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N-SITE MODELLING OF A 3D VISCOPLASTIC POLYCRYSTAL USING FAST FOURIER TRANSFORM

Ricardo A. Lebensohn
Instituto de Física Rosario (UNR-CONICET)
27 de Febrero 210 Bis, 2000 Rosario, Argentina

ABSTRACT

We present a formulation to compute the local response of elastic and viscoplastic anisotropic 3D polycrystals based on the Fast Fourier Transform (FFT) method. This FFT method can be applied to a heterogeneous periodic medium but also to structures in which the size of the heterogeneities is small compared with the size of the specimen. It provides an exact solution of the Lippmann-Schwinger equations and has better numerical performance than small-scale FEM. The results of this n-site FFT formulation are here compared with the predictions obtained for the same microstructure with the 1-site selfconsistent model.

INTRODUCTION

In a recent work [1], Moulinec and Suquet developed a method to compute the overall linear (elastic) and non-linear (elastoplastic) response of heterogeneous composites based on the FFT algorithm. The FFT method – formulated, in principle, for a periodic medium – can also be applied to non-periodic materials, if the size of the heterogeneities remains small compared with the specimen size. The FFT method is a formulation of the n-site kind. It does *not* make use of any homogenization assumption. It does provide an exact solution of the equilibrium equation and has better numerical performance than small-scale FEM for the same problem. Moreover, it avoids meshing and can make direct use of the microstructure images [1]. Briefly, the FFT method is based on computing the exact expression of the Green function of a linear homogeneous comparison material. In this work, after reviewing the elastic FFT formulation, we apply it to obtain the local response of a 3D elastic polycrystal with anisotropic constituent crystallites. Afterwards, we present the extension of the FFT formulation to the viscoplastic regime and a corresponding application to a viscoplastic polycrystal with constituent grains deforming by dislocation glide. The viscoplastic extension is based on an iterative solution for a representative volume element (RVE) of the viscoplastic incompressible Lippmann-Schwinger equations, i.e. : linearized viscoplastic constitutive law, equilibrium and incompressibility equations and periodic boundary conditions across the RVE. In both cases (elastic and viscoplastic), the n-site FFT results are compared with the predictions obtained with the 1-site selfconsistent formulation for the same model polycrystal.

ELASTIC CASE

Formulation [1]

The local problem of an inhomogeneous elastic medium where the size of the heterogeneities is small compared with the size of the specimen of interest can be solved by considering a heterogeneous RVE with periodic boundary conditions, i.e. :

$$\begin{cases} \sigma(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \varepsilon(\mathbf{x}) & \text{in RVE} \quad (1a) \\ \sigma_{ij,j} = 0 & \text{in RVE} \quad (1b) \\ \text{periodic boundary conditions} & \text{across RVE} \quad (1c) \end{cases}$$

Defining a homogeneous comparison medium of stiffness C^o, system (1) is formally equivalent to:

$$\begin{cases} \sigma(\mathbf{x}) = C^o : \varepsilon(\mathbf{x}) + \tau(\mathbf{x}) & \text{in RVE} \quad (2a) \\ \sigma_{ij,j} = 0 & \text{in RVE} \quad (2b) \\ \text{periodic boundary conditions} & \text{across RVE} \quad (2c) \end{cases}$$

where the perturbation field associated with the heterogeneity is given by: $\tau(\mathbf{x}) = \delta C(\mathbf{x}) : \varepsilon(\mathbf{x})$ with $\delta C(\mathbf{x}) = C(\mathbf{x}) - C^o$. Combining the constitutive equation (2a) and equilibrium equation (2b) we get:

$$C^o_{ijkl}\, u_{kl,j}(\mathbf{x}) + \tau_{ij,j}(\mathbf{x}) = 0 \tag{3}$$

Solving (3) by means of the Green function method gives:

$$C^o_{ijkl}\, G_{km,lj}(\mathbf{x}) + \delta_{im}\delta(\mathbf{x}-\mathbf{x}') = 0 \tag{4}$$

The local strain fluctuation $\tilde{\varepsilon} = \varepsilon - E$ can be obtained as a convolution in the cartesian space:

$$\tilde{\varepsilon}_{ij}(\mathbf{x}) = \text{sym}\left(\int_{R^3} G_{ik,jl}(\mathbf{x}-\mathbf{x}')\ \tau_{kl}(\mathbf{x}')\, d\mathbf{x}' \right) \tag{5}$$

Calling $\Gamma^o_{ijkl} = \text{sym}\left(G_{ik,jl}\right)$ and using the symbolic representation for convolution we obtain:

$$\tilde{\varepsilon} = \Gamma^o * \tau \tag{6}$$

If (6) is transformed into the Fourier space, it gives a (tensor) product:

$$\hat{\tilde{\varepsilon}} = \hat{\Gamma}^o : \hat{\tau} \tag{7}$$

where $\hat{\Gamma}^o$ can be readily calculated as:

$$\hat{\Gamma}^o_{ijkl} = -\frac{1}{2}\left(\xi_l \xi_j A'^{-1}_{ik} + \xi_l \xi_i A'^{-1}_{jk}\right) \tag{8}$$

where ξ is a point in Fourier space and:

$$\hat{G}_{ik} = A'^{-1}_{ik} = \left[\xi_l \xi_j C^o_{ijkl}\right]^{-1} \tag{9}$$

Algorithm [1]

The 3D RVE can be divided into a regular grid $\{\mathbf{x}_d\}$ defined by:

$$\{\mathbf{x}_d\} = \left\{ \left((i_1 - 1)\cdot\frac{L_1}{N_1}, (i_2 - 1)\cdot\frac{L_2}{N_2}, (i_3 - 1)\cdot\frac{L_3}{N_3} \right); i_q = 1,...N_q\ ,\ q = 1,3 \right\} \tag{10}$$

where L_q and N_q are the wavelength and the number of points along each space direction. If a strain E is prescribed to the RVE, the algorithm can be initialized with: $\tilde{\varepsilon}^0(\mathbf{x})=0$ and $\sigma^0(\mathbf{x})=C^0:E\ ;\ \forall \mathbf{x}\in\{\mathbf{x}_d\}$. Iteration (i+1) – provided $\tilde{\varepsilon}^i, \sigma^i$ are known – consists in:

1- $\tau^i(\mathbf{x}_d)=\sigma^i(\mathbf{x}_d)-C^0:\varepsilon^i(\mathbf{x}_d)$

2- $\hat{\sigma}^i=\mathrm{fft}(\sigma^i)\ ;\ \hat{\tau}^i=\mathrm{fft}(\tau^i)$

3- Convergence test: is equilibrium fulfilled?

4- $\hat{\tilde{\varepsilon}}^{i+1}=\hat{\Gamma}^0:\hat{\tau}^i \quad \text{with} \quad \hat{\tilde{\varepsilon}}^{i+1}\big|_{(\xi=\bar{0})}=0$

5- $\tilde{\varepsilon}^{i+1}=\mathrm{fft}^{-1}\left(\hat{\tilde{\varepsilon}}^{i+1}\right)$ and $\sigma^{i+1}(\mathbf{x}_d)=C(\mathbf{x}_d):\left(E+\tilde{\varepsilon}^{i+1}(\mathbf{x}_d)\right)$

In the latter, *fft* and *fft*$^{-1}$ denote the application of direct and inverse discrete Fast Fourier Transform algorithms, respectively. Concerning step #3, a measure of the error in the equilibrium condition can be obtained by taken Fourier transform to: $\sigma_{ij,j}=0$. This leads to the following convergence condition:

$$\frac{\left\langle\left|\xi_j\hat{\sigma}^i_{ij}\right|\right\rangle}{\left\|\hat{\sigma}^i(\xi=\bar{0})\right\|}<10^{-4} \tag{11}$$

where <.> denotes spatial average and $\left\|\hat{\sigma}^i(\xi=\bar{0})\right\|$ is an appropriate normalization factor.

Results

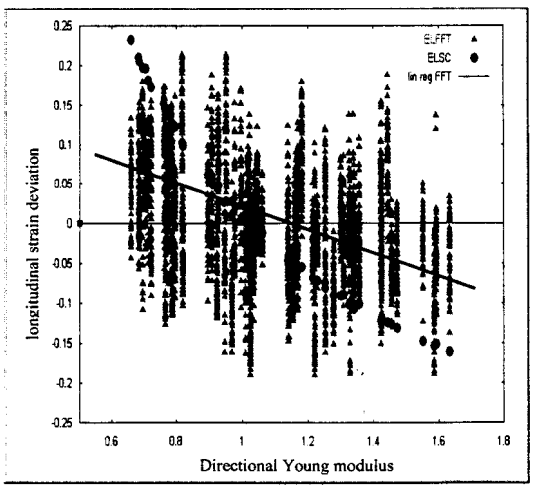

Figure 1: Relative longitudinal strain deviation calculated with 1-site ELSC and FFT vs. Directional Young modulus for a Cu polycrystal under uniaxial tension. Straight line: linear regression of FFT points.

Figure 1 shows a comparison between the 1-site elastic selfconsistent (ELSC) model and the n-site elastic FFT formulation. Both calculations were performed for a Cu polycrystal with 64 randomly oriented grains under uniaxial tension. In the FFT case the grains were cubes arranged in a 4x4x4 structure. Using a grid of 16x16x16 Fourier points, each grain contained 64 points. The ELSC gives one spot while the FFT gives 64 spots per grain. The ELSC predictions show a monotonic behavior as a function of the directional Young modulus with negative slopes. The regression line In the FFT case also shows a negative but less pronounced slope. We conclude that in the FFT case not only the orientation but also the neighbourhoods are playing a role in dictating the local behavior. Finally, it can be observed that the overall dispersions of the local strain predicted by both models are of same magnitude (± 20 % aprox.).

VISCOPLASTIC CASE

Formulation

The local non-linear behavior of a anisotropic polycrystal deforming by dislocation glide can be described in terms of a tangent approximation [2]:

$$\sigma'(\mathbf{x}) = M^{tg^{-1}}(\mathbf{x}) : \dot{\varepsilon}(\mathbf{x}) + S^{o}(\mathbf{x}) \tag{12}$$

$$M^{tg}(\mathbf{x}) = n\,\gamma_o \sum_s \frac{m^s(\mathbf{x}) \otimes m^s(\mathbf{x})}{\tau_o^s(\mathbf{x})} \left(\frac{m^s(\mathbf{x}) : \sigma'(\mathbf{x})}{\tau_o^s(\mathbf{x})} \right)^{n-1} \tag{13}$$

where in (13) we used the well-known viscoplastic law (see [2] for details). The homogeneous comparison medium may also have a tangent behavior:

$$\Sigma' = L_o^{tg} : \dot{E} + S^{oo} \tag{13}$$

Considering incompressibility, the equivalent to system (2) in viscoplasticity becomes:

$$\begin{cases} L^{tg}_{o\,ijkl}\, \dot{u}_{k,lj} + \tau_{ij,j} - p_{,i} = 0 & \text{in RVE} \quad (14a) \\ \dot{u}_{k,k} = 0 & \text{in RVE} \quad (14b) \\ \text{periodic boundary conditions} & \text{across RVE} \quad (14c) \end{cases}$$

where the perturbation field is now defined by:

$$\tau_{ij} = \tilde{\sigma}'_{ij} - L^{tg}_{o\,ijkl}\, \tilde{\varepsilon}_{kl} \tag{15}$$

where $\tilde{\varepsilon} = \dot{\varepsilon} - \dot{E}$ and $\tilde{\sigma}' = \sigma' - \Sigma'$ are the local fluctuation in strain-rate and deviatoric stress respectively. System (14) can be also solved by means of the Green function method, i.e.:

$$\begin{cases} L^{tg}_{o\,ijkl}\, G_{km.lj}(\mathbf{x}) - H_{m,i}(\mathbf{x}) + \delta_{im}\delta(\mathbf{x}-\mathbf{x}') = 0 \\ G_{km.k}(\mathbf{x}) = 0 \end{cases} \tag{16}$$

$$\tilde{\varepsilon}_{ij}(\mathbf{x}) = \text{sym}\left(\int_{R^3} G_{ik,jl}(\mathbf{x}-\mathbf{x}')\ \tau_{kl}(\mathbf{x}')\, d\mathbf{x}' \right) \tag{17}$$

$$\tilde{\varepsilon} = \Gamma^o * \tau \quad \Rightarrow \quad \hat{\tilde{\varepsilon}} = \hat{\Gamma}^o : \hat{\tau} \tag{18}$$

Taking Fourier transform to (16) we obtain:

$$\begin{cases} \xi_i \xi_j\, L^{tg}_{o\,ijkl}\, \hat{G}_{km} - i\xi_i \hat{H}_m = \delta_{im} \\ \xi_k \hat{G}_{km} = 0 \end{cases} \tag{19}$$

System (19) can be written in the following matricial form [3]:

$$\underbrace{\begin{vmatrix} & & & \xi_1 \\ & A'_{ik} & & \xi_2 \\ & & & \xi_3 \\ \xi_1 & \xi_2 & \xi_3 & 0 \end{vmatrix}}_{A''_{(4x4)}} \times \begin{vmatrix} & \hat{G}_{km} & \\ -i\hat{H}_1 & -i\hat{H}_2 & -iH_3 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{vmatrix} \tag{20}$$

from where:

$$\begin{aligned} \hat{G}_{jk} &= A''^{-1}_{jk} \qquad j,k = 1,3 \\ -i\hat{H}_j &= A''^{-1}_{4j} \qquad j = 1,3 \end{aligned} \tag{21}$$

The local fluctuation of the pressure field is given by:

$$\tilde{p}(\mathbf{x}) = \int_{R^3} H_{i,j}(\mathbf{x}-\mathbf{x}')\ \tau_{ij}(\mathbf{x}')\,d\mathbf{x}' \tag{22}$$

$$\tilde{p} = H_{i,j} * \tau_{ij} \quad \Rightarrow \quad \hat{\tilde{p}} = \hat{H}_{i,j}\ \hat{\tau}_{ij} \tag{23}$$

$$\hat{\tilde{p}} = \left(-i\hat{H}_i\right)\xi_j\ \hat{\tau}_{ij} \tag{24}$$

The equilibrium statement in Fourier space is now written as:

$$\frac{\left\langle \left| \xi_i \hat{\sigma}'_{ij} - \xi_i \hat{\tilde{p}} \right| \right\rangle}{\left\| \hat{\sigma}(\xi=\bar{0}) \right\|} < 10^{-4} \tag{25}$$

Algorithm

As for the reference medium, a Voigt average is assumed: $L_o^{tg} = \left\langle M^{tg^{-1}}(\mathbf{x}) \right\rangle$. If a strain-rate $\dot{E}$ is prescribed to the RVE, the algorithm can be initialized with: $\tilde{\varepsilon}^o(\mathbf{x}) = 0$ while to get $\sigma'^o(\mathbf{x})$ we solve $\dot{E} = \gamma_o \sum_s m^s(\mathbf{x}) \left(\frac{m^s(\mathbf{x}) : \sigma'^o(\mathbf{x})}{\tau_o^s(\mathbf{x})} \right)^n \forall \mathbf{x} \in \{\mathbf{x}_d\}$. With $\tilde{\varepsilon}^i, \sigma'^i$ being known, iteration (i+1) reads:

1- $\tau^i(\mathbf{x}_d) = \tilde{\sigma}'^i(\mathbf{x}_d) - L_o^{tg} : \tilde{\varepsilon}^i(\mathbf{x}_d)$

2- $\hat{\sigma}'^i = \mathrm{fft}\left(\sigma'^i\right)$; $\hat{\tilde{p}}^i = \left(-i\hat{H}_i\right)\xi_j\ \hat{\tau}^i_{ij}$; $\hat{\tau}^i = \mathrm{fft}\left(\tau^i\right)$

3- Convergence test: is equilibrium fulfilled? (see (25))

4- $\hat{\tilde{\varepsilon}}^{i+1} = \hat{\Gamma}^o : \hat{\tau}^i$ with $\hat{\tilde{\varepsilon}}^{i+1}\Big|_{(\xi=\bar{0})} = 0$

5- $\tilde{\varepsilon}^{i+1} = \mathrm{fft}^{-1}\left(\hat{\tilde{\varepsilon}}^{i+1}\right)$ and to get σ'^{i+1} solve: $\dot{E} + \tilde{\varepsilon}^{i+1}(\mathbf{x}_d) = \gamma_o \sum_s m^s(\mathbf{x}_d) \left(\frac{m^s(\mathbf{x}_d) : \sigma'^{i+1}(\mathbf{x}_d)}{\tau_o^s(\mathbf{x}_d)} \right)^n$

Results

Figure 1 shows a comparison between the 1-site viscoplastic selfconsistent (VPSC) [2] model

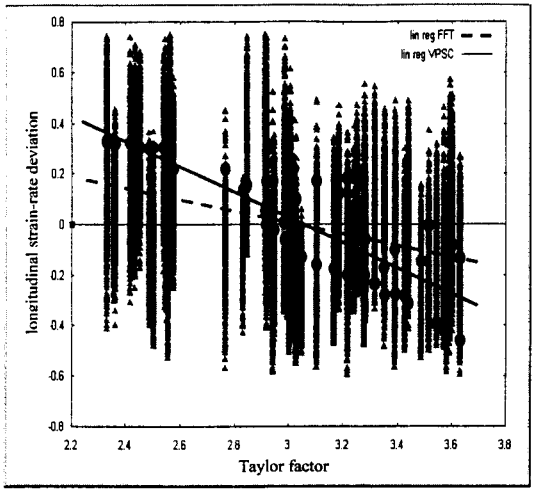

Figure 2: Relative longitudinal strain-rate deviation calculated with 1-site VPSC and FFT vs. Taylor factor for a fcc polycrystal under uniaxial tension. Straight lines: linear regression of VPSC and FFT points.

and the n-site viscoplastic FFT formulation. As in the elastic case, both calculations were performed for a fcc polycrystal with 64 randomly oriented grains under uniaxial tension. In the FFT case the grains were cubes arranged in a 4x4x4 structure. We used a grid of 32x32x32 Fourier points, so each grain contained 512 points. The regression line of the VPSC points displays a negative slope as a function of the Taylor factor (TF). (the VPSC output shows two branches at high TF). As in the elastic case, the regression line of the FFT points also shows a negative but less pronounced slope, due to neighbourhood effects. The overall dispersion of the local strain-rate predicted by n-site FFT formulation is twice higher than in the 1-site VPSC case.

CONCLUSION AND PERSPECTIVES

The FFT formulation has been applied to solve the local response of an elastic anisotropic polycrystal and the method has been extended to the viscoplastic regime. The numerical performance of the method (in a single-processor machine) is largely superior to a FEM calculation since the FFT method does not involve inversions of large matrices as FEM does. For instance, the viscoplastic FFT calculation whose results are shown in figure 2 (that involved 32^3=32768 points) took 2 minutes in a PC Pentium III 450 MHz. Furthermore, the FFT algorithm can also be parallelized [1]. In a coming paper [4] we will present a more detailed description of the viscoplastic FFT formulation (i.e.: influence of the spatial resolution and the choice of comparison medium on the convergence, etc.) together with new applications to more realistic microstructures in order to get predictions of texture development, subgrain formation, intragranular distribution of stored energy, etc.

REFERENCES

[1] **Moulinec, H. and Suquet P.**, *A numerical method for computing the overall response of nonlinear composites with complex microstructures*, Comput. Methods Appl. Mech. Engrg. Vol.157, 1998, pp. 69-94.

[2] **Lebensohn R.A. and Tomé C.N.**, *A selfconsistent approach for the simulation of plastic deformation and texture development of polycrystals: application to Zirconium alloys*, Acta Metall. Mater. Vol. 41, 1993, pp. 2611-2624.

[3] **Lebensohn R.A., Turner P.A, Signorelli J.W., Canova G.R. and Tomé C.N.**, *Calculation of intergranular stresses based on a large strain viscoplastic selfconsistent polycrystal model*, Mod. Sim. Mat. Sci. Eng. Vol. 6, (1998) pp. 447-465.

[4] **Lebensohn R.A.**, under preparation.