Macroscopic response of strongly anisotropic porous viscoplastic single crystals

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Abstract

A recently developed iterated homogenization procedure (Agoras and Ponte Castañeda, 2013) is generalized for porous viscoplastic single crystals and applied to characterize the effective behavior of low-symmetry high-anisotropy porous HCP single crystals (e.g., ice), focusing on the complex coupled effects of the porosity, void shape and crystal anisotropy. Consistent estimates for the average strain rate in the voids are also obtained and their implications for the evolution of the microstructure are explored. The intrinsic effect of the strong crystal anisotropy of porous ice is deduced from comparisons with corresponding results for porous isotropic materials, and found to be significant. In particular, as a consequence of the strong crystal anisotropy of ice, the porosity growth is found to be quite fast at low stress triaxiality, while the void distortion rates can be more significant at high stress triaxialities. Finally, the coupling between the “morphological” anisotropy induced by the void shape and the underlying crystalline anisotropy is investigated and found to have significant effects on the void growth and the void distortion, leading to significantly different behaviors for porous ice and porous isotropic materials.

Keywords: homogenization, anisotropy, crystal plasticity, porous materials

1. Introduction

Most metals and minerals—both man-made and natural—appear in the polycrystalline form. Micro-defects, such as intra/inter-granular voids and cracks, which are usually distributed with random positions and orientations in the crystalline material, have significant effects on the macroscopic behavior, as well as on their failure. It is then of great interest to be able to characterize the effective response of such porous crystalline materials in terms

of the known properties of their constituents and statistical information about their microstructures. In this work, the focus will be on the case where the voids exist either within a homogeneous single-crystal material, or within single-crystal grains of a polycrystalline material, and the size of the voids is much smaller than that of the single crystal (grains), so that the stress and strain fields around the voids develop as if they were embedded in an infinitely large single-crystal matrix subjected to homogeneous loading conditions. The objective of this paper is to develop a constitutive model for the macroscopic response of porous viscoplastic single crystals with random microstructures, by means of a generalization of the recently developed iterated nonlinear homogenization method (Ponte Castañeda, 2012; Agoras and Ponte Castañeda, 2013).

A classical subject in mechanics of materials that calls for such constitutive models is the ductile fracture of crystalline metals and alloys, where it has been evidenced both theoretically and experimentally that the nucleation, growth and coalescence of microvoids play a significant role in the creep fracture of such materials (e.g., Crépin et al., 1996; Srivastava et al., 2012). Another particularly important subject is the study of the grain-scale behavior of polycrystalline ice, which is of great scientific and practical values for further understanding the large-scale geophysical phenomena such as the flow of glaciers (Schulson and Duval, 2009). Since microvoids exist predominantly within the ice single-crystal grains, the constitutive model proposed in this work provides a useful tool for investigating the effects of the intra-granular voids on the macroscopic behavior of ice.

Over the years, important progress has been made to characterize the behavior of porous single crystals. On one hand, the effect of the crystal orientation on the void growth has been studied by means of full-field, unit-cell simulations based on the finite element method (O’regan et al., 1997; Yerra et al., 2010; Ha and Kim, 2010; Srivastava and Needleman, 2015). On the other hand, a few models have been proposed to describe the macroscopic behavior of porous single crystals. Han et al. (2013) developed a yield function for porous single crystals containing spherical voids based on the variational homogenization method developed by deBotton and Ponte Castañeda (1995) and ad hoc modifications inspired by the limit analysis of the Gurson (1977) type model. Paux et al. (2015) proposed a Gurson-type yield criterion by means of a regularized form of the Schmid law and limit-analysis calcula-

tions. These approaches all show satisfactory agreements with the corresponding unit-cell calculations for porous FCC single crystals from the work of Han et al. (2013). However, they all involve fitting of parameters to finite element simulations of porous FCC single crystals, which have not been calibrated for other types of single crystals (e.g., BCC, HCP and etc.). In this sense, the homogenization models to be developed in this work are more general since they are entirely predictive, involving no fitting parameters, and are applicable for porous single crystals of general type. Estimates for porous single crystals were developed by Idiart and Ponte Castañeda (2007a), making use of a generalization of the rigorous variational (VAR) homogenization methods of Ponte Castañeda (1991) and deBotton and Ponte Castañeda (1995). In particular, estimates were obtained for the effective flow stress of 2D porous single crystals containing cylindrical voids subjected to anti-plane shear loadings. More recently, Mbiakop et al. (2015) developed a modified variational (MVAR) homogenization model, and used it to characterize the effective yield potential of 3D porous single crystals containing general ellipsoidal voids under general loading conditions. The model was derived by using the VAR procedure of Ponte Castañeda (1991), together with an ad hoc modification, enforcing the agreement of the MVAR model with the Gurson model for the special case of spherical voids with infinite number of equi-angular slip systems subjected to purely hydrostatic loadings. The MVAR model has been found to be in good agreement with the unit-cell calculations for a wide range of parameters. However, the limiting factor of this approach is the assumption of equal flow stresses for all available slip systems made in its derivation, which makes it unsuitable for porous crystals with large anisotropy, such as porous ice, where the non-basal slip systems are known to have much larger flow stresses than the basal slip systems.

In this work, the homogenization method to be developed is based entirely on the non-linear variational homogenization method, albeit used in a novel iterated fashion (Ponte Castañeda, 2012; Agoras and Ponte Castañeda, 2013), and has the capability of providing bounds and estimates that remain accurate for porous single crystals with general crystal anisotropy, general ellipsoidal voids, subjected to general loading conditions. Here, for illustrative purposes, the model is applied to porous hexagonal closed-packed (HCP) single crystals, including porous ice, and the effects of the porosity, void shape and crystal

anisotropy on the new estimates for the flow potential are investigated in some detail. In addition, the average strain rate in the voids is also computed to explore the implications for the evolution of the microstructure.

2. Homogenization framework for porous single crystals

In this work, porous single crystals are idealized as two-phase materials with single-crystal matrix (phase 1) and vacuous inclusions (phase 2). In addition, separation of length scales is assumed implying that the size of the voids is much smaller than the size of the specimen and the scale of variation of the applied loadings. Furthermore, the porous single crystal is assumed to have statistically uniform and ergodic microstructure. As shown in Fig. 1, consider porous single crystals containing ellipsoidal voids (phase 2) that are aligned in a certain direction, but distributed randomly in the surrounding crystal matrix with two-point probability functions for their centers characterized by “ellipsoidal symmetry” (Willis, 1977; Ponte Castañeda and Willis, 1995). In general, the shape of the ellipsoid characterizing the distribution can be different from the shape of the ellipsoid characterizing the voids (Ponte Castañeda and Willis, 1995; Agoras and Ponte Castañeda, 2013). However, differences between the shape of the voids and that of the distribution are expected to have effects on the macroscopic response that are of second order in the volume fraction and will not be considered here for simplicity (Agoras and Ponte Castañeda, 2014; Song et al., 2015).

According to the above hypothesis, the microstructure of the porous single crystal can be completely characterized by the set of microstructural variables

$$\mathbf{s} \equiv \{f, w_1, w_2, \mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3\}, \quad (1)$$

where f is the volume fraction of the voids (or porosity), $w_1 = a_3/a_1$, $w_2 = a_3/a_2$ are the two aspect ratios characterizing the shape (and distribution) of the voids (a_1 , a_2 and a_3 are respectively the lengths of the three semi-axes of the ellipsoid), and $\mathbf{n}_1$, $\mathbf{n}_2$ and $\mathbf{n}_3$ are unit vectors along the three principal directions of the ellipsoid. It should be mentioned that, in general, the voids (and their distribution) are of arbitrary ellipsoidal shape, where $w_1 \neq w_2 \neq 1$ and $\mathbf{n}_i \neq \mathbf{e}_i$, leading to additional “morphological” anisotropy superimposed on the underlying anisotropy of the single-crystal matrix.

Figure 1: Schematic representation of a porous single crystal consisting of aligned, ellipsoidal voids (solid lines) that are distributed with the same ellipsoidal symmetry (dotted lines) in a single-crystal matrix.

Single crystals are assumed to deform by multi-glide along K slip systems. For simplicity, the constitutive behavior of the single-crystal matrix (phase 1) is taken to be viscoplastic, and the effects of elasticity are neglected. Then, the local constitutive response of the single crystal can be described by

$$\mathbf{D} = \frac{\partial u^{(1)}(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}}, \quad u^{(1)}(\boldsymbol{\sigma}) = \sum_{k=1}^K \phi_{(k)}(\tau_{(k)}), \quad (2)$$

where $u^{(1)}$ is the stress potential for the crystal matrix, $\boldsymbol{\sigma}$ is the Cauchy stress and $\mathbf{D}$ is the Eulerian strain rate. The convex functions $\phi_{(k)}$ ($k = 1, \dots, K$) characterize the response of the K slip systems, and depend on the resolved shear (or Schmid) stresses

$$\tau_{(k)} = \boldsymbol{\sigma} \cdot \boldsymbol{\mu}_{(k)}, \quad \text{where} \quad \boldsymbol{\mu}_{(k)} = \frac{1}{2} (\mathbf{n}_{(k)} \otimes \mathbf{m}_{(k)} + \mathbf{m}_{(k)} \otimes \mathbf{n}_{(k)}). \quad (3)$$

Here, the $\boldsymbol{\mu}_{(k)}$ are the second order Schmid tensors, with $\mathbf{n}_{(k)}$ and $\mathbf{m}_{(k)}$ denoting respectively the unit vectors normal to the slip plane and along the slip direction of the k th slip system. The slip potentials $\phi_{(k)}$ are given by the common power-law form

$$\phi_{(k)}(\tau) = \frac{\dot{\gamma}_0 (\tau_0)_{(k)}}{n+1} \left| \frac{\tau}{(\tau_0)_{(k)}} \right|^{n+1}, \quad k = 1, \dots, K, \quad (4)$$

where $\dot{\gamma}_0$ denotes the reference strain rate, $(\tau_0)_{(k)} > 0$ is the reference flow stress of the k th slip system and n is the creep exponent. Note that $(\tau_0)_{(k)}$ can be very different for each

slip system, which may lead to extreme anisotropic behavior of the crystal matrix. Also note that the creep exponent n is taken to be the same for all slip systems and, hence, the stress potential $u^{(1)}$ is a homogeneous function of degree $n + 1$ in $\boldsymbol{\sigma}$. However, n could in general be different for different slip systems, but here it will be assumed to be the same for simplicity. In particular, two limiting cases as n tends to 1 and ∞ are of special interest, since they correspond to linearly viscous and rigid ideally plastic behavior for the single crystal, respectively. On the other hand, the stress potential of the voids (phase 2) is such that $u^{(2)}(\boldsymbol{\sigma}) = 0$ if $\boldsymbol{\sigma}$ is identically zero, while $u^{(2)}(\boldsymbol{\sigma}) = \infty$ otherwise.

Given the local constitutive behavior of each phase, as well as the prescribed microstructural information (1), the effective response of the porous single crystal can be described by the constitutive relation between the macroscopic Eulerian strain rate $\overline{\mathbf{D}}$ and the macroscopic Cauchy stress $\overline{\boldsymbol{\sigma}}$, as given by

$$\overline{\mathbf{D}} = \frac{\partial \tilde{u}(\overline{\boldsymbol{\sigma}})}{\partial \overline{\boldsymbol{\sigma}}}, \quad \tilde{u}(\overline{\boldsymbol{\sigma}}) \equiv \min_{\boldsymbol{\sigma} \in \mathcal{S}(\overline{\boldsymbol{\sigma}})} \langle u(\mathbf{x}, \boldsymbol{\sigma}) \rangle. \quad (5)$$

Here $\tilde{u}$ is the effective stress potential of the porous single crystal, $\mathcal{S}(\overline{\boldsymbol{\sigma}})$ is the associated “statically admissible” set, including all $\boldsymbol{\sigma}$ fields that are divergence free, satisfy the traction continuity condition $\boldsymbol{\sigma} \mathbf{n} = \mathbf{0}$ on the void boundaries, and are such that $\langle \boldsymbol{\sigma} \rangle = \overline{\boldsymbol{\sigma}}$. It should be noted that the symbol $\langle . \rangle$ denotes the volume average over the total volume occupied by a representative volume element of the porous single crystal.

From the homogeneity of the local potential (4) in $\boldsymbol{\sigma}$, it follows that the effective potential (5) of the porous single crystal is homogeneous of degree $n + 1$ in $\overline{\boldsymbol{\sigma}}$. Then, the effective behavior of the porous single crystal can be completely characterized by a single equi-potential surface in $\overline{\boldsymbol{\sigma}}$ space, i.e., $\tilde{u}(\overline{\boldsymbol{\Sigma}}) = \text{const}$, where any other equi-potential surface is just a homothetic surface (Leblond et al., 1994). In particular, the *gauge surface* of the porous single crystal is defined by

$$\tilde{u}(\overline{\boldsymbol{\Sigma}}) = \frac{\dot{\gamma}_0 \tau_0^{-n}}{n + 1}, \quad (6)$$

where τ_0 is a reference flow stress, which can be chosen to be, e.g., one of the reference flow stresses $(\tau_0)_{(k)}$ ($k = 1, \dots, K$). Note that the normal to the gauge surface indicates the direction of the plastic flow. Also, in the limit of ideally plasticity ($n \rightarrow \infty$), the gauge surface tends to the standard yield surface.

Alternatively, the gauge surface can be obtained by introducing a gauge factor Γ , such that the effective stress potential can be written in the form

$$\tilde{u}(\bar{\boldsymbol{\sigma}}) = \frac{\dot{\gamma}_0 \tau_0}{n+1} \left(\frac{\Gamma(\bar{\boldsymbol{\sigma}})}{\tau_0} \right)^{n+1}, \quad (7)$$

where Γ is a homogeneous function of degree 1 in $\bar{\boldsymbol{\sigma}}$, which depends on the creep exponent n , the microstructural variables $\mathbf{s}$ defined in (1), and the reference flow stresses $(\tau_0)_{(k)}$, $k = 1, \dots, K$. Then, for any prescribed macroscopic stress $\bar{\boldsymbol{\sigma}}$, the normalized stress tensor

$$\bar{\boldsymbol{\Sigma}} = \frac{\bar{\boldsymbol{\sigma}}}{\Gamma(\bar{\boldsymbol{\sigma}})} \quad (8)$$

will always lie on the gauge surface. In other words, the stress tensor $\bar{\boldsymbol{\Sigma}}$ on the gauge surface can be obtained by computing the effective stress potential $\tilde{u}$ for arbitrary $\bar{\boldsymbol{\sigma}}$, determining the corresponding gauge factor $\Gamma(\bar{\boldsymbol{\sigma}})$ from (7), and normalizing $\bar{\boldsymbol{\sigma}}$ according to (8). Similarly, it is useful to introduce the corresponding normalized macroscopic strain rate

$$\bar{\mathbf{E}} = \frac{\bar{\mathbf{D}}}{\dot{\gamma}_0 (\Gamma(\bar{\boldsymbol{\sigma}})/\tau_0)^n} = \frac{\partial \Gamma(\bar{\boldsymbol{\sigma}})}{\partial \bar{\boldsymbol{\sigma}}}. \quad (9)$$

Note that $\bar{\mathbf{E}}$ is independent of the magnitude of $\bar{\boldsymbol{\sigma}}$, and depends only on the direction of $\bar{\boldsymbol{\sigma}}$.

In this work, estimates for the effective stress potential $\tilde{u}$ are obtained by means of the iterated homogenization approach (Agoras and Ponte Castañeda, 2013) in combination with the nonlinear Variational Homogenization (VH) method developed by deBotton and Ponte Castañeda (1995), and will be referred to here as the Iterated Variational Homogenization (IVH) method. It should be mentioned that the VH method makes use of the effective property of a suitably chosen porous “linear comparison composite” (LCC)—with *uniform* matrix properties and microstructure identical to that of the nonlinear porous single crystal of interest—to estimate the effective behavior of the nonlinear composite. However, while this method is known to yield rigorous bounds, they tend to be overly stiff estimates for the effective behavior of porous single crystals, especially at low porosity, high stress triaxiality and high nonlinearity (Agoras and Ponte Castañeda, 2013). The key idea of IVH is to construct the porous microstructure iteratively in a self-similar fashion (see Fig. 2 and associated discussions in Agoras and Ponte Castañeda, 2013), in such a way that, at each iteration level, the IVH involves an LCC with identical microstructure to the corresponding

nonlinear composite and with a linear single-crystal matrix, allowing for a *non-uniform* distribution of the matrix phase in the LCC, thus leading to improved estimates, which retain their bounding character.

In particular, the viscous compliance tensor of the LCC crystal matrix at the i th level is assumed to be of the form

$$\mathbb{M}_{[i]}^{(1)} = \sum_{k=1}^K \alpha_{(k)}^{[i]} \boldsymbol{\mu}_{(k)} \otimes \boldsymbol{\mu}_{(k)}, \quad i = 1, \dots, N, \quad k = 1, \dots, K, \quad (10)$$

where the $\alpha_{(k)}^{[i]}$ are the slip compliances (which will be specified later), and N is the total number of iterations in the IVH procedure. Furthermore, the effective behavior of each level LCC is computed by means of the estimates of Ponte Castañeda and Willis (1995) (to be referred to here as PCW estimates), which are given by expression (19) in the Appendix.

In their final form, the IVH estimates for the effective stress potential $\tilde{u}$ of the nonlinear porous single crystal can be written as

$$\tilde{u}^{IVH}(\bar{\boldsymbol{\sigma}}) = (1 - f^{\frac{1}{N}}) \sum_{i=1}^N f^{\frac{N-i}{N}} \left(\sum_{k=1}^K \phi_{(k)}(\hat{\tau}_{(k)}^{[i]}) \right). \quad (11)$$

In expression (11), the $\hat{\tau}_{(k)}^{[i]}$ are the second moment variables defined by

$$\hat{\tau}_{(k)}^{[i]} = \sqrt{\boldsymbol{\mu}_{(k)} \cdot \langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle_{[i]}^{(1)} \boldsymbol{\mu}_{(k)}}, \quad i = 1, \dots, N, \quad k = 1, \dots, K, \quad (12)$$

where the $\langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle_{[i]}^{(1)}$ ($i = 1, \dots, N$) denote the second moments of the stress fields in the matrix of the LCC at level i , which can be computed by means of (22) in the Appendix. In addition, the slip compliances $\alpha_{(k)}^{[i]}$, as determined by the application of VH method in terms of the LCC at each level, are given by the closure conditions

$$\alpha_{(k)}^{[i]} = \frac{\phi'_{(k)}(\hat{\tau}_{(k)}^{[i]})}{\hat{\tau}_{(k)}^{[i]}}, \quad i = 1, \dots, N, \quad k = 1, \dots, K. \quad (13)$$

In fact, $\tilde{u}^{IVH}$ is known to be a lower bound for the effective potential of the porous single crystals, the accuracy of which improves progressively with increasing N . However, the fast convergence of IVH with increasing values of N (Agoras and Ponte Castañeda, 2013) allows the use of relatively small numbers of iterations N to get accurate results, and thus, $N = 10$ is used in this work, which can be shown to give sufficiently accurate predictions for porous single crystals.

The macroscopic constitutive behavior, as well as the average strain rate in the voids of the nonlinear porous single crystal can then be obtained directly from those of the LCC (Idiart and Ponte Castañeda, 2007b; Agoras and Ponte Castañeda, 2013). In particular, the IVH estimates for the macroscopic strain rate $\overline{\mathbf{D}}$ of the nonlinear porous single crystal under the applied loading $\overline{\boldsymbol{\sigma}}$ is given by

$$\overline{\mathbf{D}} = \frac{\partial \tilde{u}^{IVH}}{\partial \overline{\boldsymbol{\sigma}}}(\overline{\boldsymbol{\sigma}}) = \tilde{\mathbb{M}} \overline{\boldsymbol{\sigma}}, \quad (14)$$

where $\tilde{\mathbb{M}} \equiv \tilde{\mathbb{M}}_{[N]}$ is the PCW estimate for the effective viscous compliance tensor of the N -level LCC, as given by (19). Moreover, the corresponding IVH estimate for the average strain rate in the voids $\overline{\mathbf{D}}^{(2)}$ is determined by

$$\overline{\mathbf{D}}^{(2)} = \mathbb{A}^{(2)} \overline{\mathbf{D}}, \quad (15)$$

with $\mathbb{A}^{(2)}$ denoting the PCW strain-rate concentration tensor, which is given by (23) together with (24) in the Appendix.

Given the normalized macroscopic strain rate $\overline{\mathbf{E}}$, as defined by (9), we define correspondingly the normalized average strain rate in the voids by $\overline{\mathbf{E}}^{(2)} = \mathbb{A}^{(2)} \overline{\mathbf{E}}$. Furthermore, by using appropriate evolution laws for the porosity f and the aspect ratios of the voids w_α ($\alpha = 1, 2$) (Gurson, 1977; Ponte Castañeda and Zaidman, 1994), we define the normalized porosity growth rate $\dot{f}$ and the normalized rate of change of the void aspect ratios $\dot{w}_\alpha$ ($\alpha = 1, 2$), which are respectively of the form

$$\dot{f} = (1 - f) \overline{E}_{kk}, \quad \dot{w}_\alpha = w_\alpha (\mathbf{n}_3 \otimes \mathbf{n}_3 - \mathbf{n}_\alpha \otimes \mathbf{n}_\alpha) \cdot \overline{\mathbf{E}}^{(2)}, \quad \alpha = 1, 2. \quad (16)$$

3. Application to porous HCP single crystals

In this section, we investigate the predictions of the IVH estimates for the instantaneous macroscopic response of porous HCP single crystals, focusing on the effect of the crystal anisotropy, the porosity and the void shape, with particular emphasis on porous ice crystals. In addition, consistent IVH estimates for the average strain rate in the voids are computed to explore the implications for the evolution of the microstructure.

Ice single crystals belong to the class of low-symmetry, HCP crystals, with a c/a ratio of 1.629, and a creep exponent n of 3. The relevant slip systems are the three basal

slips ($\{0001\} \langle 11\bar{2}0 \rangle$), the three prismatic slips ($\{10\bar{1}0\} \langle 11\bar{2}0 \rangle$) and the six second-order ($\{11\bar{2}2\} \langle 11\bar{2}3 \rangle$) pyramidal- $\langle c+a \rangle$ slips, which will be denoted by labels A, B and C, respectively. In addition, the basal slips are taken to be the “soft” slip systems, with reference flow stress τ_A , while the prismatic and pyramidal slips are taken to be the “hard” slip systems, with the same reference flow stresses $\tau_B = \tau_C = M\tau_A$. For ice, $M = 60$ (Duval et al., 1983), but in this work we will consider values of M such that $1 \leq M \leq 60$ to investigate the effect of the anisotropy of HCP single crystals more generally.

First, we examine the effect of various parameters on the gauge surfaces of porous HCP crystals for loading conditions of the type

$$\bar{\Sigma} = \bar{\Sigma}_m \mathbf{I} + \bar{\Sigma}_a \left(-\frac{1}{3} \mathbf{e}_1 \otimes \mathbf{e}_1 - \frac{1}{3} \mathbf{e}_2 \otimes \mathbf{e}_2 + \frac{2}{3} \mathbf{e}_3 \otimes \mathbf{e}_3 \right), \quad (17)$$

combining the hydrostatic stress $\bar{\Sigma}_m$ and the axisymmetric shear stress $\bar{\Sigma}_a = \bar{\Sigma}_{33} - \bar{\Sigma}_{11} = \bar{\Sigma}_{33} - \bar{\Sigma}_{22} = \pm \bar{\Sigma}_e$, where $\bar{\Sigma}_e$ is the macroscopic equivalent stress. For simplicity, it is further assumed that the symmetry axis $\mathbf{e}_3$ of the macroscopic loading (17) is aligned with the $\langle c \rangle$ -axis of the ice single crystal. At this stage, recall that the gauge surface is defined by (6), and τ_0 is chosen to be τ_A for all results shown below. In addition, note that the lower bound $\tilde{u}^{IVH}$ on the effective stress potential translates into an outer bound on the gauge surface.

Figure 2(a) shows gauge surfaces for porous HCP crystals, as predicted by the IVH and Taylor method. In particular, Fig. 2(a) depicts the $\bar{\Sigma}_m - \bar{\Sigma}_a$ cross sections of gauge surfaces for porous crystals with porosity $f = 1\%$, void aspect ratios $w_1 = w_2 = 1$ and contrast parameter $M = 1$. Corresponding IVH results are also shown for a viscoplastic porous isotropic material with isotropic matrix characterized by the power-law stress potential

$$u^{\text{iso}}(\boldsymbol{\sigma}) = \frac{\dot{\gamma}_0 \sigma_0}{n+1} \left(\frac{\sigma_e}{\sigma_0} \right)^{n+1}, \quad (18)$$

where $\sigma_0 = 1.657\tau_A$ denotes the reference flow stress, $n = 3$ is the creep exponent, and σ_e is the equivalent stress. Note that τ_0 is chosen such that in the linear case ($n = 1$), the constitutive relation (2), together with (4), for the isotropic HCP single crystal reduces to the isotropic power-law relation (18). We observe from Fig. 2(a) that the effective behavior of the porous crystal with $M = 1$ is similar to that of the porous isotropic material: the porous isotropic material exhibits a somewhat softer response at high stress triaxiality

Figure 2: IVH results for the $\bar{\Sigma}_a - \bar{\Sigma}_m$ cross sections of the gauge surfaces for porous HCP single crystals subjected to axisymmetric loadings (17). (a) Comparisons of the IVH and Taylor gauge surfaces for the porous HCP crystal with porosity $f = 1\%$, void aspect ratios $w_1 = w_2 = 1$ and contrast parameter $M = 1$. Plots are also shown for the effect of the (b) void shape, as defined by the aspect ratios w_1 and w_2 , (c) crystal anisotropy, as defined by the contrast parameter M , and (d) porosity f on the gauge surfaces for porous HCP crystals...

$X_\Sigma = \overline{\Sigma}_m/\overline{\Sigma}_e$ and a slightly stiffer response at low stress triaxiality. The Taylor estimate assumes a uniform strain rate in the phases, leading to two straight lines parallel to the horizontal hydrostatic axis, and providing an outer bound for the gauge surface of porous HCP crystals. The corresponding IVH gauge surface lies within the Taylor gauge surface for all ranges of stress state, leading to a tighter outer bound that is finite for all stress states. It should be mentioned that similar results for the gauge surface of the porous crystal with $M = 1$ can be obtained by means of the MVAR method developed by Mbiakop et al. (2015). However, we should emphasize that the MVAR method was designed for crystals with values of $M \sim 1$ and becomes progressively less accurate with increasing crystal anisotropy (values of M), while the IVH method has the advantage of providing estimates that are valid and should remain accurate for arbitrary crystal anisotropy.

Figure 2(b) shows the effect of the void shape on the IVH gauge surfaces for porous ice ($M = 60$) with fixed porosity $f = 1\%$. In particular, three different void shapes are considered: a spherical void shape with aspect ratios $w_1 = w_2 = 1$, a prolate void shape with $w_1 = w_2 = 5$, and an oblate void shape with $w_1 = w_2 = 0.2$. Note that the symmetry axes of the spheroidal voids are assumed to be aligned with the direction of the unit vector $\mathbf{e}_3$ and, hence, also aligned with the direction of the $\langle c \rangle$ -axis of the ice single crystal. First, it is observed that the gauge surface of porous ice with $w_1 = w_2 = 1$ and $M = 60$ becomes much larger and tilted with respect to the vertical deviatoric axis, when compared with the corresponding result for $M = 1$ in Fig. 2(a). In addition, we observe from Fig. 2(b) that changing the void shape changes both the size and shape of the gauge surface, suggesting that changes in void shape should have strong *anisotropic* hardening or softening effects. Furthermore, we found that the effect of the void shape exhibits a strong dependence on the crystal anisotropy. For instance, when subjected to purely hydrostatic loadings, porous ice ($M = 60$) with prolate voids ($w_1 = w_2 = 5$) is stiffer than that with spherical voids ($w_1 = w_2 = 1$), while it is the other way around for $M = 1$ (the corresponding results are not shown due to limitations of space). As expected, the IVH results corresponding to three different void shapes all lie within the Taylor outer bound (two straight lines parallel to the horizontal hydrostatic axis), which is independent of the void shape.

Figure 2(c) demonstrates the effect of the crystal anisotropy on the IVH gauge surfaces

for porous HCP crystals with porosity $f = 1\%$, void aspect ratios $w_1 = w_2 = 1$ and different values of the contrast parameter ($M = 1, 5, 10, 20, 60$). The main observation from Fig. 2(c) is that increasing M leads to the expansion of the gauge surface and, hence, to stronger behavior for the porous crystals, as expected. However, the gauge surface changes its shape and rotates counterclockwise as M increases, implying a strong distortional hardening effect with increasing values of M . The above observation has important implications on the plastic anisotropy. For instance, when the porous crystal is subjected to purely hydrostatic loading, the direction of the induced plastic flow, as determined by the normal to the gauge surface, changes significantly with increasing values of M . It should also be mentioned that when $M \rightarrow \infty$, the corresponding gauge surface tends to infinity, suggesting that non-basal slip is required for the overall plastic response of porous HCP crystals, under loading condition (17).

Figure 2(d) shows the effect of the porosity on the gauge surfaces for porous ice ($M = 60$) with void aspect ratios $w_1 = w_2 = 1$, where three values of porosity ($f = 1\%, 10\%$ and 25%) are considered. As expected, increasing f leads to the contraction of the gauge surface for all loading directions and, thus, to softer behavior. However, the reduction of the gauge surface with increasing values of f is more significant at high stress triaxialities, inducing a dramatic change in the shape of the gauge surface. In particular, for high porosity (e.g., $f = 25\%$), the shape of the gauge surface is nearly elliptical, whereas for low porosity (e.g., $f = 1\%$), the gauge surface tends to become flat near the vertical deviatoric axis and develops a markedly non-elliptical shape.

For completeness, results for the normalized macroscopic strain rate $\overline{E}_a = \frac{2}{3}(\overline{E}_{33} - \overline{E}_{11}) = \frac{2}{3}(\overline{E}_{33} - \overline{E}_{22}) = \pm \overline{E}_e$, as determined by expression (9), are presented in Figs. 2(e) and 2(f), corresponding to the cases considered in Figs. 2(c) and 2(d), respectively. In particular, Fig. 2(e) depicts plots of $\overline{E}_a$ as a function of the stress triaxiality X_Σ and the contrast parameter M , for porous crystals with porosity $f = 1\%$ and aspect ratios $w_1 = w_2 = 1$. For comparison purposes, the corresponding result for a porous isotropic material is also presented in Fig. 2(e). In this context, it should be mentioned that, for all values of X_Σ considered in the following, $\overline{\Sigma}_a \geq 0$ is assumed, so that $X_\Sigma = \overline{\Sigma}_m / \overline{\Sigma}_e = \overline{\Sigma}_m / \overline{\Sigma}_a$. The corresponding results for $\overline{\Sigma}_a < 0$ can be easily obtained by symmetry considerations. It can be seen that the

Figure 2: ...Results are also shown for the normalized macroscopic strain rate $\bar{E}_a$ (defined by (9)) corresponding to the cases considered in Figs. 2(c) and 2(d), as functions of the stress triaxiality X_Σ , for different values of the (e) contrast parameter M and (f) porosity f .

IVH estimate of $\bar{E}_a$ for $M = 1$ is similar to that for the porous isotropic material, in agreement with the similarity of the corresponding gauge surfaces observed in Fig. 2(a). On the other hand, $\bar{E}_a$ decreases with increasing values of M , indicating a strong effect of increasing crystal anisotropy, as already observed in Fig. 2(c). In addition, $\bar{E}_a$ reaches its maximum value at $X_\Sigma = 0$ for all values of M , implying that the porous HCP crystal with $M = 1$ undergoes the largest amount of shear deformation under purely deviatoric loadings, as expected on physical grounds. On the other hand, Fig. 2(f) shows plots of $\bar{E}_a$ as a function of the stress triaxiality X_Σ and the porosity f , for porous ice ($M = 60$) with void aspect ratios $w_1 = w_2 = 1$, where various porosities ($f = 1\%$, 10% and 25%) are considered. Similar to the findings in Fig. 2(e), E_a reaches its maximum value under purely deviatoric loadings, independent of the porosity f . However, as f increases, the curve for E_a becomes progressively more asymmetric with respect to the vertical deviatoric axis $X_\Sigma = 0$, consistent with the developing asymmetry of the corresponding gauge surfaces with respect to the vertical axis $\bar{\Sigma}_m = 0$ ($X_\Sigma = 0$) in Fig. 2(d), and indicating a strong anisotropic effect induced by the porosity change.

Next, we present results for the porosity growth rate $\dot{f}$ and the rate of change of the void

shape $\dot{w}$, as defined by the normalization (16), and explore their implications for the evolution of the microstructure. For simplicity, we will only consider the case of initially spheroidal voids ($w_1 = w_2$) here, and the symmetry axes of the voids are assumed to be aligned with those of the applied loading (17), leaving the cases of more general orientations for future consideration. Due to the symmetry of the problem considered, $\dot{w}_1 = \dot{w}_2 = \dot{w}$, indicating that the initially spheroidal voids will remain spheroidal in shape under loading condition (17), but will, in general, change their size and aspect ratios. It should be mentioned that the normalized results shown for $\dot{f}$ and $\dot{w}$ depend only on the direction of the applied stress $\bar{\sigma}$, so that multiplication of $\bar{\sigma}$ by a scalar will not change the results. In addition, larger values of $\dot{f}$ imply a faster growth of the porosity and, in particular, $\dot{f} > 0$ indicates that the porosity increases and $\dot{f} < 0$ indicates that the porosity decreases. On the other hand, larger magnitudes of $\dot{w}$ indicate more significant void distortion rates and, in particular, $\dot{w} > 0$ means that the voids are becoming more prolate, while $\dot{w} < 0$ means that the voids are becoming more oblate.

Figures 3(a) and 3(b) show respectively the effect of the crystal anisotropy on $\dot{f}$ and $\dot{w}$ for porous HCP crystals with porosity $f = 1\%$, void aspect ratios $w_1 = w_2 = 1$ and different values of the contrast parameter ($M = 1, 5, 10, 20, 60$). For comparison purposes, corresponding results for porous isotropic materials are also incorporated in the figures. It can be seen from Fig. 3(a) that, for all cases considered, the porosity grows faster at high stress triaxiality, as expected. The $\dot{f}$ curve for the porous HCP crystal with $M = 1$ is similar to that for the porous isotropic material, consistent with the previous observations from Figs. 2(a) and 2(e). However, as M increases, $\dot{f}$ tends to increase at small values of stress triaxiality, and to decrease at large (positive and negative) values of stress triaxiality, indicating that increasing crystal anisotropy facilitates the void growth at low stress triaxiality, while it suppresses it at high stress triaxiality. On the other hand, we observe from Fig. 3(b) that while $\dot{w}$ is symmetric with respect to the vertical axis ($X_\Sigma = 0$) for the porous isotropic material, the corresponding curves for the porous HCP crystals become progressively more asymmetric with increasing values of M , due to the correspondingly increasing crystal anisotropy. In particular, for the porous isotropic material $\dot{w}$ tends to zero as $X_\Sigma \rightarrow \infty$, suggesting that the void distortion rate becomes insignificant at high stress triaxiality, whereas the magnitude

Figure 3: IVH results for the normalized growth rates of the porosity $\dot{f}$ and the aspect ratios $\dot{w}$ (as defined by (16)), as functions of X_Σ , for porous HCP single crystals subjected to axisymmetric loadings (17). Plots are shown for (a) $\dot{f}$ and (b) $\dot{w}$ for different values of the contrast parameter M , as well as for (c) $\dot{f}$ and (d) $\dot{w}$ for different values of the initial porosity f ...

of $\dot{w}$ for porous ice ($M = 60$) can be quite large, indicating significant void distortion rates, even at high stress triaxiality.

Figures 3(c) and 3(d) demonstrate the effect of the initial porosity f on $\dot{f}$ and $\dot{w}$, respectively, for porous ice ($M = 60$) with void aspect ratios $w_1 = w_2 = 1$. Three values of the initial porosity ($f = 1\%, 10\%$ and 25%) are considered in each figure. We observe from Fig. 3(c) that for a given fixed value of X_Σ , the dependence of $\dot{f}$ on the initial porosity f is qualitatively the same for porous ice as for the porous isotropic materials (which is not shown here, for brevity). However, due to the strong anisotropy of the ice single crystal, the corresponding results for $\dot{f}$ lose their symmetry with respect to the origin. In particular, the porosity growth for porous ice can be quite significant even at low stress triaxiality. In fact, the value of $\dot{f}$ at $X_\Sigma = 0$ is comparable to that at high stress triaxiality. This behavior of porous ice is significantly different from that of the porous isotropic material, since the void growth rate for the latter case is always zero at $X_\Sigma = 0$. On the other hand, Fig. 3(d) shows that, for all values of f , the void distortion rates, as described by $\dot{w}$, are more significant at high stress triaxiality than at low stress triaxiality. In particular, note that the value of $\dot{w}$ at $X_\Sigma = 10$ is several times greater than that at $X_\Sigma = 0$ for $f = 1\%$. This is unlike the case of porous isotropic materials, where $\dot{w}$ tends to become relatively small at high stress triaxiality. Furthermore, we observe that the effect of the initial porosity f on $\dot{w}$ is significant at high stress triaxiality, where it is observed that the void distortion is much faster for lower initial porosity, while the effect of f on $\dot{w}$ is negligible at low stress triaxiality.

Finally, Figs. 3(e) and 3(f) show respectively the effect of the initial void shape on $\dot{f}$ and $\dot{w}$, for porous ice ($M = 60$) with initial porosity $f = 1\%$. For comparison purposes, corresponding results for porous isotropic materials are also shown in Fig. 3(g) and Fig. 3(h), respectively. First, we observe from Fig. 3(g) that the results for $\dot{f}$ for porous isotropic materials with non-spherical voids are asymmetric with respect to the origin, due to the “morphological” anisotropy induced by the void shape. In addition, the $\dot{f}$ curve for porous isotropic materials with prolate voids ($w_1 = w_2 = 5$) approximately lies between that with oblate voids ($w_1 = w_2 = 0.2$) and spherical voids ($w_1 = w_2 = 1$). However, this is not the case for porous ice, where the order of the corresponding results for $w_1 = w_2 = 5$ and $w_1 = w_2 = 1$ are interchanged (see Fig. 3(e)). The above facts strongly suggest that the effect of the void

(e)

(f)

(g)

(h)

Figure 3: ... (e) $\dot{f}$ and (f) $\dot{w}$ for different initial void shapes. For comparison purposes, corresponding results are also shown for the porous isotropic materials for (g) $\dot{f}$ and (h) $\dot{w}$ for different initial void shapes.

shape on the porosity growth depends crucially on the crystal anisotropy, indicating a strong coupling between the “morphological” anisotropy and the crystal anisotropy. Similarly, it can be seen from Fig. 3(h) that the $\dot{w}$ curves for porous isotropic materials with non-spherical voids are asymmetric with respect to $X_\Sigma = 0$ due to the above-mentioned “morphological” anisotropy. In particular, for porous isotropic materials with $w_1 = w_2 = 5$, $\dot{w}$ decreases monotonically with increasing values of X_Σ , becoming negative for $X_\Sigma > 1.25$, while the opposite is true for $w_1 = w_2 = 0.2$. However, Fig. 3(f) shows that all of the three $\dot{w}$ curves for porous ice with different void shapes exhibit qualitatively similar behaviors, indicating that the extreme anisotropy induced by the crystal matrix prevails over the “morphological” anisotropy induced by the void shape, so that the dependence of $\dot{w}$ on the stress triaxiality X_Σ for ice is qualitatively unaffected by the void shape.

4. Concluding remarks

In this paper, a generalization of a recently developed iterated variational homogenization (IVH) method (Agoras and Ponte Castañeda, 2013) has been developed to generate bounds for the effective flow potential of porous viscoplastic single crystals. The method was then implemented for low-symmetry, high-anisotropy porous HCP single crystals, such as porous ice, to investigate the macroscopic response of these materials under axisymmetric loadings. In general, it was found that the overall size, shape and orientation of the macroscopic gauge surfaces depends sensitively on the instantaneous values of the porosity, void shape and crystal anisotropy, suggesting strong distortional hardening/softening effects in the macroscopic response of these materials under finite-strain loading conditions (leading to evolution of the microstructure). In particular, it was observed that strong crystal anisotropy could significantly affect the dependence of the gauge surfaces on the porosity and void-shape parameters. For example, it was found that while changing the void shape from spherical to prolate has a softening effect on the effective behavior for porous crystals with low anisotropy ($M = 1$)—in agreement with earlier results (Agoras and Ponte Castañeda, 2013; Mbiakop et al., 2015)—the opposite is true for porous crystals with high anisotropy, such as ice ($M = 60$), with prolate voids leading to a stronger response than spherical voids. In addition, consistent IVH estimates for the average strain rate in the voids were

computed to explore their implications for the evolution of the microstructure. Thus, it was found that strong crystal anisotropy may lead to fast porosity growth at low stress triaxiality and to significant void distortion rates at high stress triaxiality, which is in contrast to the corresponding results for porous isotropic materials. Furthermore, it was found that the dependence of the porosity growth and void distortion on the initial void shape is also strongly affected by the crystal anisotropy. In fact, the crystal anisotropy largely dominates over the effect of the void shape, leading to significantly different behaviors for porous ice and porous isotropic materials. The fact that the IVH model predicts a complex coupled effect of the “morphological” anisotropy and crystal anisotropy provides strong encouragement for its further development into the finite-strain regime, thus accounting for evolving microstructures by incorporating the effects of the lattice rotation, void growth as well as the matrix hardening, building on the earlier models of Agoras and Ponte Castañeda (2014) and Song et al. (2015) for porous isotropic materials. These developments will be considered in future publications. Finally, it is noted that the IVH method can also be used for high-symmetry crystals. Indeed, preliminary results for porous FCC crystals indicate fairly good agreement with FEM results based on unit cell calculations (Srivastava and Needleman, 2015). These results will also be published in future papers.

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Appendix: Detailed expressions for the IVH method

In this Appendix, detailed expressions for the IVH method are provided, which are generalizations of the corresponding expressions in the work of Agoras and Ponte Castañeda (2013). In this context, it is important to mention that these expressions are obtained by means of the PCW estimates of Ponte Castañeda and Willis (1995) for the LCC at each iteration step. In addition, it is assumed for simplicity that the shape and orientation of the voids are identical to those of their distribution. However, more general cases with different

shapes and orientations of the voids and their distribution can be accounted for, as was done, for example, by Agoras and Ponte Castañeda (2013).

We begin by recalling that the viscous compliance tensor $\mathbb{M}_{[i]}^{(1)}$ of the matrix of the i -level LCC is given by (10), while the effective compliance tensor $\tilde{\mathbb{M}}_{[i]}$ of the i -level LCC is given by

$$\tilde{\mathbb{M}}_{[i]} = \mathbb{M}_{[i]}^{(1)} + c_{[i]}^{(2)} \left[\left(\tilde{\mathbb{M}}_{[i-1]} - \mathbb{M}_{[i]}^{(1)} \right)^{-1} + (1 - c_{[i]}^{(2)}) \mathbb{Q}_{[i]} \right]^{-1}, \quad i = 1, \dots, N, \quad (19)$$

where the $c_{[i]}^{(2)}$ ($i = 1, \dots, N$) are the incremental volume fractions required to satisfy the condition $f = \prod_{i=1}^N c_{[i]}^{(2)}$, which will be simply chosen as $c_{[i]}^{(2)} = f^{1/N}$ ($i = 1, \dots, N$), and the $\mathbb{Q}_{[i]}$ ($i = 1, \dots, N$) are fourth-order microstructural tensors, depending on the matrix property $\mathbb{M}_{[i]}^{(1)}$ and the shape and orientation of the voids (see Nebozhyn et.al, 2001 for their corresponding expressions). It should be mentioned that $\tilde{\mathbb{M}}_{[0]} \rightarrow \infty$ in (19), representing the compliance tensor of the vacuum inclusion in the first level LCC.

Following the work of Agoras and Ponte Castañeda (2013), the macroscopic stress $\bar{\sigma}_{[i]}$ of the i -level LCC can be written in the form

$$\bar{\sigma}_{[i]} = \left[\prod_{j=i+1}^N \mathbb{B}_{[j]}^{(2)} \right] \bar{\sigma}, \quad i = 1, \dots, N-1, \quad \text{and} \quad \bar{\sigma}_{[N]} = \bar{\sigma}, \quad (20)$$

where the corresponding stress concentration tensors are provided by

$$\mathbb{B}_{[i]}^{(2)} = \left[\mathbb{I} + (1 - c_{[i]}^{(2)}) \mathbb{Q}_{[i]} \left(\tilde{\mathbb{M}}_{[i-1]} - \mathbb{M}_{[i]}^{(1)} \right) \right]^{-1}, \quad i = 2, \dots, N, \quad (21)$$

with $\mathbb{I}$ denoting the fully symmetric fourth-order identity tensor. Given expressions (19), (20) and (21), the second moment of the stress field in the matrix of the i -level LCC can be computed via

$$\langle \sigma \otimes \sigma \rangle_{[i]}^{(1)} = \frac{1}{1 - c_{[i]}^{(2)}} \bar{\sigma}_{[i]} \cdot \frac{\partial \tilde{\mathbb{M}}_{[i]}}{\partial \mathbb{M}_{[i]}^{(1)}} \bar{\sigma}_{[i]}, \quad i = 1, \dots, N. \quad (22)$$

On the other hand, the iterated PCW estimates for the average strain-rate field in the voids can also be obtained, following the work of Agoras and Ponte Castañeda (2013), and is given by $\bar{\mathbf{D}}^{(2)} = \mathbb{A}^{(2)} \bar{\mathbf{D}}$, where $\mathbb{A}^{(2)}$ is the associated strain-rate concentration tensor, determined by

$$\mathbb{A}^{(2)} = \prod_{i=1}^N \mathbb{A}_{[i]}^{(2)}, \quad (23)$$

with

$$\mathbb{A}_{[i]}^{(2)} = \left[c_{[i]}^{(2)} \mathbb{I} + (1 - c_{[i]}^{(2)}) \left[\left(\mathbb{M}_{[i]}^{(1)} - \mathbb{M}_{[i]}^{(1)} \mathbb{Q}_{[i]} \mathbb{M}_{[i]}^{(1)} \right) \left(\tilde{\mathbb{M}}_{[i-1]} \right)^{-1} + \mathbb{M}_{[i]}^{(1)} \mathbb{Q}_{[i]} \right] \right]^{-1}, \quad i = 1, \dots, N. \quad (24)$$

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