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SOME NUMERICAL ASPECTS OF FINITE ELEMENT MODELS FOR POLYCRYSTALLINE HOMOGENIZATION

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An interesting option to predict the macroscopic plastic response of a polycrystalline metal is the use of homogenization models based on crystal plasticity (CP) models for the grain behavior. The main advantage of these models over standard phenomenological approximations (J_2 theory, etc.) is the ability to include the effect of the microstructure (grain shapes, orientations, size distributions, etc) and its evolution on the anisotropic flow stress and hardening behavior.

In order to capture the local stress and strain fields accurately and to analyze the influence of the actual grain shape and local details of the grain spatial distribution, computational homogenization arises as an ideal tool. Computational homogenization is based on the numerical simulation of the mechanical behavior of a representative volume element (RVE) of the material microstructure. The numerical solution of the boundary value problem is generally done by the finite element method [1, 2, 3]

In this study several aspects related to the finite element implementation of computational homogenization of polycrystals will be analyzed and some methodologies will be proposed to improve the efficiency and accuracy of the polycrystalline models. In relation with the CP model, an efficient implementation of visco-plastic laws for very high strain rate sensitivity exponents will be developed. Regarding the geometric representation of the RVE, complex microstructures defined by voxels and represented by cubic elements will be compared with microstructures formed by Voronoi teselations meshed with tetrahedral elements. Finally, an alternative formulation of the finite element model based on superelements defined by the grain polygons will be proposed. The resulting polycrystalline model will be used to predict the mechanical behavior and texture evolution of nano-Ti under large deformations.

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