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Inverse homogenization problem: Evaluation of elastic and electrical (thermal) properties of composite constituents

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ABSTRACT

The methodology of evaluation of the elastic and electrical/thermal properties of composite constituents from measurements of the overall properties of heterogeneous material is proposed and verified by comparison with experimental data available in the literature and with results of direct Finite Element Method (FEM) simulations. A theoretical approach is based on the solution of the inverse homogenization problem in the frameworks of the Non-Interaction approximation, Maxwell and Mori-Tanaka-Benveniste micromechanical models. Sensitivity of the results to the shape of inhomogeneities and contrast in matrix/inhomogeneities properties is discussed. It is observed that reconstruction of matrix properties is generally more accurate in comparison with properties of inhomogeneities.

1. Introduction

This work is motivated by needs in rock mechanics and mechanics of nanocomposites. In rock mechanics, reliable data on rock thermal and elastic properties are required for basin and petroleum system modeling, interpretation of temperature logging data, etc. However, sometimes, consolidated cores cannot be recovered even during the well drilling in highly porous and/or fractured reservoirs and the necessity to evaluate the properties of rock cuttings becomes of primary importance. In mechanics of nanocomposites, very often properties of small inhomogeneities differ significantly from the properties of bulk materials and must be evaluated independently (see Fig. 1 for examples). Moreover, interphase zones in such composites play a significant role but there are no reliable methods to estimate these properties. Certainly, similar problems appear in other applications as well. To the best of our knowledge, they have never been systematically studied. Our paper attempts to fill this gap and proposes an approach based on the solution of inverse homogenization problem – expression of the properties of inhomogeneities or matrix in terms of the properties of a matrix or inhomogeneities, overall effective properties of a composite and available microstructural information.

Inverse problems of micromechanics usually appear in the context of recovery of microstructural information from the effective properties. The extraction of microstructural information from the effective properties involves uncertainties due to an obvious non-uniqueness in this inverse problem (Sevostianov, Gorbatikh, & Kachanov, 2001). The extent of uncertainty strongly depends on the type of the overall anisotropy; it is reduced if partial information on defect shapes or on the overall porosity becomes independently available. In rock mechanics, the problem of interest is the recovery of information on crack systems from the effective moduli (Hood & Schoenberg, 1989) and wave-speed data is often used in

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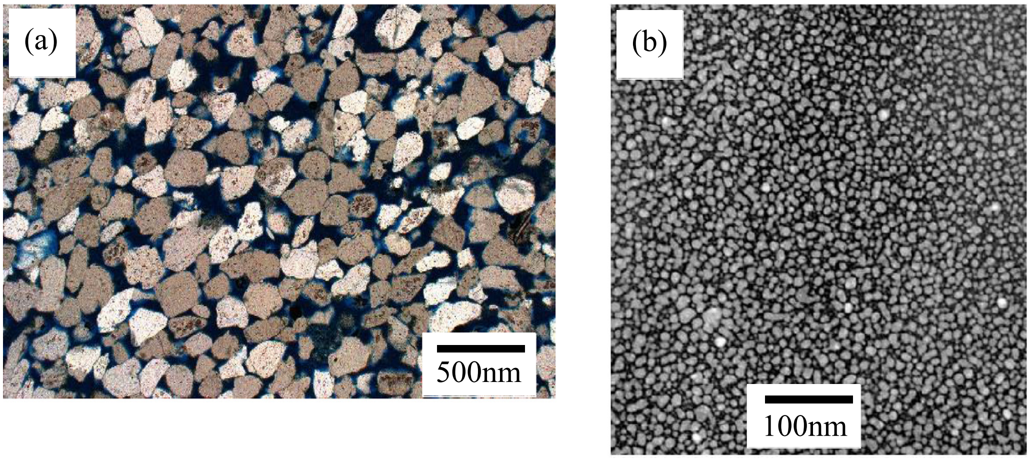

Fig. 1. Examples of (a) sand stone specimens (colored cross-section, light color corresponds to the grains of quartzite, dark–porous space) (Chen et al., 2017); (b) FE-SEM microstructure of alumina–17 vol.% SiC nanocomposites sintered by spark plasma sintering (SPS) at 1400 °C (Borrell, Álvarez, Torrecillas, Rocha, & Fernández, 2012). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

this context (Sayers & Kachanov, 1995). Monitoring of microstructure is an important problem in biomedical applications, for example, in connection with the evolution of microstructure of bones due to aging and other factors (Burr et al., 1995). Evaluation of the effective thermal or hydraulic conductivity of a random mixture of two different materials from the known effective permittivity of the same mixture was discussed in (Cherkaev, 2001). Author proposed to obtain geometrical information of microstructure from spectral measurements in the Stieltjes representation of the effective complex permittivity. (Bonifasi-Lista & Cherkaev, 2009) proposed the recovery of porosity of bone from measurements of its effective electrical properties. The microstructural information was obtained from the spectral measure in the Stieltjes representation of the bone effective complex permittivity or complex conductivity and can be recovered from the measurements over a range of frequencies. Several numerical algorithms of recovery of the microstructural information from measured transport properties of composite materials were suggested in (McPhedran, McKenzie, & Milton, 1982). The inverse Bruggeman homogenization problem was solved using Newton–Raphson technique to extract geometrical information of dielectric columnar thin film, characterized macroscopically by relative permittivity dyadic, at the nanoscale (Mackay & Lakhtakia, 2009). In (Zhang, Cherkaev, & Lamoureux, 2011), the authors used numerical rational approximation of Bruggeman continuous spectral density for estimation of fractions of components in a composite from simulated effective permittivity of the medium.

In the present work, we discuss inverse homogenization procedure in a different context – to reconstruct information on the elastic properties and electrical/thermal conductivities of composite constituents while effective properties and morphology are presumed to be known. Although this problem is easier than the inverse problem on recovery of geometrical parameters, the key issues that arise in its context do not seem to have been adequately discussed in literature. Our approach is based on the concept of property contribution tensors discussed in Section 2 and applied to the systems containing randomly oriented mixture of ellipsoidal inhomogeneities using Non-Interaction approximation, Mori-Tanaka and Maxwell schemes. In Section 3 we present the inversion of these schemes for elastic problems while in Section 4 we consider thermal conductivity. Procedure of generation and further numerical homogenization of representative volume elements (RVEs) is presented in Section 5. Theoretical predictions of the properties of inhomogeneities according to various homogenization techniques are compared with numerical results in Section 5; application to the experimental data of composites with glass inhomogeneities is presented in Section 6. Sensitivity analysis of approximations with respect to the variation in volume fraction, material properties, and shape of inhomogeneities is presented in Section 7. Finally, conclusions and remarks are drawn in Section 8.

2. Theoretical background

In this section, we provide a brief overview of the theoretical approach to the inverse homogenization procedure. It is based on the concept of property contribution tensors for a single inhomogeneity that have been first introduced in the context of elastic properties of a material containing ellipsoidal pores (Horii & Nemat-Nasser, 1983).

2.1. Elasticity problem

In the context of effective elastic properties, we consider a volume V containing matrix material and an isolated inhomogeneity of volume V_1. The volume V is subjected to uniform traction boundary conditions on $\partial V : \boldsymbol{t}|_{\partial V} = \boldsymbol{\sigma}^0 \cdot \mathbf{n},$ where