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Effective conductivity tensor of ordered and disordered composite media: exact relations and numerical simulations

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Abstract

Generic three-dimensional (3D) exact relations were found recently (Phys. Rev. B (2002) 184416) between macroscopic or bulk effective moduli of composite systems with related microstructures which are, in general, different. As an example of possible application of these relations, a new numerical approach is proposed for simulations of composite systems with oblate inclusions: The initially anisotropic shape of the inclusions can be transformed to spherical, but the local conductivity tensor $\hat{\sigma}_2$ of the host in the initial system should be replaced by the corresponding transformed value $\hat{\mu}_2$. We simulate large 3D networks of circuit elements in this new μ-system using relaxation, network-reduction, and other methods. The effective value of the conductivity, $\hat{\sigma}_e$, of the initial σ-system, can be found from the effective value $\hat{\mu}_e$ of the transformed μ-system, using our exact relations. We propose to apply this approach for simulations of the phase transition in the high-T_c superconducting granular ceramics.

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Despite the considerable progress made in the theory of disordered and percolating media, the main tool for studying such systems remains numerical simulations. The only analytical results for such media are the expressions obtained in the effective medium approximation (EMA) [1–3] and Keller's exact relations [4,5]. Both are widely used in current researches but both have strong restrictions on their applicability. The first (EMA) does not work in the vicinity of the percolation threshold, while the second (Keller's theorem) is valid only in 2D systems. Recently we found a generic three-dimensional (3D) exact relations between macroscopic or bulk effective moduli of composite systems with different microstructures [6]. These relations are valid for both ordered and disordered composite media. As an example of possible application of these relations, a set of Keller-like quasi-3D relations were derived recently for the case of columnar-shaped parallel inclusions [6–8].

Here we present another possible application of these relations: A new numerical approach is developed in order to perform simulations of composite systems with oblate inclusions. The initially anisotropic shape of inclusions can be transformed to spherical, but the local conductivity tensor $\hat{\sigma}_2$ of the host in the initial system must be replaced by another value $\hat{\mu}_2$. We simulate large 3D networks of circuit elements in this new μ-system using relaxation, network-reduction, and other methods. The effective value of the conductivity, $\hat{\sigma}_e$, of the initial σ-system, can be found from the effective value $\hat{\mu}_e$ of the transformed μ-system, using our exact relations.

Let us consider a pair of two-constituent composite media which differ in their microstructure as well as in their constituent physical properties. Let the first system is characterized by the local conductivity tensors $\hat{\sigma}_1$ (inclusions), $\hat{\sigma}_2$ (host), and by the volume averaged effective conductivity tensor $\hat{\sigma}_e$ (for details see e.g. Ref. [9]), while the second system is characterized by the other set of conductivity tensors $\hat{\mu}_1$, $\hat{\mu}_2$, and $\hat{\mu}_e$, respectively. As proven in Ref. [6], if

$$\frac{\delta\sigma_{\alpha\beta}}{\sqrt{\sigma^{(2)}_{\alpha\alpha}\sigma^{(2)}_{\beta\beta}}} = \frac{\delta\mu_{\alpha\beta}}{\sqrt{\mu^{(2)}_{\alpha\alpha}\mu^{(2)}_{\beta\beta}}} \quad (\text{where } \delta\hat{\sigma} \equiv \hat{\sigma}^{(2)} - \hat{\sigma}^{(1)})\,, \tag{1}$$

then the macroscopic analogue of this relation is also valid:

$$\frac{\delta\sigma^{(e)}_{\alpha\beta}}{\sqrt{\sigma^{(2)}_{\alpha\alpha}\sigma^{(2)}_{\beta\beta}}} = \frac{\delta\mu^{(e)}_{\alpha\beta}}{\sqrt{\mu^{(2)}_{\alpha\alpha}\mu^{(2)}_{\beta\beta}}}\,. \tag{2}$$

Here we assumed that the off-diagonal parts of $\hat{\sigma}$ and $\hat{\mu}$ are related as: $\sigma^{(2)}_{\alpha\beta} = -\sigma^{(2)}_{\beta\alpha}$, $\mu^{(2)}_{\alpha\beta} = -\mu^{(2)}_{\beta\alpha}$, for $\alpha \neq \beta$. Relation (2) can be simplified when $\alpha = \beta$, or if we assume $\sigma^{(2)}_{\alpha\beta} \Big/ \sqrt{\sigma^{(2)}_{\alpha\alpha}\sigma^{(2)}_{\beta\beta}} = \mu^{(2)}_{\alpha\beta} \Big/ \sqrt{\mu^{(2)}_{\alpha\alpha}\mu^{(2)}_{\beta\beta}}$. In those cases

$$\text{if } \frac{\sigma^{(1)}_{\alpha\beta}}{\sqrt{\sigma^{(2)}_{\alpha\alpha}\sigma^{(2)}_{\beta\beta}}} = \frac{\mu^{(1)}_{\alpha\beta}}{\sqrt{\mu^{(2)}_{\alpha\alpha}\mu^{(2)}_{\beta\beta}}}, \quad \text{then } \frac{\sigma^{(e)}_{\alpha\beta}}{\sqrt{\sigma^{(2)}_{\alpha\alpha}\sigma^{(2)}_{\beta\beta}}} = \frac{\mu^{(e)}_{\alpha\beta}}{\sqrt{\mu^{(2)}_{\alpha\alpha}\mu^{(2)}_{\beta\beta}}}\,. \tag{3}$$

The pair of microstructures under consideration are related to each other by the coordinate rescaling transformation: Thus, if L_α is a characteristic size in the direction

α in the first system and $\mathscr{L}_\alpha$ is the analogous value in the second system, then these lengths will be related to each other by

$$\mathscr{L}_\alpha = L_\alpha \sqrt{\mu^{(2)}_{\alpha\alpha}/\sigma^{(2)}_{\alpha\alpha}} \ . \tag{4}$$

If the tensors $\hat{\sigma}_2$ and $\hat{\mu}_2$ have diagonal elements that are not proportional to each other, then an initial spherical shape of inclusions will be transformed to an ellipsoidal shape.

Relations (1)–(3) can be used for *numerical simulations* of composites with oblate inclusions. It is clear from the above consideration that the initially anisotropic shape of inclusions can be transformed to a spherical shape. The condition, that in the re-scaled coordinates the shape of the inclusions will be spherical, is $\mathscr{L}_\alpha = \mathscr{L}_\beta$, where $\alpha, \beta = x, y, z$. After taking into account Eq. (4), this gives $L_\alpha\sqrt{\mu^{(2)}_{\alpha\alpha}/\sigma^{(2)}_{\alpha\alpha}} = L_\beta\sqrt{\mu^{(2)}_{\beta\beta}/\sigma^{(2)}_{\beta\beta}}$. Thus, instead of the composite with conductivity tensor $\hat{\sigma}^{(2)}$ and oblate shape of the inclusions, we can consider a composite with spherical inclusions but a different conductivity tensor $\hat{\mu}^{(2)}$, satisfying

$$\mu^{(2)}_{\alpha\alpha}/\mu^{(2)}_{\beta\beta} = (L_\beta/L_\alpha)^2 \left(\sigma^{(2)}_{\alpha\alpha}/\sigma^{(2)}_{\beta\beta}\right) \ . \tag{5}$$

We then construct a random 3D resistor network in order to perform Monte Carlo simulations of the conductor/superconductor composite with host conductivity tensor $\hat{\mu}_2$ and calculate the effective conductivity $\hat{\mu}_e$ of the considered system. The effective conductivity tensor $\hat{\sigma}_e$ can then be found from Eq. (3):

$$\sigma^{(e)}_{\alpha\alpha} = (\sigma^{(2)}_{\alpha\alpha}/\mu^{(2)}_{\alpha\alpha})\mu^{(e)}_{\alpha\alpha} \ . \tag{6}$$

In Fig. 1 we plot $\hat{\rho}_e = 1/\hat{\sigma}_e$ vs. the volume fraction p_1 of the superconducting inclusions. We believe that the method described here is a powerful tool for numerical

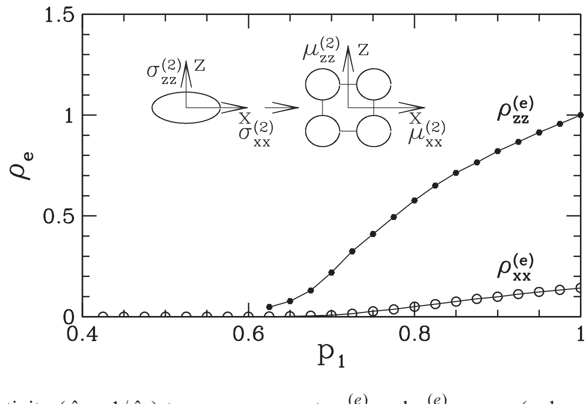

Fig. 1. Effective resistivity ($\hat{\rho}_e = 1/\hat{\sigma}_e$) tensor components $\rho^{(e)}_{zz}$ and $\rho^{(e)}_{xx}$ vs. p_1 (volume fraction of perfectly conducting inclusions), obtained by numerical simulations. In the calculations were used the following values of the host conductivity tensor in the re-scaled system: $\mu^{(2)}_{zz}=1$, $\mu^{(2)}_{xx}=1/5$ (in dimensionless units), $\mu^{(2)}_{yy}=\mu^{(2)}_{xx}$, $\mu^{(2)}_{\alpha\beta}=0$ for $\alpha \neq \beta$. If in the initial system $\sigma^{(2)}_{zz}=1$, $\sigma^{(2)}_{xx}=7$, and $L_x/L_z=\sqrt{35}$, then [according to Eqs. (5), (6)] $\sigma^{(e)}_{zz}=\mu^{(e)}_{zz}$ and $\sigma^{(e)}_{xx}=35\mu^{(e)}_{xx}$, from what we obtain $\hat{\rho}_e = 1/\hat{\sigma}_e$. The discrete network is constructed as described in Ref. [10]. The x- and z-axis lie along the principal axes of spheroidal inclusion.

simulation of the resistive phase transition in high-T_c superconducting ceramics with highly anisotropic grains (in addition to our recent EMA studies of such superconductors [11]).

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