International Journal of Solids and Structures 50 (2013) 2115–2131

Contents lists available at SciVerse ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

A yield function for single crystals containing voids

X. Han [a,b], J. Besson [a], S. Forest [a,*], B. Tanguy [b], S. Bugat [c]

[a] Centre des Matériaux, Mines ParisTech, CNRS UMR 7633, BP 87, 91003 Evry cedex, France
[b] Laboratoire de Comportement mécanique des Matériaux Irradiés, CEA Saclay, 91191 Gif-sur-Yvette cedex, France
[c] EDF R&D - Neutronic, NICT, Scientific Calculations Department, 1 avenue du General de Gaulle 92141 Clamart, France

ARTICLE INFO

Article history:
Received 16 May 2012
Received in revised form 27 October 2012
Available online 19 March 2013

Keywords:
Porous media
Single crystal
Variational approach
Yield criterion
Unit cell model

ABSTRACT

A yield function for single crystals containing voids has been developed based on a variational approach. This first yield function is phenomenologically extended by modifying the dependence on the mean stress and introducing three adjustable parameters. Unit cell finite element calculations are performed for various stress triaxiality ratios, main loading directions and porosity levels in the case of a perfectly plastic FCC single crystal. The three model parameters are adjusted on the unit cell calculations so that a very good agreement between simulation results and the proposed model is obtained.

1. Introduction

In crystalline metals, void nucleation, growth and coalescence lead to ductile fracture. Since the last forty years, building on the earliest works by Mc Clintock (1968); Rice and Tracey (1969); and Gurson (1977), much effort has been made to improve the prediction of damage evolution and fracture of porous ductile materials at macro and mesoscopic scales. The role of various characteristic features such as porosity, viscoplasticity, void shape, plastic anisotropy of the matrix has been studied. Some reviews were recently provided by Pineau and Pardoen (2007); Besson (2010); Benzerga and Leblond (2010). Two main approaches have been proposed to develop models for ductile damage growth. The first one is based on the seminal work by Gurson (1977) which uses an upper bound approach, following Tvergaard and Needleman (1984), Gologanu and Leblond (1993), Leblond et al. (1994), Benzerga and Besson (2001), Monchiet et al. (2007), Monchiet et al. (2008). The second approach is based on variational formulation of the homogenization theory using the concept of linear-comparison material, see Ponte Castañeda (1991); DeBotton and Ponte Castañeda (1995); Liu et al. (2005); Danas and Ponte Castañeda (2009) and Lebensohn et al. (2011).

Theoretical results obtained following these approaches can be verified using unit cell calculations first introduced in the pioneering work by Koplik and Needleman (1988). This versatile methodology allows to easily study the effect of various parameters on void growth and coalescence such as hardening rate (Faleskog et al., 1998; Gao et al., 1998; Lecarme et al., 2011), void shape or cell shape (Pardoen and Hutchinson, 2000), void population (Faleskog and Shih, 1997,Fabrègue and Pardoen, 2008 and Fritzen et al., 2012), void distribution (Bandstra and Koss, 2008), and second phase particles (Steglich and Brocks, 1997; Steglich et al., 1999).

The effect of the anisotropy of matrix behaviour on void growth was investigated in relation to the anisotropic plastic properties of metal sheets, see in particular (Benzerga et al., 2004) and more recently (Monchiet et al., 2008). Typically, a Hill-type yield criterion was assumed for the matrix in the latter references. The situation is quite different in the presence of voids embedded in a single crystalline matrix. The case of single crystals containing voids (hereafter referred to as porous single crystals) has only been studied recently using the unit cell methodology either based on FE simulations (Schacht et al., 2003; Yerra et al., 2010; Ha and Kim, 2010), or based on slip line theory in the case of simple cylindrical voids (Kysar et al., 2005; Gan et al., 2006; Gan and Kysar, 2007). Besides, the analysis of ductile fracture in single crystals has been performed at smaller scales for nano and micro-voids by means of Discrete Dislocations Dynamics in (Huang et al., 2007; Hussein et al., 2008; Segurado and Llorca, 2009; Segurado and Llorca, 2010 and Huang et al., 2012), and Molecular Dynamics in (Potirniche et al., 2006; Zhao et al., 2009; Traiviratana et al., 2008; Tang et al., 2010b and Tang et al., 2010a). However a set of constitutive equations describing the overall behaviour of porous single crystals is still lacking in the literature. The previously mentioned papers do

* Corresponding author at: Centre des Matériaux, Mines ParisTech, UMR CNRS 7633, BP 87, 91003 Evry cedex, France.
E-mail address: samuel.forest@ensmp.fr (S. Forest).

0020-7683/$ - see front matter © 2013 Published by Elsevier Ltd.
http://dx.doi.org/10.1016/j.ijsolstr.2013.02.005

not provide an overall yield function for porous single crystals. There is currently a real need for such a yield function that would be simple enough to allow straightforward Finite Element implementation for carrying out structural computations of ductile fracture in single and poly-crystals. It could be used for instance to reproduce experimental facts showing accelerated anisotropic growth of cavities in single crystals as observed in Crépin et al. (1996).

The purpose of the present work is to develop a model to describe the yield function of porous single crystals. Such models could be used to represent ductility of stainless steel (304/316 series) used for core internals of Fast Breeder Reactor and PWR nuclear power plants in which intragranular voids develop and lead to the phenomenon of swelling due to high irradiation levels (Foster and Strain, 1974; Seran et al., 1984; Dubuisson, 2011 and Renault et al., 2011), also that of Ni based single crystal superalloys used in turbo-engines components (Wang et al., 2006). The model is theoretically motivated using a micromechanical analysis based on the variational approach by (Ponte Castañeda and Suquet, 1998). It is extended on a phenomenological basis to match trends obtained for rate-independent material (e.g. Gurson–Tvergaard–Needleman model). Unit cell calculations are used to adjust and validate the model. Various loading directions and porosity levels (from 0.5% to 10%) are used.

The single crystal constitutive framework is recalled in Section 2.1. The proposed yield function for porous single crystal is presented in Section 2.2. The Section 3 is dedicated to the identification methodology of the corresponding material parameters from unit cell computations. The results and validation of the approach are provided in Section 4 in terms of crystal orientation, loading conditions and void volume fraction. The micromechanical motivation of the model is explained in Appendix A.

2. Proposed model for porous single crystals

The analysis given in this paper is limited to the small deformation framework, as it is the case in standard limit analysis.

2.1. Model for the single crystal matrix

In this work, which essentially deals with yielding of porous single crystals, a very simple law is used to describe the constitutive behaviour of the single crystal matrix. For each slip system $s = 1 \dots N$, the resolved shear stress, τ_s is expressed as:

$$\tau_s = \underline{\sigma} : \underline{m}_s \quad \text{with } \underline{m}_s = \frac{1}{2}\left(\vec{l}_s \otimes \vec{n}_s + \vec{n}_s \otimes \vec{l}_s\right) \tag{1}$$

where $\underline{\sigma}$ is the Cauchy stress tensor acting on the single crystal volume element. $\vec{l}_s$ and $\vec{n}_s$ are the unit vectors along the slip direction of the slip system s and normal to the slip plane, respectively. The total number of slip systems is N. For each slip system a yield surface can be defined as:

$$\psi_s = |\tau_s| - \tau_0 \tag{2}$$

Provided that $\psi_s \geqslant 0$, the slip rate for each slip system s is given as:

$$\dot{\gamma}_s(\tau_s) = \dot{\gamma}_0 \left(\frac{\psi_s}{\tau_0}\right)^n = \dot{\gamma}_0 \left(\frac{|\tau_s| - \tau_0}{\tau_0}\right)^n \tag{3}$$

where $\dot{\gamma}_0, \tau_0$ and n are material parameters. τ_0 represents the critical resolved shear stress (CRSS) of the slip system. For the sake of simplicity each slip system is assumed to have the same CRSS but the model presented here can be easily extended in order to take into account different CRSS as well as self and cross hardening. Using the normality rule, the plastic strain rate tensor, $\underline{\dot{\varepsilon}}_p$, is expressed as:

$$\underline{\dot{\varepsilon}}_p = \sum_s \dot{\gamma}_s \frac{\partial \psi_s}{\partial \underline{\sigma}} = \sum_s \dot{\gamma}_s \text{sign}(\tau_s) \underline{m}_s \tag{4}$$

2.2. Model for the porous single crystal

One considers here a single crystal containing spherical voids. The void volume fraction is referred to as f in the following. Based on the variational formulation proposed by Ponte Castañeda and Suquet (1998), it is shown in Appendix A that an effective scalar resolved stress acting on each slip system $\tau_s^*(\underline{\sigma}, f)$ can be defined as a function of the applied stress and the porosity level, such that:

$$\tau_s^* - \frac{1}{1-f}\left(\tau_s^2 + \frac{2}{45} f \sigma_{eq}^2 + \frac{3}{20} f \sigma_m^2\right)^{\frac{1}{2}} \overset{\text{def.}\tau_s^*}{=} 0 \tag{5}$$

where σ_m (resp. σ_{eq}) is the mean stress (resp. von Mises stress) of the macroscopic stress tensor $\underline{\sigma}$. τ_s^{*2} is expressed as a quadratic form of $\underline{\sigma}$. Note that the notations used here for the overall yield functions are different from those in Appendix A: Small letters are used for the stress and strain quantities instead of capital letters, because there is no reference any more to the micromechanical variational analysis. Similar yield functions were obtained in the case of a voided solid made of an isotropic von Mises matrix (Leblond et al., 1994). The quadratic dependence in (5) is known to be inadequate in the case of plastic solids since the seminal works of Mc Clintock (1968) and Rice and Tracey (1969). An exponential dependence on the mean stress should be preferred. Using the second order Taylor expansion of $\cosh(x) = 1 + \frac{1}{2}x^2$, other definitions of the effective scalar resolved stress τ_s^* can be proposed so that it better corresponds to models derived from the Gurson (1977) model. Following the concept of a scalar stress measure (Besson et al., 2001), which can be explicitly or implicitly defined, another expression for τ_s^* can be worked out from the following expression which takes into account the mean stress dependence as in Gurson type models:

$$\left(\frac{\tau_s^2}{\tau_s^{*2}} + \frac{2}{45} f \frac{\sigma_{eq}^2}{\tau_s^{*2}}\right) + 2f \cosh\left(\sqrt{\frac{3}{20}} \frac{\sigma_m}{\tau_s^*}\right) - 1 - f^2 \overset{\text{def.}\tau_s^*}{=} 0 \tag{6}$$

τ_s^* is found by solving this equation. Another solution, based on the recent development by Monchiet et al. (2007) would be to define τ_s^* based on the following equation:

$$\frac{\tau_s^2}{\tau_s^{*2}} + 2f \cosh\left(\sqrt{\frac{3}{20}\frac{\sigma_m^2}{\tau_s^{*2}} + \frac{2}{45}\frac{\sigma_{eq}^2}{\tau_s^{*2}}}\right) - 1 - f^2 \overset{\text{def.}\tau_s^*}{=} 0 \tag{7}$$

In the following the Gurson-like formulation will be used (Eq. 6). It is however well known that the original Gurson (1977) model could not well represent the behaviour of actual voided cells as simulated using finite element calculations (Brocks et al., 1995; Kuna and Sun, 1996 and Fritzen et al., 2012) so that empirical modifications have to be introduced to better represent the cell behaviour (Tvergaard and Needleman, 1984 and Faleskog et al., 1998). Accordingly, the following definition for τ_s^* is proposed:

$$\left(\frac{\tau_s^2}{\tau_s^{*2}} + \alpha \frac{2}{45} f \frac{\sigma_{eq}^2}{\tau_s^{*2}}\right) + 2q_1 f \cosh\left(q_2 \sqrt{\frac{3}{20}} \frac{\sigma_m}{\tau_s^*}\right) - 1 - q_1^2 f^2 \overset{\text{def.}\tau_s^*}{=} 0 \tag{8}$$

where α, q_1 and q_2 are parameters that need to be adjusted. q_1 and q_2 play a similar role as in the work by Tvergaard and Needleman (1984) whereas α is a new parameter weighting the relative contribution of the resolved shear stress on each slip system and the usual isotropic equivalent von Mises stress measure. The identification of these parameters will be done in the following based on unit cell simulations of voided single crystals. In all cases, $\tau_s^* = |\tau_s|$ for $f = 0$ so that the yield surface of the single crystal matrix is retrieved.

For each slip system, the yield surface is then defined as:

$$\psi_s^* = \tau_s^* - \tau_0 = 0 \tag{9}$$