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A model for porous single crystals with cylindrical voids of elliptical cross-section

A. Mbiakop, A. Constantinescu, K. Danas *

Laboratoire de Mécanique des Solides, CNRS UMR7649 & Département de Mécanique, École Polytechnique, 91128 Palaiseau Cedex, France

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ABSTRACT

This work presents a rate-dependent constitutive model for porous single crystals with arbitrary number of slip systems and orientations. The single crystal comprises cylindrical voids with elliptical cross-section at arbitrary orientations and is subjected to general plane-strain loadings. The proposed model, called modified variational model (MVAR), is based on the nonlinear variational homogenization method, which makes use of a linear comparison porous single crystal material to estimate the response of the nonlinear porous single crystal. The MVAR model is validated by periodic finite element simulations for a large number of parameters including general in-plane crystal anisotropy, general in-plane void shapes and orientations, various creep exponents (i.e., nonlinearity) and general plane strain loading conditions. The MVAR model, which at the present state involves no calibration parameters, is found to be in good agreement with the finite element results for all cases considered in this work. The model is then used in a predictive manner to investigate the complex response of porous single crystals in several cases with strong coupling between the anisotropy of the crystal and the (morphological) anisotropy induced by the shape and orientation of the voids.

1. Introduction

Voids originating in the manufacturing process have an important effect on the lifetime as well as deformability of materials and play an important role on the constitutive response of metallic alloys. Indeed, as recently indicated by experimental observations (Srivastava et al., 2012) at high enough temperatures on tensile specimens, the growth of initially present processing induced voids in a nickel based single crystal superalloy as well as in standard polycrystals played a significant role in limiting creep life. The presence of voids (or cracks) in metals is known to be one of the major causes of ductile failure, as addressed in pioneering works by Mc Clintock (1968), Rice and Tracey (1969) and Gurson (1977). Most of the studies so far have been carried out in the context of two-phase material systems comprising an isotropic rate-(in) dependent matrix phase (metal usually described by von Mises yield criterion or creep potential) and a voided phase (pores of spherical, spheroidal or arbitrary ellipsoidal shapes). The models proposed previously for ductile damage growth use either limit analysis (see for instance Tvergaard and Needleman, 1984; Gologanu and Leblond, 1993; Leblond et al., 1994; Monchiet et al., 2007; Madou and Leblond, 2012a,b) based on Gurson (1977) work, or a variational homogenization theory using the concept of a linear comparison composite (see for instance Ponte Castañeda, 1991a; deBotton and Ponte Castañeda, 1995; Danas and Ponte Castañeda, 2009a).

Far fewer results have been obtained for rate-(in) dependent anisotropic matrix systems, generally based on a phenomenological Hill-type matrix (see Benzerga and Besson, 2001; Benzerga et al., 2004; Monchiet et al., 2008; Keralavarma et al., 2011). The case of porous single crystals have only been studied through discrete dislocations dynamic by Huang et al. (2007, 2012), Hussein et al. (2008), Segurado and Llorca (2010) and molecular dynamics at smaller scales (Traiviratana et al., 2008; Zhao et al., 2009; Tang et al., 2010a,b), or using finite element simulations (Yerra et al., 2010; Ha and Kim, 2010). Such anisotropic matrix systems have known slip directions and contain usually a small volume fraction of impurities. When these material systems are subjected to external loads impurities fail or decohere leading to the creation of pores, which in turn evolve in size, shape and orientation (Srivastava and Needleman, 2012). This complex evolution of microstructure together with the evolution of the rate-dependent matrix anisotropy is critical in the prediction of the eventual

* Corresponding author.
E-mail addresses: mbiakop@lms.polytechnique.fr (A. Mbiakop), andrei.constantinescu@lms.polytechnique.fr (A. Constantinescu), kdanas@lms.polytechnique.fr (K. Danas).

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fracture of the specimen under monotonic and cyclic loading conditions.

Nevertheless, there have been only a handful of models for porous single crystals which deal with special void geometries, loading conditions and slip system orientations. Such studies involve the study of cylindrical voids with circular cross-section in a rigid-ideally plastic face-centered cubic (FCC) single crystals using slip line theory (Kysar et al., 2005; Gan et al., 2006; Gan and Kysar, 2007), the study two dimensional "out of plane" cylindrical voids with circular cross-section subjected to anti-plane loadings (Idiart and Ponte Castañeda, 2007) and that of spherical voids (Han et al., 2013; Paux et al., 2015). While each one of these studies has its own significant contribution to the understanding of the effective response of porous single crystals none of them is general enough in the sense of arbitrary void shapes and orientations and general loading conditions.

In this regard, the scope of the present work is to develop a two-dimensional model in plane-strain loading conditions that is able to deal with general in-plane crystal anisotropy, arbitrary elliptical void shapes and orientations and general plane strain loading conditions. While this model is not three-dimensional it represents a necessary step towards this direction. It allows for a fully analytical treatment of the problem and thus provides a good insight of the effective response in such highly nonlinear and highly anisotropic systems. A three-dimensional model is then feasible using the same theory that is developed in the present work and.

More specifically, in Section 2, we use the variational linear comparison composite theory of Ponte Castañeda (1991a) to provide a fully analytical model, called the modified variational (MVAR) model (see Danas and Aravas, 2012), in two-dimensions. Subsequently, in Section 4, we present in detail the finite element (FE) periodic unit-cells which will be used to assess the MVAR model as well as to visualize the underlying deformation fields in the context of porous single crystals. In Sections 5 and 6, we present comparison between the MVAR predictions and the FE results for a wide range of crystal anisotropy, arbitrary elliptical void shapes and orientations, porosities, creep exponents and general plane-strain loading conditions. Finally, we conclude with Section 7.

2. Theory

Consider the RVE (representative volume element) Ω to be a two-phase porous single crystal with each phase occupying a sub-domain $\Omega^{(r)}$ $(r=1,2)$. The vacuous phase is identified with phase 2 and the non-vacuous phase (i.e., single crystal matrix) is denoted as phase 1. At this point it is important to note that we make use of the hypothesis of separation of length scales which implies that the size of the voids (microstructure) is much smaller than the size of the single crystal and the variation of the loading conditions at the level of the single crystal. In the following, the brackets $\langle\cdot\rangle$ and $\langle\cdot\rangle^{(r)}$ define volume averages over the RVE (Ω) and the phase r ($\Omega^{(r)}$), respectively.

2.1. Microstructure

The present study focuses on two-dimensional (2D) porous single crystals containing polydisperse cylindrical voids aligned with the x_3-axis. The voids are randomly and uniformly distributed in the transverse plane x_1–x_2. This material is subjected to plane-strain loading in the x_3-direction. In this regard, we first define the relevant microstructural variables, which serve to describe the volume fraction of the vacuous phase as well as the shape, orientation and the distribution of the voids embedded uniformly in the matrix phase. For simplicity, we will also consider that the shape and orientation of the distribution function is identical to the shape and orientation of the voids themselves (see Danas and Ponte Castañeda, 2009a). However, this analysis can be readily extended to distribution of a different shape and orientation than the voids (Ponte Castañeda, 1995; Kailasam and Ponte Castañeda, 1998). Thus, as shown in Fig. 1, the internal variables characterizing the state of the microstructure are:

- The porosity or volume fraction of the voids $f=V_2/V$, where $V=V_1+V_2$ is the total volume, with V_1 and V_2 being the volume occupied by the matrix and the vacuous phase, respectively.
- The aspect ratio $w=a_2/a_1$, with $2a_i$ $(i=1,2)$ denoting the lengths of the principal axes of the representative elliptical void, in the plane $1-2$. The cases $w=1$ and $w\neq 1$ correspond to voids with circular and elliptical cross-sections, respectively.
- The in-plane orientation unit vectors $\mathbf{n}^{(i)}$ $(i=1,2)$, defining an orthonormal basis set, which coincides with the principal axes of the representative elliptical void. As a consequence of the 2D representation of the microstructure the two orientation vectors $\mathbf{n}^{(i)}$ can be easily parameterized in terms of a single Euler angle, ψ,

$$\mathbf{n}^{(1)}=\cos\psi\,\mathbf{e}_1+\sin\psi\,\mathbf{e}_2,\quad \mathbf{n}^{(2)}=-\sin\psi\,\mathbf{e}_1+\cos\psi\,\mathbf{e}_2. \tag{2.1}$$

The above set of the microstructural variables can then be denoted by the set $s_\alpha=\{f,w,\psi\}$.

2.2. Effective behavior: general considerations

The local constitutive behavior of the matrix phase is characterized by an anisotropic, convex stress potential $U_1\equiv U$ while the stress potential of the porous phase $U_2\equiv 0$. As a consequence of the Hill–Mandel lemma (Hill, 1963; Mandel, 1964), the effective stress potential $\widetilde{U}$ for a porous medium is reduced to

$$\widetilde{U}(\overline{\boldsymbol{\sigma}},s_\alpha)=(1-f)\min_{\boldsymbol{\sigma}\in S(\overline{\boldsymbol{\sigma}})}\langle U(\boldsymbol{\sigma})\rangle^{(1)}, \tag{2.2}$$

where

$$S(\overline{\boldsymbol{\sigma}})=\left\{\boldsymbol{\sigma},\operatorname{div}(\boldsymbol{\sigma})=0\text{ in }\Omega,\ \boldsymbol{\sigma}\mathbf{n}=0\text{ on }\partial\Omega^{(2)},\ \langle\boldsymbol{\sigma}\rangle=\overline{\boldsymbol{\sigma}}\right\} \tag{2.3}$$

is the set of statically admissible stresses that are compatible with the average stress $\overline{\boldsymbol{\sigma}}$ and a traction free void surface.

Subsequently, the effective strain-rate tensor can be expresses as

$$\overline{\mathbf{D}}=\frac{\partial\widetilde{U}}{\partial\overline{\boldsymbol{\sigma}}}(\boldsymbol{\sigma}). \tag{2.4}$$

The above described problem is non-trivial since it involves, in general, nonlinear constitutive relations for the constituents as well as random spatial distributions of the voids and thus the goal of the present work is to propose approximate, albeit robust and rigorous, homogenized models. In the next sections, we define the local constitutive response of the single crystal matrix and we provide both analytical and numerical estimates of the effective response of such porous single crystals.

2.3. Constitutive behavior of the constituents

Let us consider a reference single crystal which undergoes viscoplastic deformation on a set of K preferred crystallographic slip systems. At this stage, for simplicity in the homogenization procedure elasticity effects are neglected. Then, these systems are