. The second approach corresponds to the case in which the local constitutive relation can be expressed by means of quantities defined in the current configuration only (e.g., Equation 1). In this case, the use of two grids is needed, one computational grid, in which the required FFT's are computed, and one grid of material points, which are convected according to the calculated displacement field. Interpolation is used to transfer field values between the grids, as needed. The applicability of these updating schemes to polycrystals is currently being explored.

An elasto-viscoplastic extension of the FFT-based formulation is also under development. For this, a Euler-implicit time discretization is needed to solve the problem incrementally in time. While the details of the EVP-FFT implementation for polycrystals will be reported in future publications, it is worth mentioning here a couple (among several) of potential applications of such a formulation.

By keeping the elasticity in the problem, it will be possible to translate the computed elastic strains into the lattice spacing changes that are measureable in a diffraction experiment, performing in this way a "numerical" diffraction computation. The predictions resulting from an FFT-based computation will have an important advantage compared with the present state-of-the-art modeling of internal strains, based on homogenization (e.g., Reference 27). In such mean-field computations, lattice spacing changes are computed using non spatially-resolved information on grain-average elastic strains and average grain orientations only. With the proposed full-field approach, the elastic fields will show variations inside each grain, and, as plastic deformation proceeds, the intragranular misorientation and the dislocation density distributions (which can also be efficiently estimated from the micromechanical fields) will increase. This intragranular heterogeneity will affect the angular contribution of different diffraction volumes and, therefore, the profile of simulated diffractograms. This improved capability of the EVP-FFT model will provide a tool for a more refined line profile analysis. Also, the resulting space-resolved predictions of elastic strains will be amenable to direct comparison with local strains measured using novel 3-D x-ray diffraction techniques.[3,4] The EVP-FFT method will also enable problems involving localization of plastic flow to be studied with direct input from microstructural images, which is essential for investigating damage initiation and growth. For example, fatigue cracks are often observed starting from heterogeneities such as voids or brittle particles, and relating variability in fatigue lifetime to microstructural variability remains a significant challenge.[28]

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