Fast Fourier Transform-based micromechanical modeling of polycrystals with direct input from microstructural images

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FFT-based formulation for polycrystals: fast prediction of mechanical behavior of 3-D polycrystalline materials

CP-FEM (mesh, integration points)

FFT-based method (voxels)

local (single crystal) constitutive equation for each voxel

numerically-generated

Advantages of a FFT-based approach:

- **Easier preprocessing:** no meshing involved, voxelized data used as is
- **Faster computation:** FFT algorithm very efficient
- **Direct validation:** fields mapped on a regular grid, c.f. EBSD, DIC, etc

Disadvantages:

Restricted boundary condition
Fourier grid non-conformal to grain boundaries
Proposed by Suquet and co-workers, for linear (Moulinec & Suquet, 1994) and nonlinear composites (Moulinec & Suquet 1998, Michel-Moulinec-Suquet, 2000, 2001), and adapted for polycrystals (PX):


→ dilatational VP PXs (Lebensohn et al., Phil Mag 2011).


→ finite-strain EVP PXs (Eisenlohr, Diehl, Lebensohn, Roters, IJP, 2013).

Based on the equivalence between the micromechanical response of a heterogeneous medium and a homogenous medium with eigenstrains.

Non-linear problems are treated similarly to linear problems, using the concept of “Linear Reference Material”.
FFT-based approach for elastically heterogeneous materials (*)

\[ \sigma(x) = C(x) : \epsilon(x) \]

local elasticity

\[ \sigma(x) = \sigma(x) + C^0 : \epsilon(x) - C^0 : \epsilon(x) = \]

\[ = C^0 : \epsilon(x) + \Delta C : \epsilon(x) = C^0 : \epsilon(x) + \tau(x) \]

stiffness of a linear reference medium

\[ \tau(x) = \Delta C : \epsilon(x) \]
polarization (heterogeneity) field

function of solution requires iterative procedure to adjust

\[ \epsilon_{ij}(x) = E_{ij} + \text{sym} \left( \int_{R^3} G_{ik, jl}(x - x') \tau_{kl}(x') \, dx' \right) \Rightarrow \hat{\epsilon} = \Gamma^0 \ast \tau \Rightarrow \hat{\epsilon} = \hat{\Gamma}^0 : \hat{\tau} \Rightarrow \text{FFT!} \]

Upon convergence: \( \sigma(x), \epsilon(x) \)

FFT-based approach for viscoplastic polycrystals (VP-FFT) (*)

E.g. viscoplastic FFT with input from EBSD:

\[ \dot{\varepsilon}(x) = \dot{\gamma}_0 \sum_s \mathbf{m}^s(x) \left( \frac{\sigma^s(x)}{\tau^s(x)} \right)^n \times \text{sgn} \left( \mathbf{m}^s(x) \cdot \sigma'(x) \right) \]

\[ \tau(x) = \sigma'(x) - \mathbf{L}^0 \dot{\varepsilon}(x) \]

\[ \tilde{\varepsilon}(x) = \Gamma^0 \left( \mathbf{L}^0 \right) \ast \tau \Rightarrow \tilde{\varepsilon}(x) = \hat{\Gamma}^0 : \hat{\tau} \Rightarrow \dot{\varepsilon}(x) = \dot{E} + \text{FT}^{-1} \hat{\Gamma}^0 : \hat{\tau} \]

**FEM-FFT comparison** [1]

- FEM and FFT solvers implemented within the same finite-strain framework [2]
- Identical constitutive model: elasto-viscoplastic single crystal (fcc) behavior
- At the same resolution, FEM and FFT predict similar strain distributions, but FFT strain fields are more heterogeneous
- At higher resolutions (unreachable with FEM within decent computation times), FFT predicts very detailed strain localization pattern

↓

Our ability to solve the problem with higher spatial resolution allows us uncovering new and relevant features of the micromechanical response

Porosity evolution in 3-D: synthetic polycrystal vs. isotropic matrix (*)

Microstructural effects on void growth:
Qualitative comparison with experiments

\[ \hat{\varepsilon}_{eq}(x)/\hat{\varepsilon}_{eq} \]

\[ \phi = 11\% \]

shocked Cu (**)
hard link → no coalescence

Taylor factor

\[
\begin{array}{cc}
\text{Min} & \text{Max} \\
2.26886 & 2.54903 \\
2.54903 & 2.93101 \\
2.93101 & 3.11208 \\
3.11208 & 3.36316 \\
3.36316 & 3.87420 \\
\end{array}
\]

soft link → coalescence


(**) Escobedo et al, J. Appl. Phys., 2011
VP-FFT calculation with input from 2-D data: misorientation in Cu polycrystal


Grains with orientations near transition line may be “pulled” towards different stable orientations → prone to develop higher misorientations, in average

Intragranular misorientation → orientation-dependent (highest near [110])
Image-based modelling using 3-D orientation information

FIB-EBSD → voxelized 3-D grain orientation maps → FFT analysis (*)

pure Ni

VM stress
VM strain-rate

 (*) Rollett, Lebensohn et al., MSMSE, 2010
Measured Polycrystal (IN100) (*)

FFT simulations

von Mises Stress

Von Mises Strain Rate

Euclidean Distance Maps

Stresses vs distance from features

High stresses concentrate near grain boundaries, triple junctions, etc. However, low stress points also cluster near boundaries.

(*) Rollett, Lebensohn et al., MSMSE, 2010
In-situ observation/modelling of orientation fields of 2-D bulk grains (*)

In general, 2-D orientation fields are stacked together to obtain a 3D volume.

Reorientation of large grains at 14%

Measured vs. predicted Kernel Average Misorientation (KAM) (*):

HEDM initial

HEDM 12% strain

FFT

mid layer

KAM [deg]

2-D EBSD: consistent with simulations

FFT model ≈ 2-D EBSD ≠ 3-D HEDM