Effective flow surface of a bi-porous material: constitutive modeling and numerical simulations

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ABSTRACT

This work is devoted to the mechanical behavior of ductile porous materials with two populations of cavities of rather different sizes and shapes. A modeling of the effective plastic flow surface following [1] is briefly recalled and the results are compared to original numerical simulations using a computational method based on augmented Lagrangians and Fast Fourier Transforms for composite materials (FFT Method, [2]).

The starting point of this study is the modeling of the mechanical behavior of the highly irradiated uranium dioxide (UO_2) studied by the French "Institut de Radioprotection et de Sûreté Nucléaire" (IRSN) to assess the behavior of fuel rods under accident conditions. UO_2 is a porous material with a complex microstructure. This is a polycrystalline material with grain size of about $10\ \mu m$. When highly irradiated, its microstructure shows, as a first approximation, two populations of cavities of rather different sizes and shapes. At the smallest scale (microscopic scale), a first population of cavities, almost spherical in shape with a typical diameter of a few nanometers can be found in the interior of the grains (referred to as *intragranular bubbles*). At a larger scale (mesoscopic scale), a second population of cavities, roughly spheroidal in shape with typical size of a few microns, can be observed at the grain boundaries (referred to as *intergranular bubbles*). These two populations of cavities contain fission gases.

At high temperature, such as those encountered in accident conditions, this porous material is almost ductile. Moreover, under such conditions, the pressures inside the cavities (due to the fission gases) and the effective thermal strain sharply increase resulting in the growth and coalescence of the cavities.

Approximate models for the effective flow surface of a bi-porous material have been proposed in [1] and are briefly recalled. An up-scaling procedure is performed in two successive steps: first from the microscopic to the mesoscopic scale, smearing out all the small spherical voids, and second from the mesoscopic to the macroscopic scale, smearing out the details of the grain boundaries and the intergranular ellipsoidal voids. The main model is based on the variational approach of Ponte Castañeda and Suquet [3] applied to a Gurson-like matrix containing randomly oriented ellipsoidal cavities. In other words, the governing equation for the flow surface of the grains containing intragranular spherical bubbles is a Gurson-like criterion. For the second step of the up-scaling, the variational (or modified secant) method is used. Central to these techniques is the notion of a linear comparison composite (LCC)

which, here, exhibits the same geometry as the original nonlinear material and whose properties are determined by a nonlinear closure condition. The LCC is comprised of a matrix phase with randomly distributed ellipsoidal pressurized cavities. The matrix phase is split into N several layers in order to refine the predictions of the model, following an idea originally introduced in [4]. As a result, the main model presented in the article of [1] is called the N-phase model.
When the two internal pressures inside the two populations of cavities coincide, the effective flow surface of the biporous material is obtained from that of the drained material by *a shift along the hydrostatic axis*. However, when the two pressures are different, the modifications brought to the effective flow surface in the drained case involve not only a shift along the hydrostatic axis but also *a change in shape and size of the surface*.
In order to check the validity of this model, two types of numerical simulations using the FFT Method have been performed. First, simulations with a Gurson matrix and ellipsoidal cavities without internal pressure have been carried out in 2D generalized plane strain. The N-phase model of [1] has been extended to this specific case for comparison. These simulations show highly localized strain fields when the overall stress is almost hydrostatic.
Then, 3D simulations with a Gurson matrix and spherical cavities with internal pressure have been carried out. The results of these simulations are in good agreement with the predictions of the model [1]. In particular, the effect of the two pressures on the effective flow surface is accurately captured.

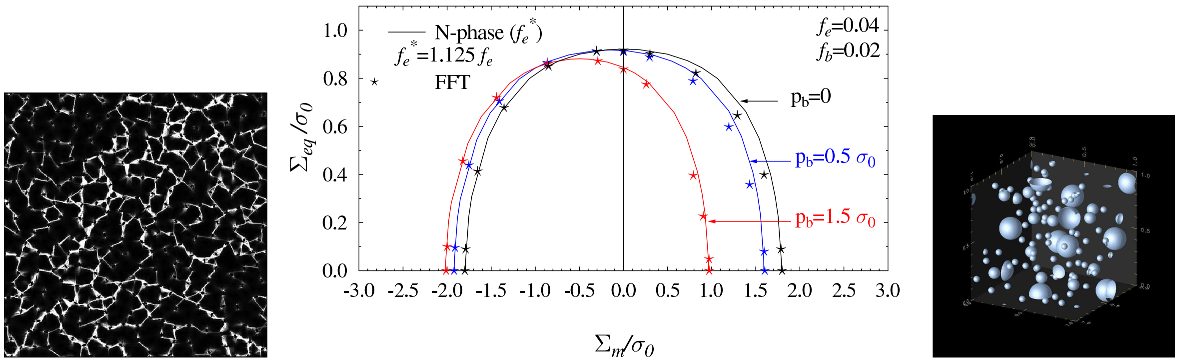

Figure 1: *Left*: 2D FFT simulation: localization of the local strain for an overall hydrostatic stress. *Medium*: Effective flow surfaces - 3D FFT simulations and model [1] (f_e intergranular porosity, f_b intragranular local porosity, p_b and p_e intra and intergranular cavity pressures, σ_o yield stress of the sane matrix, Σ_m and Σ_{eq} overall hydrostatic and von Mises stresses, $p_e = 0$). *Right*: 3D unit cell.

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