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Elastic behavior of porous media with spherical nanovoids

Xavier Haller[a,c], Yann Monerie[b,c], Stéphane Pagano[b,c], Pierre-Guy Vincent[a,c,*]

[a] Institut de Radioprotection et de Sûreté Nucléaire, B.P. 3, 13115 Saint-Paul-lez-Durance Cedex, France
[b] Laboratoire de Mécanique et Génie Civil, Université de Montpellier, CNRS, CC 048 Place Eugène Bataillon, 34095 Montpellier Cedex, France
[c] Laboratoire de Micromécanique et Intégrité des Structures, IRSN-CNRS-UM, B.P. 3, 13115 Saint-Paul-lez-Durance Cedex, France

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ABSTRACT

This study is devoted to the effective elastic properties of nanoporous media containing spherical nanovoids. Nanocomposites materials are strongly dependent on their nanometric characteristic lengths. This size effect cannot be directly modeled using the classical homogenization schemes based on the Eshelby inclusion problem. However recent studies have extended the continuum mechanics and well-known micromechanical models to the nanoscale. In this paper, it is shown that these models can be replaced in a unified framework using the morphologically representative pattern-based approach of Stolz and Zaoui (1991) and therefore can be generalized to more complex microstructures. Following this approach, new bounds and estimates are derived. Two particular cases are treated: (i) the case of an ellipsoidal spatial distribution of the voids, (ii) the case of a biporous material containing both spherical nanovoids and randomly oriented spheroidal microvoids. The second case is typical of the microstructure of the irradiated uranium dioxide (UO_2). Thereby, the associated result could be used for determining the poro-elastic properties of these doubly voided materials.

1. Introduction

Nanoporous materials can be classified into the category of nanocomposites materials in which the characteristic length is typically of the order of a few nanometers (<100 nm, Paliwal and Cherkaoui (2012)). The particularity of this kind of materials is the high surface/volume ratio. Indeed, atoms near a surface are in a different local environment than those in the bulk: their coordination number is less than that of the bulk atoms and their energy is different (Duan et al., 2005a; 2005b; Paliwal and Cherkaoui, 2012; Wang et al., 2011). Therefore there is a disturbed region sometimes called the *interfacial region* whose thickness is of the order of few atomic layers (about one nanometer), which has a local elastic behavior different from that of the bulk (Paliwal and Cherkaoui, 2012; Wang et al., 2011). The impact of surfaces is often negligible in classical continuum mechanics but becomes predominant when the number of surface atoms is high as in nanocomposite materials (Brisard et al., 2010a; Duan et al., 2005a; 2005b; Le Quang and He, 2008; Paliwal and Cherkaoui, 2012; Wang et al., 2011). In particular, such surface effects have to be considered when deriving a model for the effective elastic behavior of these materials. The main consequence of the surface effects is a strong dependency of the effective properties to the nanometer characteristic length (Duan et al., 2005b; Paliwal and Cherkaoui, 2012; Sharma and Ganti, 2004). The present study is devoted to the modeling of the elastic properties of porous materials which exhibits cavities whose characteristic length is in the nanometer range.

Indeed, this is the case of the irradiated uranium dioxide (UO_2), which is commonly used as a nuclear fuel. The modeling of its mechanical behavior from up-scaling methods has recently motivated several studies (see for example Julien et al. (2011); Vincent et al. (2008); Vincent et al. (2009a, 2009b); Vincent et al. (2014a, 2014b)). This material contains intragranular cavities whose radii range between one and ten nanometers and pore density from 10^{23} m^{-3} to 10^{24} m^{-3} (Kashibe et al., 1993). Jelea et al. (2011) have carried out atomistic simulations and have determined the elastic moduli of a system built with periodic UO_2 elementary cells containing spherical nanocavities. Their results are compared to classical homogenization schemes in elasticity (Mori–Tanaka and self-consistent) and experimental data. Although there is a good agreement between the different results, it was shown that a surface effect exists at the scale of nanometric intragranular cavities in UO_2 and the results obtained from the homogenization approach could be improved by taking into account these surface effects.

* Corresponding author at: Institut de Radioprotection et de Sûreté Nucléaire, B.P. 3, 13115 Saint-Paul-lez-Durance Cedex, France. Tel.: +33 4 42 19 97 61; fax: +33 4 42 19 91 66.
E-mail addresses: xavier.haller@irsn.fr (X. Haller), yann.monerie@umontpellier.fr (Y. Monerie), stephane.pagano@umontpellier.fr (S. Pagano), pierre-guy.vincent@irsn.fr (P.-G. Vincent).

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Description of the disturbed region. The first step to derive a micromechanical model with surface effects consists in giving a mechanical description to the disturbed region. There are mainly two ways to model this region. The first way is a zero thickness approach and the disturbed region is treated as an 'interface'. The interface stress model or 'imperfect coherent interface model' assumes that the traction vector is discontinuous across the surface and the displacement is continuous (Brisard et al., 2010a; 2010b; Duan et al., 2005a; 2005b; 2005c; 2006; 2007; Le Quang and He, 2008; Paliwal and Cherkaoui, 2012; Sharma and Ganti, 2004; Wang et al., 2005; 2011; 2007). This model is a limit case of a thin and stiff interphase (Wang et al., 2005) and is often used to model the disturbed region for nanocomposite materials.

The second way describes the disturbed region as an 'interphase' (Marcadon, 2005; Paliwal and Cherkaoui, 2012), i.e. as a classical three-dimensional coating. Although this approach is less used than the interface stress model, it makes no assumption concerning the stiffness and the thickness of the disturbed region. However it often leads to more complex analytical results.

Homogenization process. Once the description of the interfacial region is chosen, it has to be integrated in the homogenization process to derive models. Most of the classical micromechanical models are based on the Eshelby inclusion problem (Eshelby, 1957) and cannot deal with surface effects. Relatively recent works (Brisard et al., 2010a; 2010b; Duan et al., 2005b) have extended these classical models to the case of nanocomposite materials, particularly the Hashin (1962) composite sphere assemblage model, the Mori and Tanaka (1973) model, and the generalized self-consistent model (Christensen and Lo, 1979). These models, developed by analogy with their classical counterparts, are based on a *modified* inclusion problem in which the perfect interface[1] between the spherical inclusion and the surrounding medium is replaced by an imperfect coherent interface (as stated above, the term *coherent* means that the displacement field is continuous across the interface). The solving of this problem generally leads to non-uniform deformation fields inside the inclusion. This generalization of the classical results is limited to the case of materials containing nanospherical inclusions isotropically distributed inside the bulk. However, it is shown in the sequel that they can be derived in the theoretical framework of the morphologically representative pattern (MRP) theory (Bornert, 1996a; 1996b; 2001; Bornert et al., 1996; Stolz and Zaoui, 1991) and thus extended to the case of materials with more complex microstructures such as an ellipsoidal spatial distribution of voids.

Morphologically representative pattern. The MRP theory extends the classical approach: it allows us to take some finer details of the microstructure into account and particularly the local arrangement of the phases. It is convenient in the case of nanoparticulate composites (also called materials with an inclusion-matrix morphology[2]), in which the disturbed region is included between the matrix and the heterogeneities and locally perturbs the mechanical fields. The establishment of the effective elastic moduli through this approach requires the solving of auxiliary problems related to heterogeneous inclusions embedded in an infinite medium. In the case of the spherical inclusions or voids, these auxiliary problems are similar to those solved by Duan et al. (2005b) and correspond to a single spherical inclusion coated with a disturbed region (modeled as an interface or an interphase) surrounded by a matrix phase. It is shown here that the MRP approach delivers a better understanding concerning the assumptions underlying in the already existing models.

[1] A perfect interface (or a perfect bonding condition) means that the traction vector and the displacement are continuous across two adjacent media.

[2] The material is made of a predominant phase in which heterogeneities (inclusions, voids or *heterogeneous* inclusions) are included.

The present study is organized as follows. The interface stress model typically used for nanomaterials is shortly described in Section 2. In Section 3, the theory and the main results concerning the MRP approach are summarized. This section is also devoted to a direct use of the MRP theory in the case of nanoporous materials and it is shown that the existing models can be directly derived from the MRP approach. Section 4 deals with some original results, corresponding to particular cases that can be easily treated following the MRP theory. It illustrates the ability of the MRP approach to catch the effective elastic properties of materials containing nanospherical voids. Two particular cases are discussed in this section: (i) spheroidal spatial distributions of voids, (ii) a biporous medium containing spherical nanovoids together with larger spheroidal voids. The second case is typical of the microstructure of irradiated UO_2 and the results are then plotted with characteristic moduli for this material.

2. Nanomaterials: modeling of the disturbed region with the interface stress model

As already stated, the interface stress model is intensively used in the case of nanomaterials. It assumes a traction vector jump across the interface whereas the displacement is continuous. This model has been proposed by Gurtin and Murdoch (1975) developing a theoretical framework for the mechanical behavior of material surfaces.

The Gurtin and Murdoch model consists in a set of two equations: a surface constitutive law and a balance equation. The surface constitutive law is assumed to be composed of two parts: a surface internal stress, called by analogy with liquids a 'surface tension', which is independent on the external loading and an elastic part whose moduli are distinct from those of the bulk. The elastic behavior is often assumed to remain isotropic in the tangent plane. For polycristals with intragranular nanocavities, such as the irradiated UO_2, due to the crystal anisotropy, the mechanical behavior of the disturbed region around each cavity is probably not isotropic. It is unlikely that the disturbed region is in a particular crystallographic orientation and it is certainly randomly oriented. Although the hypothesis of an isotropic elastic behavior of the disturbed region is not really equivalent to the case of randomly oriented disturbed regions, the complexity generated by anisotropy to develop non-numerical micromechanical models would be higher than the gain of precision by taking account of it (Duan et al., 2005b; Paliwal and Cherkaoui, 2012). As a result, the elastic behavior of the surface is commonly considered as isotropic.

The surface between two media (1 and 2) is denoted by Γ. The unit normal vector to Γ (oriented from 1 to 2) is denoted by $\boldsymbol{n}$ and the two vectors $\boldsymbol{t}_t$ and $\boldsymbol{t}_b$ are unit vectors contained in the tangent plane to Γ. These three vectors are assumed to be pairwise orthogonal and $(\boldsymbol{t}_t, \boldsymbol{t}_b, \boldsymbol{n})$ forms a vector basis for 3 dimensional vectors ($\boldsymbol{n} = \boldsymbol{t}_t \wedge \boldsymbol{t}_b$). The couple $(\boldsymbol{t}_t,\ \boldsymbol{t}_b)$ is a basis for surface tangent vectors. The second-order identity tensor in the tangent plane $\boldsymbol{i}_T$ and the fourth-order identity tensor in the tangent plane $\mathbb{I}_T$ are defined as:

$$\boldsymbol{i}_T = \boldsymbol{i} - \boldsymbol{n} \otimes \boldsymbol{n} \tag{1}$$

$$\mathbb{I}_T = \sum_{\alpha,\beta=t,b} \Big[\boldsymbol{t}_\alpha \otimes \boldsymbol{t}_\alpha \otimes \boldsymbol{t}_\alpha \otimes \boldsymbol{t}_\alpha + \frac{1}{2}\left(\boldsymbol{t}_\alpha \otimes \boldsymbol{t}_\beta \otimes \boldsymbol{t}_\alpha \otimes \boldsymbol{t}_\beta + \boldsymbol{t}_\alpha \otimes \boldsymbol{t}_\beta \otimes \boldsymbol{t}_\beta \otimes \boldsymbol{t}_\alpha\right) \Big] \tag{2}$$

where $\boldsymbol{i}$ is the classical second-order identity tensor ($i_{kl} = 1$ if $k = l$, $i_{kl} = 0$ otherwise) and $\otimes$ denotes the tensor product. The two tensors $\boldsymbol{i}_T$ and $\mathbb{I}_T$ can be seen as projectors onto the surface, in the sense that they serve to extract the tangential parts of vectors or