A comparison between different methods for the numerical simulation of polycrystalline aggregates

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ABSTRACT

The macroscopic behavior of polycrystalline materials is largely influenced by the shape, the arrangement and the orientation of crystallites. Different methods have thus been developed to determine the effective behavior of such materials as a function of their microstructural features. In this work, which focuses on polycrystalline materials with an elastic-viscoplastic behavior, the self-consistent (SC) method [1], the finite element (FE) method and the spectral (FFT) method [2] are compared. These common methods are used to determine the effective behavior of different 316L polycrystalline aggregates subjected to various loading conditions (uniaxial tension, cyclic tension/compression).

Independently on the loading conditions, no significant difference is observed between the SC, FE and FFT methods at the macroscopic scale. The application of the FE method however requires important computational ressources while the SC method provides reasonable estimates within very short computation times. Also, while kinematical compatibility constraints are equally fulfilled with the FE and FFT methods, static equilibrium conditions are better respected with the FFT method. At the microscale, some discrepancies exist between the SC method and the other methods. Indeed, since the SC method does not explicitly account for neighborhood effects, it fails in providing an accurate description of the mechanical response associated with a specific crystallite. The SC method nevertheless gives a reasonable description of the average response obtained for a group of crystallites with identical features (e.g. shape, crystallographic orientation).

References

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[2] H. Moulinec, P. Suquet, A numerical method for computing the overall response of non- linear composites with complex microstructure, Computer Methods in Applied Mechanics and Engineering 157, 69–94, 1998.