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Evaluation of the effective elastic and conductive properties of a material containing concave pores

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ABSTRACT

We calculate effective properties of a porous material with non-ellipsoidal concave pores. The pore shape is described by equation of a supersphere $x^{2p} + y^{2p} + z^{2p} = 1$ that is convex when $p > 0.5$ and concave when$p < 0.5$. Compliance and resistivity contribution tensors for a superspherical pore are calculated using finite element method and approximated by analytical expressions for $p < 1$. These tensors are used to evaluate effective elastic and conductive properties of a material with superspherical pores via non-interaction approximation, Mori–Tanaka scheme and Maxwell scheme. We show that the geometrical parameters entering expressions for the elastic moduli and conductivity are the same and establish cross-property connection for such materials. These connections coincide with ones for a material with spherical pores.

1. Introduction

In this paper we develop a semi-analytical approach to evaluate effective elastic properties and thermal conductivity of a material containing pores of non-ellipsoidal shape focusing on concave superspherical pores. The key quantities in the problem of the effective elastic and conductive properties of a heterogeneous material are property contribution tensors that give the extra strain or temperature gradient produced by introduction of the inhomogeneity into the material subjected to uniform stress field or heat flux. Alternatively, one can use the dual stiffness contribution tensor or conductivity contribution tensor (see Sevostianov & Kachanov, 2007).

Although various materials science applications require quantitative characterization of inhomogeneities of irregular shape, most of the existing results are based on Eshelby's (1957, 1961) solution for an ellipsoidal inhomogeneity. While for 2-D non-elliptical inhomogeneities many analytical and numerical results have been obtained (see Zimmerman, 1986; Kachanov, Tsukrov, & Shafiro, 1994; Tsukrov & Novak 2002, 2004), only a limited number of numerical results and approximate estimates are available for non-ellipsoidal 3-D shapes. Compliance contribution tensors for several examples of pores of irregular shape typical for carbon–carbon composites have been calculated by Drach et al. (2011) using FEM. The authors showed that pores of irregular shapes can be sometimes approximated by ellipsoids (in agreement with earlier experimental works of Prokopiev & Sevostianov, 2006, 2007). It is difficult, however, to make any conclusions from the results of Drach et al. (2011) (Tables 1 and 2 in their paper) regarding effect of any particular irregularity factor. In the narrower context of irregularly shaped cracks, certain results were

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obtained by Sevostianov and Kachanov (2002); Grechka, Vasconselos, and Kachanov (2006); Mear, Sevostianov, and Kachanov (2007); Kachanov and Sevostianov (2012).

The only analytical model that can account for concave shape of the pores has been developed by Sevostianov and Giraud (2012) and applied by Giraud and Sevostianov (2013) to calculation of the overall elastic properties of oolitic rock. This approach, however is based on computational results of Sevostianov, Kachanov, and Zohdi (2008) where stability of the calculations is rather poor and, as we discuss below, the accuracy of the calculations is insufficient.

The property contribution tensor is used as the basic building block to evaluate effective elastic and conductive properties of a material containing concave superspherical pores. For this goal we use (1) Mori–Tanaka (Mori & Tanaka, 1973) scheme in the form given by Benveniste (1986) and (2) Maxwell scheme (Maxwell, 1873) in the form proposed by Sevostianov and Giraud (2013). These schemes, in particular, are known to have good agreement with experimental data on elastic and conductive properties of porous materials.

1.1. Remark on Eshelby tensor

Some results have been obtained in the context of calculation of Eshelby tensor for a non-ellipsoidal inclusion. We mention results of Rodin (1996) for polyhedral shapes, Onaka (2001) for a concave supersphere; Onaka, Sato, and Kato (2002) for a toroidal inclusion and Chen, Giraud, Sevotianov, and Grgic (2015) for a convex supersphere. We have to point out however, that Eshelby tensor for non-ellipsoidal inhomogeneities is irrelevant for the problem of effective properties of heterogeneous material. Unfortunately, several publications already appeared where authors erroneously try to calculate effective properties of materials with non-ellipsoidal inhomogeneities using Eshelby tensor (see, for example Hashemi, Avazmohammadi, Shodja, & Weng (2009) where results of Onaka (2001) are used to calculate effective properties of a composite with cuboidal inhomogeneities). This mistake is a consequence of the misleading overestimation of the role of Eshelby tensor in micromechanics.

2. Property contribution tensors for a superspherical inhomogeneity

2.1. Compliance and resistivity contribution tensors

Compliance and resistivity contribution tensors have been first introduced in the context of pores and cracks by Horii and Nemat-Nasser (1983) (see also detailed discussion in the book of Nemat-Nasser & Hori, 1993). Components of this tensor were calculated for 2-D pores of various shape and 3-D ellipsoidal pores by Kachanov et al. (1994). For general case of elastic inhomogeneities, these tensors were introduced and calculated for ellipsoidal shapes by Sevostianov and Kachanov (1999, 2002). In this section we briefly describe the physical meaning of the compliance contribution tensor and discuss how it may be calculated for a superspherical pore.

We consider a homogeneous isotropic elastic material (matrix), with the compliance tensor $\boldsymbol{S}^0$ containing an inhomogeneity, of volume V_*, of a different material with the compliance tensor $\boldsymbol{S}^1$. The compliance contribution tensor of the inhomogeneity is a fourth-rank tensor $\boldsymbol{H}$ that gives the extra strain (per reference volume V) due to the presence of the inhomogeneity:

$$\Delta\,\boldsymbol{\varepsilon} = \frac{V_*}{V}\boldsymbol{H}:\boldsymbol{\sigma}^\infty, \quad \text{or,}\ \ \text{in components,}\quad \Delta\varepsilon_{ij} = \frac{V_*}{V}H_{ijkl}\sigma_{kl}^\infty \tag{2.1}$$

where σ_{kl}^∞ are remotely applied stresses that are assumed to be uniform within V in the absence of the inhomogeneity. For an ellipsoidal inhomogeneity, its compliance contribution tensor is expressed in terms of tensor $\boldsymbol{Q}$ - one of two Hill's tensors (Hill, 1965, Walpole, 1969) as

$$\boldsymbol{H} = [(\boldsymbol{S}^1 - \boldsymbol{S}^0)^{-1} + \boldsymbol{Q}]^{-1}, \tag{2.2}$$

Sevostianov and Kachanov (2011) showed that the far-field asymptotics of the elastic fields generated by an inhomogeneity determines its contribution to the effective elastic properties and vice versa. The latter result, in particular, allows formulation of the Maxwell homogenization scheme in its terms (Sevostianov & Giraud, 2013).

For a pore, the additional strain due to its presence is calculated as an integral over the pore boundary $\partial\Omega$

$$\Delta\varepsilon_{ij} = \frac{-1}{2V}\int_{\partial\Omega}(u_i n_j + u_j n_i)dS \tag{2.3}$$

where $\boldsymbol{u}$ and $\boldsymbol{n}$ denote displacements on the pore boundary and a unit normal to it (directed inwards the pore). The representation (2.3) directly follows from application of the divergence theorem to a solid containing a pore (see, for example, Kachanov et al., 1994).

The resistivity contribution tensor has been introduced by Sevostianov and Kachanov (2002) in the context of the cross-property connection between elastic and conductive properties of heterogeneous materials. We assume that the background material of volume V with the isotropic thermal conductivity k_0 contains an isolated inhomogeneity of volume V_1 with the isotropic thermal conductivity k_1. Limiting cases $k_1 = 0$ and $k_1 = \infty$ correspond to an insulating and a superconducting inhomogeneities. Assuming linear relation between temperature gradient ∇T and the heat flux vector $\boldsymbol{q}$ per volume (Fourier law) for both