Fast Fourier transform-based modelling for the determination of micromechanical fields in polycrystals

Ricardo A. Lebensohn, Anthony D. Rollett, Pierre Suquet

Keeping up with emerging characterization methods of crystalline materials: Fast Fourier Transform-based modelling for the determination of micromechanical fields in polycrystals

Ricardo A. Lebensohn, Anthony D. Rollett and Pierre Suquet

Abstract

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.

1- 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 Focus-Ion-Beam (FIB) combined with Electron Back-Scattering Diffraction (EBSD) now provides a way (although destructive) to characterize local orientations in 3-D (e.g. [1]) with nanometric spatial resolution. Moreover, novel synchrotron-based X-ray diffraction techniques can now be used for in-situ measurement of the positions, shapes, and crystallographic orientations (e.g. [2]) , and even local strains of bulk grains in an aggregate [3-4], with micrometric and sub-micrometric resolution.

From a modelling 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, to its full extent. 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.

As a contribution to facing this challenge, in this overview we report 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, e.g. 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 numerically-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 [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 a FEM calculation is roughly of the same order as the total number of voxels in the image, give an idea of the daunting task that a routinely 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.

2- 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, 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].

Briefly, 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 Green functions 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. For details of the formulation, the interested reader is referred to 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 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 in iteratively adjusting two strain (or strain-rate) and two stress fields. By construction, one the strain fields is compatible and one 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 consider 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:

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

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]. In what follows, we discuss and show some applications of this VP-FFT formulation.

3- Applications to viscoplastic polycrystals

The FFT-based formulation for viscoplastic polycrystals, based on the constitutive representation given by Eq. (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 duplicate 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. [19]), and the orientation dependence of strain localization in strongly heterogeneous polycrystals (e.g. [20]). Among these applications, it is worth mentioning a recent study on dilatational plasticity of porous polycrystalline materials [21], in which the effect on void growth of the crystallinity of the material surrounding intergranular 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 of 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].

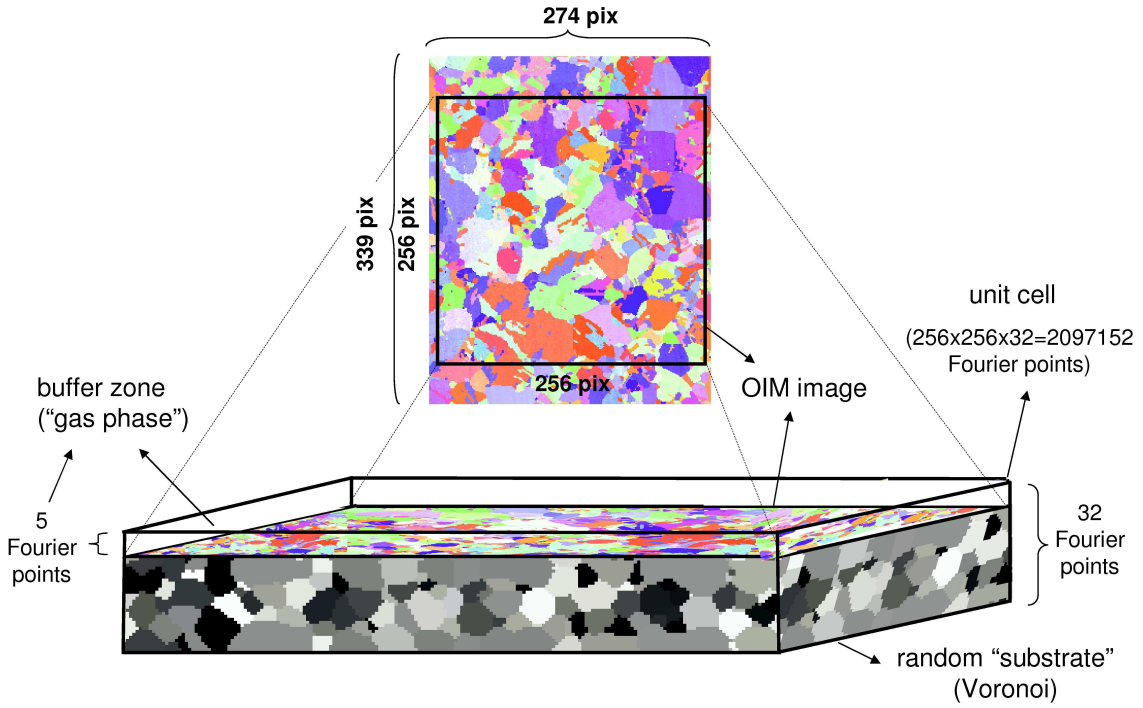

Figure 1: Schematic representation of the 3-D unit cell used in the FFT-based simulations of local orientation and misorientation evolution, with direct input from EBSD images [12].

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 Cu polycrystal deformed in tension. 2-D EBSD was used to characterize the local orientations measured in an area of about 500x500 microns, located on one of the flat surfaces of a recrystallized copper sample, with a spatial resolution of 2 microns, before and after 11% deformation. Since in this case the actual 3-D microstructure of the bulk of the sample was not known, 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 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 Ref. [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 exactly 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, in order to reproduce the actual free surface condition on 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).

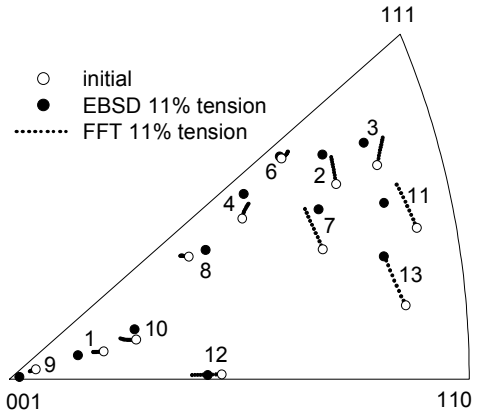

Figure 2: Inverse pole figure of the measured initial orientation and the final average orientation and trajectories predicted with the FFT-based approach for the 13 largest grains in the image [12].

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

Table 1: Average misorientation of the 13 largest grains after 11% tensile strain, measured by EBSD and predicted with the FFT-based approach [12].

Figure 2 shows in an inverse pole figure representation 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, using an explicit microstructure update scheme, rigorous for the crystallographic orientations and the CRSS, and including an uniform stretching approximation for the grain morphology that maintains the required regularity of the Fourier grid as deformation proceeds (see Ref. [12] for details).

Grains in the region close to the <001>-corner rotate towards the stable orientation <001>. Grains with initial orientations close to the upper half of the <001>-<111>-line exhibit rotations along this line towards 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 towards 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. In Table 1 we report 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.

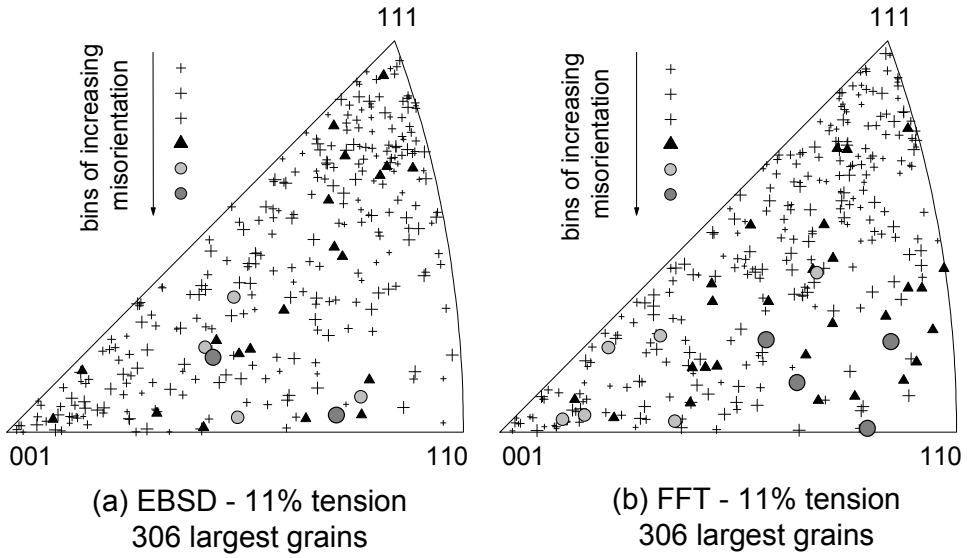

Figure 3: Inverse pole figures of the average orientations and misorientations of the 306 largest grains after 11% tensile strain, (a) measured by EBSD, and (b) predicted with the FFT-based approach. The misorientations were grouped in bins of equal size, and different symbols were assigned to each bin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

To elucidate whether an orientation dependence of the average misorientations does exist (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 towards 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> towards the stable orientations. This observation can be explained in the following terms: depending on their initial orientation, the grains of an fcc polycrystal in tension are attracted towards 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> towards the mid section of the <001>-<111>-line, can be pulled

simultaneously towards 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 towards different stable orientations. This conflicting attraction towards two completely different orientations may be accommodated by the development of relative higher misorientations between different grain's sub-domains, which corresponds to the concept of transition band [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 (a IN100 nickel alloy sample) measured by serial-sectioning [23]. From the original image of dimensions 389×146×184 voxels, a subset of 128x128x128 voxels was extracted for input of the VP-FFT model.

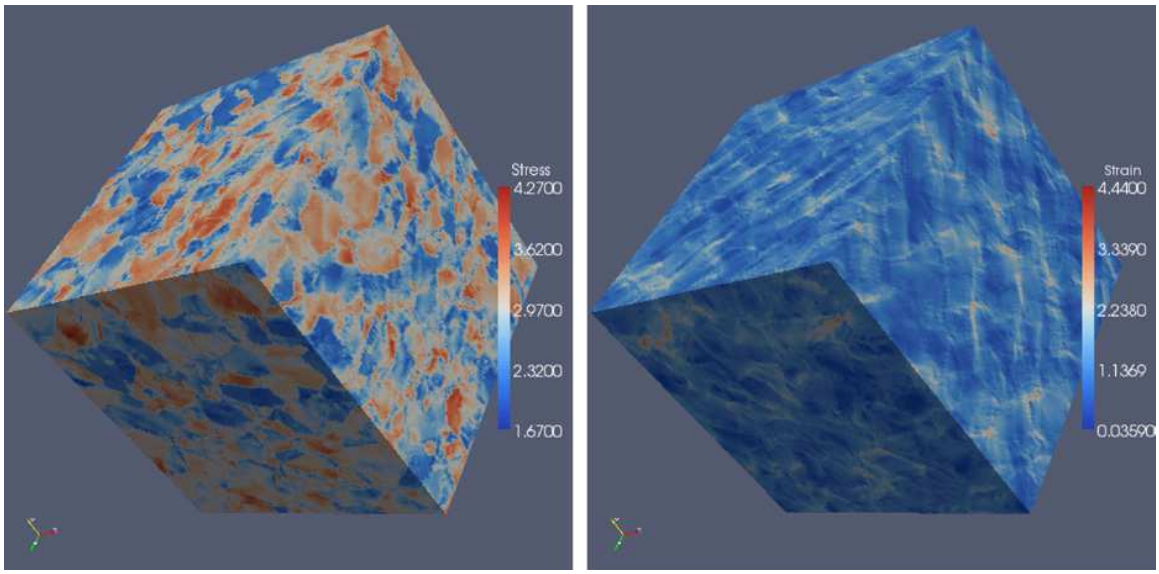

Figure 4: Von Mises equivalent stress and strain-rate on the surface of the simulation volume for the measured nickel alloy polycrystal [23].

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. [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, 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. Further extreme values statistical analysis of the predicted micromechanical fields and its correlation with other microstructural features, like crystallographic orientation, can be found in Ref. [23].

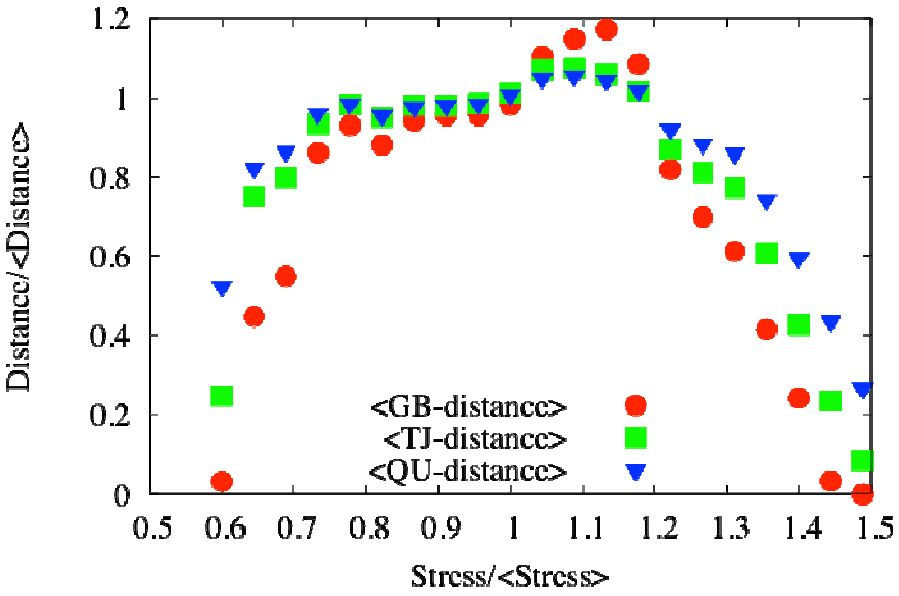

Figure 5: Average normalized distances for the three different microstructural features: grain boundaries (GB), triple lines (TJ) and quadruple point (QU) for each stress class [23].

4- Conclusion and Perspectives

The examples above show 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 has proven to be a useful tool for solving different problems involving plastically-deforming polycrystals. The existing numerical implementation of the model is currently being improved, e.g. 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. Moreover, experiments are underway to non-destructively 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 in 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. Eq. (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, an 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) potential applications of such 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 a FFT-based computation will have an important advantage compared with the present state-of-the-art modelling of internal strains, based on homogenization (e.g. [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 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 of 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].

Acknowledgments

R.A.L. acknowledges support from LANL's Joint DoD/DOE Munitions Technology Program and ASC Physics & Engineering Models, Materials Project. A.D.R. acknowledges support from the User Productivity Technology Transfer and Training Program (PETTT) of the High Performance Computing Modernization Office, by the Office of Basic Energy Sciences under Award Number DE-FG02-09ER46645, and by the MRSEC program of the National Science Foundation under Award Number DMR-0520425. P.S. acknowledges support from the French Agence Nationale de la Recherche under contract BLAN08-3 373405 (ELVIS project).

References

[1] M.D. Uchic, M.A. Groeber, D.M. Dimiduk and J.P. Simmons, "3-D Microstructural Characterization of Nickel Superalloys via Serial-Sectioning using a Dual Beam FIB-SEM," *Scripta Mater*., 55 (2006), pp. 23-28.

[2] E.M. Lauridsen, S.R. Dey, R.W. Fonda and D. Juul-Jensen, "Nondestructive approaches for 3-D materials characterization," *JOM*, 58 (2006), pp. 40-44.

[3] J.S. Park, P. Revecz, A. Kazimirov and M.P.Miller, "A Methodology for Measuring In-Situ Lattice Strain of Bulk Polycrystalline Material Under Cyclic Load," *Rev. Sci. Instrum.*, 78 (2007), p. 023910.

[4] J. Oddershede *et al*., "Determining grain resolved stresses in polycrystalline materials using three-dimensional X-ray diffraction," *J. Appl. Crystallogr*. 43 (2010), pp. 539-549.

[5] H. Moulinec and P. Suquet, "A fast numerical method for computing the linear and nonlinear mechanical properties of composites," *C. R. Acad Sci Paris II* (1994), 318, pp. 1417-1423.

[6] H. Moulinec and P. Suquet, "Numerical method for computing the overall response of nonlinear composites with complex microstructure," *Comput. Meth. Appl. Mech. Eng*., 157 (1998), pp. 69-94.

[7] F. Roters *et al*., "Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications," *Acta mater.* 58 (2010), pp. 1152-1211.

[8] J.C. Michel, H. Moulinec and P. Suquet, "A computational method based on augmented Lagrangians and fast Fourier transforms for composites with high contrast," *Comput. Model. Eng. Sci.* 1 (2000) pp.79-88.

[9] J.C. Michel, H. Moulinec and P. Suquet, "A computational scheme for linear and non-linear composites with arbitrary phase contrast," *Int. J. Numer. Methods Eng.* 52 (2001), pp. 139-158.

[10] R.A. Lebensohn, "N-site modelling of a 3-D viscoplastic polycrystal using Fast Fourier Transform," *Acta Mater.* 49 (2001), pp. 2723-2737.

[11] R.A. Lebensohn, Y. Liu and P. Ponte Castañeda, "On the accuracy of the self-consistent approximation for polycrystals: comparison with full-field numerical simulations," *Acta Mater.* 52 (2004), pp. 5347-5361.

[12] R.A. Lebensohn, R. Brenner, O. Castelnau and A.D. Rollett, "Orientation image-based micromechanical modelling of subgrain texture evolution in polycrystalline copper," *Acta Mater.* 56 (2008), pp. 3914-3926.

[13] Y.U. Wang, Y.M.M. Jin and A.G. Khachaturyan, "Phase field microelasticity theory and modeling of elastically and structurally inhomogeneous solid," *J. Appl. Phys.* 92 (2002), pp. 1351-1360.

[14] D.J. Eyre and G.W. Milton, "A fast numerical scheme for computing the response of composites using grid refinement, " *J. Phys. III* 6 (1999), pp. 41-47.

[15] S. Brisard and L. Dormieux, "FFT-based methods for the mechanics of composites: A general variational framework," *Comput. Mater. Sci*. 49 (2010), pp. 663-671.

[16] J. Zeman, I. Vondrejc, J. Novak and I. Marek, "Accelerating a FFT-based solver for numerical homogenization of periodic media by conjugate gradients," *J. Comput. Phys*. 229 (2010), pp 8065-8071.

[17] F. Willot and Y.P. Pellegrini, "Fast Fourier Transform computations and build-up of plastic deformation in 2D, elastic-perfectly plastic, pixelwise disordered porous media," *Continuum Models and Discrete Systems,* ed. D. Jeulin and S. Forest (Presses Mines ParisTech, 2008), pp.443-450.

[18] R.J. Asaro and A. Needleman, "Texture development and strain hardening in rate dependent polycrystals," *Acta Metall.* 33 (1985), pp. 923-953.

[19] R.A. Lebensohn, O. Castelnau, R. Brenner and P. Gilormini, "Study of the antiplane deformation of linear 2-D polycrystals with different microstructures,". *Int. J. Solids Struct*. 42 (2005), pp. 5441-5459.

[20] R.A. Lebensohn *et al*., "Modeling viscoplastic behavior and heterogenous intracrystalline deformation of columnar ice polycrystals," *Acta Mater.* 57 (2009), pp. 1405-1415.

[21] R.A. Lebensohn, M.I. Idiart, P. Ponte Castañeda and P.G. Vincent, "Dilatational viscoplasticity of polycrystalline solids with intergranular cavities," *Phil. Mag.,* submitted.

[22] I.L. Dillamore, P.L. Morris, C.J.E. Smith, W.B. Hutchinson, "Transition bands and recrystallization in metals," *Proc R Soc Lond A* 329 (1972), pp. 405-420.

[23] A.D. Rollett *et al*., "Stress hot spots in viscoplastic deformation of polycrystals," *Model. Simul. Mater. Sci. Eng.* 18 (2010), 074005, 16pp.

[24] T. Saito and J.I. Toriwaki, "New algorithms for Euclidean distance transformation of an N-dimensional digitized picture with applications," *Pattern Recognit.* 27 (1994), pp. 1551-1565.

[25] C. Hefferan *et al.*, "Statistics of high purity nickel microstructure from high energy X-ray diffraction microscopy," *Comput. Mater. Continua* 14 (2010), pp. 209-219

[26] N. Lahellec, J.C. Michel, H. Moulinec and P. Suquet, "Analysis of inhomogeneous materials at large strains using fast Fourier transforms," *IUTAM Symposium on Computational Mechanics of Solids Materials,* ed. C. Miehe (Dordretcht: Kluwer Academic, 2001) pp. 247-268.

[27] P.A. Turner, C.N. Tomé, "A study of residual-stresses in zircaloy-2 with rod texture," *Acta Metall. Mater*. 42 (1994), pp. 4143-4153.

[28] J.E. Bozek *et al.,* "A geometric approach to modeling microstructurally small fatigue crack formation: I. Probabilistic simulation of constituent particle cracking in AA 7075-T651," *Modelling Simul. Mater. Sci. Eng*. 16 (2008), p. 065007

Ricardo A. Lebensohn is a Scientist with the Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA; Anthony D. Rollett is a Professor with the Department of Materials Science and Engineering, Carnegie-Mellon University, Pittsburgh, PA 15213, USA; Pierre Suquet is a Senior Researcher with the Laboratoire de Mécanique et d'Acoustique/CNRS, 13402 Marseille, France.