# Micromechanics of polycrystals: full-field computations and second-order homogenization approaches

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Models based on crystal plasticity are increasingly used in engineering applications. Three key elements of these methods are: 1) a proper consideration of the plastic deformation mechanisms at single crystal level; 2) a representative description of the polycrystal's microstructure, and 3) an appropriate scheme to connect the microstates in the crystallites and the polycrystal's response. The latter can be based on homogenization theories, which rely on a statistical description of the microstructure, or be full-field solutions (e.g. crystal plasticity Finite Elements or spectral methods), which requires a spatial description of the microstructure.

In the first part of this talk we will present a spectral formulation based on crystal plasticity (CP) and Fast Fourier Transforms (FFT) for the determination of micromechanical fields in plastically-deformed 3-D polycrystals. This formulation, pioneered by Suquet and coworkers as a fast algorithm to compute the response of composites using as input a digital image of their microstructures (e.g. [1]), has been in turn adapted to deal with polycrystals deforming by dislocation glide [2].

Next, we will show applications of the CP-FFT formulation to the following problems: prediction of orientation-dependent intragranular misorientations in Cu polycrystals deformed in tension [3], prediction of strain localization in columnar ice polycrystals deformed in creep [4], study of effect of the matrix's crystallinity on the dilatational plastic behavior of polycrystals with intergranular cavities [5].

Finally, the CP-FFT formulation will be used to assess the accuracy of different available nonlinear homogenization approaches for the prediction of the viscoplastic behavior of polycrystalline aggregates. We will show that Ponte Castañeda's second-order formulation [6], which explicitly uses information on average intragranular field fluctuations, implemented within the widely-used ViscoPlastic Self-Consistent (VPSC) code, yields the most accurate results [7].

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