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A multi-scale homogenization model for fine-grained porous viscoplastic polycrystals: II – Applications to FCC and HCP materials

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ABSTRACT

In Part I of this work (Song and Ponte Castañeda, 2018a), a new homogenization model was developed for the macroscopic behavior of three-scale porous polycrystals consisting of random distributions of large pores in a fine-grained polycrystalline matrix. In this second part, the model is used to investigate both the instantaneous effective behavior and the finite-strain macroscopic response of porous FCC and HCP polycrystals for axisymmetric loading conditions. The stress triaxiality and Lode parameter are found to have significant effects on the evolution of the substructure, which in turn have important implications for the overall hardening/softening behavior of the porous polycrystal. The intrinsic effect of the texture evolution of the polycrystalline matrix is inferred by appropriate comparisons with corresponding results for porous isotropic materials, and found to be significant, especially at low triaxialities. In particular, the predictions of the model identify, for the first time, two disparate regimes for the macroscopic response of porous polycrystals: a porosity-controlled regime at high triaxialities, and a texture-controlled regime at low triaxialities. The transition between these two regimes is found to be quite sharp, taking place between triaxialities of 1 and 2.

1. Introduction

In the preceding paper (Song and Ponte Castañeda, 2018a), henceforth referred to as Part I, we have proposed a finite-strain model for the macroscopic behavior of three-scale porous polycrystals containing large pores randomly distributed in a fine-grained polycrystalline matrix. The model is based on the fully optimized second-order (FOSO) method of Ponte Castañeda (2015)—used in an iterated manner (Agoras and Ponte Castañeda, 2013)—and is referred to as the Iterated Second-Order (ISO) model. The ISO model consists of two main ingredients: (i) the determination of the instantaneous response of the porous polycrystals for fixed values of the substructural variables, and (ii) the prediction of the evolution of the substructural variables at finite strains.

In this model, the substructural variables characterizing the two-scale structure of the porous polycrystal are given by the set

$$\mathbf{s} \equiv \{f, w_1^p, w_2^p, \mathbf{G}^p; \mathbf{Q}^{(1,r)}, w_1^g, w_2^g, \mathbf{G}^g\}. \tag{1}$$

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Here, f is the volume fraction of the pores (porosity), $w_1^p = a_3^p/a_1^p$ and $w_2^p = a_3^p/a_2^p$ are two aspect ratios of the representative ellipsoids characterizing the shape (and distribution) of the pores (a_1^p, a_2^p and a_3^p being the lengths of the three semi-axes of the ellipsoid), $\mathbf{G}^p$ is a second-order rotation tensor characterizing the orientation of the principal axes of the pores relative to the laboratory axes (see Fig. 1(c) in Part I). In addition, the $\mathbf{Q}^{(1,\,r)}$ $(r = 1, \ldots, N)$ are rotation tensors describing the crystallographic orientation of the single-crystal phases in the polycrystalline matrix, $w_1^g = a_3^g/a_1^g$ and $w_2^g = a_3^g/a_2^g$ are the two aspect ratios characterizing the average ellipsoidal shape of the crystal grains (a_1^g, a_2^g and a_3^g being the lengths of the three semi-axes of the grain ellipsoid), and $\mathbf{G}^g$ is a second-order rotation tensor describing the orientation of the principal directions of the ellipsoidal grains relative to the laboratory axes. Of these substructural variables (1), the first four (f, w_1^p, w_2^p, and $\mathbf{G}^p$) describe the porous mesostructure of the composite (see Fig. 1(a) of Part I), while the remaining variables characterize the underlying microstructure of the polycrystalline matrix (see Fig. 1(b) of Part I).

The ISO model makes use of the effective behavior of a suitably chosen three-scale linear comparison composite (LCC)—with substructure identical to that of the nonlinear porous polycrystal of interest—to estimate the effective behavior of the nonlinear composite. In particular, the three-scale homogenization problem for the LCC is decomposed into two double-scale problems for the associated meso- and micro-structure, so that the effective behavior of the LCC can be determined by means of a two-step sequential homogenization approach. At the microscale, the effective properties of the linear polycrystalline matrix are determined by means of the self-consistent estimates (Willis, 1977), while at the mesoscale, the effective properties of the porous LCC are obtained by means of the estimates of the Ponte Castañeda and Willis (1995) type. In addition, as discussed in Section 3.2 of Part I, the iterated homogenization procedure of Agoras and Ponte Castañeda (2013) is used to "discretize" the polycrystalline matrix of the LCC, by allowing the matrix properties in the LCC to be *non-uniform*, thereby generating improved estimates for the effective behavior of the nonlinear porous polycrystal, especially for low porosities and high stress triaxialities (see also the introduction to Section 4 of Song and Ponte Castañeda, 2017a, for a similar development in the context of porous single crystals). Furthermore, consistent homogenization estimates for the strain-rate and spin fields in the pores and grains are used to develop evolution equations for the substructural variables (1), characterizing the evolution of the size, shape and orientation of the pores (at the mesoscale), as well as of the morphological and crystallographic textures of the polycrystalline matrix (at the microscale).

In this paper, we consider specific applications of the ISO model for two different types of porous polycrystals, including the porous (high-symmetry) FCC polycrystals in Section 2 and porous (low-symmetry) HCP polycrystals in Section 3. In each section, we examine both the instantaneous effective behavior of the porous polycrystals for fixed states of the substructure, as well as the finite-strain macroscopic response of the porous polycrystals with evolving substructures, under axisymmetric loading conditions for different values of the stress triaxiality and Lode parameter. The effect of the loading conditions on the substructure evolution, field fluctuations, and the overall hardening/softening behavior of the porous polycrystals is investigated in detail. In addition, the intrinsic effect of the texture evolution for the polycrystalline matrix is deduced by comparing with the corresponding results for the porous isotropic materials. Finally, some general conclusions will be drawn in Section 4.

2. Applications to porous FCC polycrystals

In this section, we employ the ISO model to study the instantaneous effective behavior and finite-strain response of porous FCC polycrystals. The corresponding results generated by the IVAR model will also be included for comparison purposes. It should be recalled that the IVAR model can be recovered from the ISO model by means of certain simplifications in the properties of the LCC (see Song, 2017 for details).

For FCC single crystals, the deformation takes place through slip on a set of four slip planes of the type {111} along three slip directions (per plane) of the type ⟨110⟩. Of these, five are linearly independent, thus allowing arbitrary plastic deformation for the single-crystal grains. For simplicity, all slip systems are assumed to be non-hardening with the same reference flow stresses, i.e., $(\tau_0)_{(k)} = \tau_0$ $(k = 1, \ldots, 12)$. In addition, the reference strain rate $\dot{\gamma}_0$ and the creep exponent n are also assumed to be identical for all slip systems.

2.1. Instantaneous effective response

In this section, we explore the instantaneous macroscopic behavior of porous FCC polycrystals for fixed states of the substructure. For simplicity, the FCC polycrystalline matrix is taken here to be *untextured*, with "equiaxed" ($w_1^g = w_2^g = 1$) single-crystal grains and *uniformly distributed* crystallographic orientations, such that the polycrystalline matrix exhibits an overall isotropic behavior.

For later use, we briefly recall the definition of *gauge surface* (Leblond et al., 1994). Given that the viscous exponent n is identical for all the available slip systems in the polycrystalline matrix, it can be shown (Ponte Castañeda and Suquet, 1998) that the effective stress potential $\widetilde{u}$ is a homogeneous function of degree $n+1$ on the macroscopic stress $\overline{\boldsymbol{\sigma}}$, so that $\widetilde{u}$ can be expressed in the form

$$\widetilde{u}(\overline{\boldsymbol{\sigma}}) = \frac{\dot{\gamma}_0 \sigma_0}{n+1} \left(\frac{\Gamma(\overline{\boldsymbol{\sigma}})}{\sigma_0} \right)^{n+1}, \tag{2}$$