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Effective flow surface of porous materials with two populations of voids under internal pressure: II. Full-field simulations

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ABSTRACT

This study is devoted to the effective plastic flow surface of a bi-porous material saturated by a fluid. Highly irradiated uranium dioxide is a typical example of such a material. In part I of this study, a GTN-type approximation of the effective plastic flow surface has been derived. In this second part, the predictions of this new model are compared with full-field numerical simulations performed with a numerical method based on Fast Fourier Transforms. This method is successfully applied to voided materials with a Gurson matrix where the voids are subjected to internal pressure. Different microstructures containing a large number of spherical or ellipsoidal voids are investigated. The deviation from isotropy of their mechanical response is measured by a new criterion.

1. Introduction

In the second part of this study devoted to the mechanical behavior of highly irradiated uranium dioxide fuel (UO_2) under accident conditions, the predictions of the analytical models proposed in the first part are compared to full-field simulations. As recalled in part I of this paper, UO_2 exhibits a very specific microstructure with two populations of voids of rather different sizes and shapes: a first population of voids, almost spherical in shape, is observed inside the grains at the lowest scale (intragranular voids), and a second population of voids, almost lenticular and located at the grain boundaries can be found at a larger scale (intergranular voids). During a reactivity initiated accident (RIA), the temperature of the fuel increases abruptly, inducing a thermal dilatation of the material and a strong increase of the pressure in the voids due to the presence of fission gases confined inside these bubbles. At the mesoscale, the matrix (where intragranular voids are already smeared out) is modeled as a pressure-sensitive ductile material governed by the Gurson–Tvergaard–Needleman (GTN) criterion (Gurson, 1977; Koplik and Needleman, 1988; Tvergaard et al., 1990). The objective of this study is to derive a criterion describing the effective flow surface of the voided material at the macroscopic scale when the intergranular voids are ellipsoidal and subjected to an internal pressure.

The analytical Gurson-like criterion (or GTN criterion) proposed in the first part of this study (Vincent et al., 2014) takes the form:

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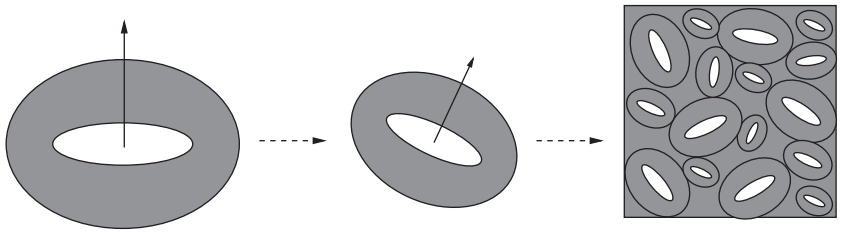

Fig. 1. *Assemblage of self-similar randomly oriented hollow ellipsoids (from (Vincent et al., 2009)). Unit pattern (left). Rotated and dilated hollow ellipsoid (center). Representative volume element (right).*

$$\frac{1}{\beta}\left(\frac{\Sigma_{eq}}{\sigma_0}\right)^2+\frac{1}{\alpha}\cosh\left(\frac{3}{2}\left(\frac{\Sigma_m}{\sigma_0}-\gamma\right)\right)-1=0, \tag{1}$$

where α, β, and γ are three functions of the parameters of the problem, namely f_b the void volume fraction of the spherical intragranular voids of very small size, f_e and w the void volume fraction and aspect-ratio of the ellipsoidal (oblate) intergranular voids, p_b and p_e the internal pressures in the intragranular and intergranular voids, respectively (see part I of this study, Vincent et al., 2014, for more details). Fritzen et al. (2013) have recently published a similar study for voided materials with a pressure-sensitive matrix of Green type. The present study differs from the latter one in three aspects: first the matrix in the present study is a Gurson material, second the voids are randomly oriented ellipsoids and third they are subjected to an internal pressure.

The approach followed to derive (1) is based on a study of an elementary volume element made of a single hollow ellipsoid and extended to an assemblage of self-similar randomly oriented ellipsoidal voids, as schematized in Fig. 1.

Since, to the best of the authors' knowledge, no comparison with experimental data is available to assess the validity of the analytical model (1), its predictions are compared here with three-dimensional full-field simulations, performed with a numerical method based on Fast Fourier Transforms. This iterative method was proposed by Moulinec and Suquet (1994, 1998) for microstructures subjected to periodic boundary conditions and does not require, at least explicitly, any meshing of the microstructure.

The organization of the paper is as follows:

- The procedure followed to generate different microstructures used in the full-field simulations is presented in Section 2.1. These microstructures must contain a large number of voids to approach overall isotropy as closely as possible. An original (to the best of our knowledge) criterion for measuring deviation from isotropy is introduced.
- A reminder on the FFT method, and its variant based on augmented Lagrangians is given in Section 3.
- Finally the results of the full-field simulations for spherical and ellipsoidal voids are presented in Sections 4.2 and 4.3 and compared with the analytical criterion (1). The agreement is found to be good, not only for the effective flow surface but also for the average dilatation-rate in the matrix which governs the evolution of the void volume fraction of both population of voids.

2. Microstructures

2.1. Microstructure generation

The full-field simulations are performed on artificially generated microstructures. The unit-cell is a unit cube. The microstructures are generated in two steps.

1. First the unit-cell is filled with spheres using an algorithm inspired by Molecular Dynamics. This algorithm proceeds iteratively. First, the spheres are randomly placed in the volume and can freely overlap. Then the distance of interpenetration between each sphere and its neighbors is calculated as the sum of the radius of the sphere and of its neighbors minus the distance between the centers of the two spheres (or zero if the spheres do not interpenetrate). For each sphere all the interprenetration distances are summed up and the center of the sphere is moved by a given fraction of this sum augmented by a small random displacement. The iterative process is stopped as soon as no interpenetration is detected between spheres. The volume fraction which can be reached by the classical Random Sequential Addition algorithm (Torquato, 2003) does not exceed 40% whereas the filling rate obtained with the above MD algorithm is about 60% for monodisperse spheres and higher for polydisperse spheres.
2. In a second step, a unit void, either a spherical void or an ellipsoidal void with random orientation, is located at the center of each sphere. All single hollow elements are self-similar and the void volume fraction in each of them is identical, chosen in such a way that the overall void volume fraction f_e is reached. Therefore each void is surrounded by a shell of matrix with a width proportional to the void size.