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Replacement relations for thermal conductivity of a porous rock

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ABSTRACT

We focus on derivation and experimental verification of the replacement relations that link the overall thermal conductivities of heterogeneous materials with the same matrix and microstructure but having inhomogeneities with different properties. First, we derive replacement inequalities based on Hashin-Shtrikman bounds that relate overall thermal conductivity of a composite to thermal conductivity of a.porous material. Hashin-Shtrikman bounds are also used to derive analogy of Gassmann equation for thermal conductivity. Then, we use formalism of property contribution tensors to obtain replacement relations for anisotropic materials containing ellipsoidal inhomogeneities. These relations coincide for different homogenization schemes – non-interaction approximation, Mori-Tanaka scheme, and Maxwell scheme, provided, that both effective conductivity of a composite and porous material are calculated in the framework of the same method. In the case of the overall isotropy, all of these relations coincide with Gassmann equation derived from Hashin-Shtrikman bounds. We check the possibility to apply these relations to 3-D non-ellipsoidal inhomogeneities on example of a supersphere using numerical simulations. The replacement relations are approximate with satisfactory accuracy for convex superspheres, while the error is significant for concave shapes. For this case, we suggest a modification that involves an extra shape factor that can be determined, for example, from comparison of the average Eshelby tensor for conductivity and conductivity contribution tensor of a pore. To verify the approach, thermal conductivity of 85 quartz sandstone specimens – dry and saturated with water and kerosene – of porosity varying from 0.14 to 0.29 is measured using optical scanning technique. The average pore shape and thermal conductivity of the dense quartz matrix are determined from best fitting of the conductivity-porosity curve for dry sandstone. Then these parameters are used in the replacement relation for sandstone saturated with water and kerosene. The comparison of the experimental data with theoretical predictions shows a good accuracy of the proposed approach.

1. Introduction

In the present paper we formulate the replacement relations used in the evaluation of overall conductive properties to the case of thermal conductivity. The replacement relations link overall properties of heterogeneous materials that have the same matrix material and microstructure while properties of the inclusions are different. They can be used to predict the change in overall thermal conductivity of a porous material upon the saturation.

The replacement relations have been first proposed by Gassmann[1] in the context of the effect of saturation on seismic properties of rock in geomechanics. He proposed to express the bulk modulus of fully saturated rock in terms of the elastic properties of dry rock. Brown and Korringa[2] generalized Gassmann equation for inhomogeneous anisotropic material. Further discussion has been done by Han and Batzle[3] who mentioned that several physical quantities (porosity, density and speed velocity) should be consistent and constrained and proposed to use Voigt-Reuss bounds and critical porosity limits constraints to get upper and lower bounds for the fluid-saturation effect. Ciz and Shapiro[4] obtained the replacement relations for the general case of anisotropic two-phase material with anisotropic constituents and specified it for bulk and shear moduli of the isotropic two-phase composite (see also[5] for corrected equation).

Sevostianov and Kachanov[6] formulated the replacement relations for anisotropic materials in terms of the property contribution tensor for elasticity problem. They showed that these relations are exact for ellipsoids and approximately accurate for certain non-ellipsoidal shapes (a cube and various 2D shapes). Chen et al.[7] further developed

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their results checking the applicability of the relations to 3-D non-ellipsoidal inhomogeneities on example of a supersphere (the shape is mathematically described by equation $|x_1|^{2p} + |x_2|^{2p} + |x_3|^{2p} = 1$). They showed that the replacement relations can be used to estimate with a satisfactory accuracy the effective elastic properties of a material containing inhomogeneities of convex shape, the error of estimation for concave inhomogeneities is significant. Saxena and Mavko[8] discussed the replacement relations under the assumption that the elastic fields inside the inhomogeneities are uniform (overall properties and properties of the constituents are isotropic). Note that this assumption is actually equivalent to the statement that the inhomogeneities are ellipsoids subjected to the uniform external field[9–11]. Saxena and Mavko[12,13] discussed the impactful applications of these relations in geophysics, they highlighted the importance of these relations in evaluating the effective properties of a heterogeneous material from those of a porous material and the benefices of calculating effective properties using Eshelby tensor.

In this context, the difference between the Eshelby tensor and the property contribution tensor need to be clarified. Eshelby tensor, referred in the first Eshelby problem, is a dimensionless quality that interrelate the resulted elastic field to the eigenstrain that would have been exist inside the inclusion. Property contribution tensor, referred in the second Eshelby problem, is used to give a quantitative description of the contribution of the inhomogeneity into the overall properties. For ellipsoids, the first and the second Eshelby problems are mathematically equivalent, all the tensors (Eshelby tensor, Hill tensor, property contribution tensor etc.) are uniform inside the inclusion/inhomogeneity (position independent) and they are linearly interrelated. For non-ellipsoids, the interrelation between the Eshelby tensor and the property contribution tensor is not valid, and the Eshelby tensor can't be used in the calculation of the overall properties.

In the context of thermal conductivity problem, Schärli and Rybach[14] compared air saturated and water saturated low-porosity granitic rocks and reported that thermal conductivity of water-saturated samples is 30% higher than "dry" conductivities. Zimmerman[15] evaluated thermal conductivity of air- and water- saturated rock using Fricke formula[16] for electrical conductivity of a material containing randomly oriented spheroidal inhomogeneities (that represents generalization of Maxwell formula[17]). In particular, Zimmerman[15] proposed a methodology to evaluate thermal conductivity of water saturated rock from the dry rock measurements and validated the prediction on experimental data for sedimentary and granitic rock data. He stated, that the procedure requires inversion of the equations and, while to of the required equations can be inverted in closed form, the final results can be obtained only numerically.

In the present paper, we derive the replacement relations analytically in closed form. First we use Hashin-Shtrikman bounds[18] to obtain replacement inequalities and analogy of Gassmann equation[1] for the case of thermal conductivity of *isotropic* material. Then we use formalism of resistivity/conductivity contribution tensors to derive these *relations for anisotropic materials containing ellipsoidal inhomogeneities*. The replacement relations constitute an important connection between Eshelby tensor (the first Eshelby problem) and the resistivity/conductivity contribution tensor (the second Eshelby problem). We check the possibility to use replacement relations for materials containing non-ellipsoidal inhomogeneities using example of a superspherical shape[7]. We show that, similarly to the elastic case, the replacement relations can be used as a good approximation for materials with convex inhomogeneities, while application to concave shapes lead to a serious error. In such cases, we propose to use modified replacement relation that involves a shape factor that can be determined experimentally. The approach is verified by comparison with experimentally measured thermal conductivities of dry and saturated sandstone. To the best of our knowledge, replacement relations have never been derived for anisotropic materials and their applicability has never been checked against the pore shape.

2. Replacement relations based on Hashin-Shtrikman bounds

Hashin-Shtrikman bounds for effective thermal conductivity k_{eff} of an isotropic statistically homogeneous two-phase material (consisting of two isotropic phases with conductivities k_0 and k_1) have the following form[18]:

$$k_1 + \frac{1-\phi}{\frac{\phi}{3k_1} + \frac{1}{k_0 - k_1}} \le k_{eff} \le k_0 + \frac{\phi}{\frac{1-\phi}{3k_0} + \frac{1}{k_1 - k_0}} \tag{2.1}$$

Where ϕ is volume concentration of the phase with conductivity k_1. For a porous material $k_1 = 0$ and the lower bound vanishes while the upper bound can be written as

$$k_0 + \frac{\phi}{\frac{1-\phi}{3k_0} + \frac{1}{k_1 - k_0}} = k_0\left(1 - \frac{3\phi}{2+\phi}\right) \tag{2.2}$$

Thus, the Hashin-Shtrikman bounds for overall conductivity k_{dry} of a porous material can be written as

$$0 \le k_{dry} \le k_0\left(1 - \frac{3\phi}{2+\phi}\right) \tag{2.3}$$

It leads to the following bounds for porosity ϕ:

$$\phi \le \frac{2(k_0 - k_{dry})}{2k_0 + k_{dry}};\ \ 1-\phi \ge \frac{3k_{dry}}{2(k_0 + k_{dry})} \tag{2.4}$$

Substitution of the expression (2.4) into the lower Hashin-Shtrikman bound (2.1) yields the following lower bound for the effective conductivity of a composite material in terms of the conductivity of porous material having the same structure:

$$k_1\left[\frac{2k_0(k_0+2k_1) + k_{dry}(7k_0 - 4k_1)}{2k_0(k_0+2k_1) - k_{dry}(2k_0 - 5k_1)}\right] \le k_1 + \frac{1-\phi}{\frac{\phi}{3k_1} + \frac{1}{k_0 - k_1}} \le k_{eff} \tag{2.5}$$

Similarly, the upper bound for the effective conductivity can be written as

$$k_{eff} \le k_0 + \frac{\phi}{\frac{1-\phi}{3k_0} + \frac{1}{k_1 - k_0}} \le k_0\left[\frac{2k_0k_1 + k_{dry}(2k_0 - k_1)}{2k_0^2 + k_{dry}k_1}\right] \tag{2.6}$$

Combining (2.5) and (2.6), we can write the replacement bounds - Hashin-Shtrikman bounds for effective conductivity of a two-phase material in terms of conductivities of two phases and conductivity of a porous material (having porosity equal to the volume concentration of the phase with conductivity k_1)

$$k_1\left[\frac{2k_0(k_0+2k_1) + k_{dry}(7k_0 - 4k_1)}{2k_0(k_0+2k_1) - k_{dry}(2k_0 - 5k_1)}\right] \le k_{eff} \le k_0\left[\frac{2k_0k_1 + k_{dry}(2k_0 - k_1)}{2k_0^2 + k_{dry}k_1}\right] \tag{2.7}$$

These bounds can be used, for example, to evaluate thermal conductivity of saturated rock if properties of the dry one, as well as properties of two phases are known while the porosity is not known. Fig. 1 compares bounds (2.7) with the Hashin-Shtrikman bounds (2.1) for the case of porous calcite either saturated with crude oil or having pores filled with saturated clay (the properties are given in Table 1). As expected, the wideness of resulting bounds is about the same as those of the original bounds (2.1). In particular, when the thermal conductivity of two constituents, k_0 and k_1, differ two times (conductivities of calcite and saturated clay), the upper and lower bounds almost coincide (Fig. 1a and b).

Hashin-Shtrikman upper bounds for effective conductivities of two statistically isotropic composites can be used to derive the analogy of Gassmann's equation for conductivity. Indeed, the upper bound

$$k_{eff} = k_0 + \frac{\phi}{\frac{1-\phi}{3k_0} + \frac{1}{k_1 - k_0}} \tag{2.8}$$