22. A. N. Pavlenko, Important Topics in Thermophysics and Physical Hydro and Gas-Dynamics [in Russian], Novosibirsk (1985), pp. 307-317.
23. Yu. A. Kirichenko, S. M. Kozlov, and N. M. Levchenko, Inzh.-Fiz. Zh., 42, No. 2, 207-213 (1982).

A SELF-CONSISTENT METHOD FOR THE DESCRIPTION OF THE GENERALIZED CONDUCTIVITY OF HETEROGENEOUS SYSTEMS

E. A. Mityushov and P. V. Gel'd

UDC 537.311.3+536.212

A generalization is presented of the self-consistent field method for the determination of the effective conductivity of heterogeneous materials based on simultaneous utilization of the field balance and flux equations. Generality of the approach being proposed and its relation to many formal solutions of the problem being discussed are illustrated.

One of the promising paths to the improvement of the exploitational characteristics of articles is related to the extensive utilization and optimization of heterogeneous material properties that are often microinhomogeneous media with inhomogeneity dimensions significantly less than the characteristic quantities for the specimen or article. Many important physical properties of similar materials such, for instance, as the kinetic, magnetic, and dielectric, can be investigated theoretically from a single aspect because of the mathematical equivalence of their description. The problem of finding regularities of the change in the heterogeneous system characteristics being discussed has received the designation of the problem of generalized conductivity [1, 2] for which a number of fundamental generalizations has been established in investigations (see [2], say). By virtue of the sufficient complexity of the problem all the known solutions have been obtained under definite simplifying assumptions of a physical or mathematical nature whereupon the equivalence of the mathematical and physical models utilized in describing the generalized conductivity has often been lost. A generalization of the known self-consistent field method [3] is presented below, that permits setting up a connection between solutions obtained under different assumptions, as well as a deeper comprehension of their physical meaning without relying here on a complex mathematical apparatus.

The crux of the self-consistent field method in the establishment of effective heterogeneous material characteristics is the equalization of the mean field in particles of a multiphase system placed alternately in a homogeneous medium with effective properties to a microscopic field. The field balance equation is the self-consistent condition (while the flux balance equation is satisfied automatically) in this method that has received extensive application in the description of statistical mixtures of particles of equally likely phases. Generalization of the result obtained in such a manner can be obtained because of the introduction of an additional conductivity parameter for the heterogeneous system with simultaneous utilization of the field and flux balance equations.

To clarify the features of the method it is expedient first to examine the solution of an auxiliary problem on determining the characteristics of a uniform homogeneous medium in which upon placement of a single spherical inclusion with i-th phase conductivity σ_i and application of an external field $\langle E\rangle$ the field in the inclusion will agree with the mean in the corresponding phase in the heterogeneous system E_i. We call this homogeneous system the comparison body and denote its conductivity by σ_c.

Using the solution of the problem of polarization of a sphere in a homogeneous infinite field [4], and taking account of the mathematical equivalence of its description and that inherent to the problem under consideration, we obtain

S. M. Kirov Ural Polytechnic Institute, Sverdlovsk. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 57, No. 1, pp. 75-80, July, 1989. Original article submitted January 7, 1988.

$$\mathbf{E}_i = \frac{3\sigma_c}{2\sigma_c + \sigma_i} \langle \mathbf{E} \rangle . \tag{1}$$

From the field balance conditions $\langle \mathbf{E} \rangle = \sum c_k \mathbf{E}_k, \ \sum c_k = 1$. Then taking account of (1) for the particular case of a two-phase system there follows

$$\langle \mathbf{E} \rangle = \frac{3\sigma_c c_1}{2\sigma_c + \sigma_1} \langle \mathbf{E} \rangle + \frac{3\sigma_c c_2}{2\sigma_c + \sigma_2} \langle \mathbf{E} \rangle$$

or

$$\frac{3\sigma_c c_1}{2\sigma_c + \sigma_1} + \frac{3\sigma_c c_2}{2\sigma_c + \sigma_2} = 1. \tag{2}$$

Here c_1, c_2 are volume concentrations of the heterogeneous system phase components.

If it is assumed that the properties of the comparison body agree with the effective ($\sigma_c = \sigma^*$), i.e., if spherical inclusions placed in a medium with effective properties are examined at once, then the self-consistent solution of the problem of generalized conduction of a two-phase statistical system can be found from (2)

$$\sigma^* = \frac{(2 - 3c_1)\sigma_2 + (2 - 3c_2)\sigma_1}{4} + \sqrt{\frac{[(2 - 3c_1)\sigma_2 + (2 - 3c_2)\sigma_1]^2}{16} + \frac{\sigma_1\sigma_2}{2}} . \tag{3}$$

Formula (3) agrees with that obtained earlier by V. I. Odelevskii [5] for materials formed by isotropic and inextensible particles distributed statistically in a homogeneous matrix. This expression was first established by Bruggeman [3] and was then derived by a number of other authors [5-10] in connection with investigating the effective characteristics of heterogeneous systems. The relationship (3) is known in the domestic literature as the Kondorskii—Odelevskii formula [11-13]. It has been used successfully repeatedly in the description of diverse physical properties of hot-stamped metal powders [14, 15], solid porous materials, and dielectrics [13] as well as other systems [5, 7, 16]. As noted, a set of methods exists for the description of the effective characteristics of heterogeneous systems underlying which are different assumptions of both a physical and a purely mathematical nature. Let us show that many of the solutions established by using them can easily be obtained by using the self-consistent method if the properties of the comparison body are here considered a variatable parameter.

To do this we use the flow balance condition $\langle \mathbf{j} \rangle = c_1\mathbf{j}_1 + c_2\mathbf{j}_2$ where $\mathbf{j}_1$ and $\mathbf{j}_2$ are mean values of the flow over the volume of the appropriate phase component in the heterogeneous system. In a form equivalent to this equality we can write

$$\sigma^* \langle \mathbf{E} \rangle = \sigma_1 c_1 \mathbf{E}_1 + \sigma_2 c_2 \mathbf{E}_2.$$

Substitution of the values of the field intensity $\mathbf{E}_i$ in the phases determined by the relationship (1) into this expression yields

$$\sigma^* \langle \mathbf{E} \rangle = 3\sigma_c \left[\frac{\sigma_1 c_1}{2\sigma_c + \sigma_1} + \frac{\sigma_2 c_2}{2\sigma_c + \sigma_2} \right] \langle \mathbf{E} \rangle$$

or

$$\sigma^* = 3\sigma_c \left[\frac{\sigma_1 c_1}{2\sigma_c + \sigma_1} + \frac{\sigma_2 c_2}{2\sigma_c + \sigma_2} \right]. \tag{4}$$

Let us execute an identical transformation in (4) by introducing the mean value of the conductivity of a two-phase system $\langle\sigma\rangle = c_1\sigma_1 + c_2\sigma_2$ into the consideration. Then

$$\sigma^* = \frac{3\sigma_c (2\sigma_c \langle \sigma \rangle + \sigma_1\sigma_2)}{(2\sigma_c + \sigma_1)(2\sigma_c + \sigma_2)},$$

or taking the relationship (2) into account

$$\sigma^* = \frac{2\sigma_c \langle \sigma \rangle + \sigma_1\sigma_2}{2\sigma_c + c_1\sigma_2 + c_2\sigma_1}.$$

Finally, adding and subtracting the value of the mean conductivity $\langle\sigma\rangle$ in the right side of this expression, we obtain

$$\sigma^* = \langle \sigma \rangle - \frac{c_1c_2(\sigma_1 - \sigma_2)^2}{2\sigma_c + c_1\sigma_2 + c_2\sigma_1}. \tag{5}$$

It is important that the solution presented agrees exactly with the formula obtained within the framework of the generalized singular approximation [17] or the method of renormalization [18-20], where the effective characteristics of a heterogeneous medium are found from the solution of an integrodifferential equation with kernels containing the second derivatives of the Green's functions of the Laplace equation. The crux of these methods is the representation of the second derivative of the Green's function as the sum of formal and singular parts and utilization of only the latter in the subsequent computations. In passing, let us note that extraction of the singular component in the kernel of the appropriate integrodifferential equation is equivalent to separating an interaction into local and nonlocal components.

Representation of the effective conductivity of heterogeneous systems by using (5) containing the variatable parameter σ_c permits description of the characteristics of two-phase materials of arbitrary structure. Thus, setting the conductivity of the comparison body equal to $\sigma_c = \infty$ and $\sigma_c = 0$ we find the upper and lower bounds of the effective conductivity values for fixed properties of the phase components of systems [21]: $\langle\sigma^{-1}\rangle^{-1} \leqslant \sigma^* \leqslant \langle\sigma\rangle$, corresponding to models of a material with parallel and sequentially arranged structural elements.

Narrower variational conductivity boundaries established by Hashin and Shtrikman [22] that agree with those calculated by the Maxwell formula for matrix systems [1, 23] are found if the conductivities of the comparison body are taken equal to $\sigma_c = \sigma_1$ and $\sigma_c = \sigma_2$. In this case

$$\langle \sigma \rangle - \frac{c_1c_2(\sigma_1 - \sigma_2)^2}{2\sigma_1 + c_1\sigma_2 + c_2\sigma_1} \leqslant \sigma^* \leqslant \langle \sigma \rangle - \frac{c_1c_2(\sigma_1 - \sigma_2)^2}{2\sigma_2 + c_1\sigma_2 + c_2\sigma_1}, \quad \sigma_2 > \sigma_1.$$

If it is considered that $\sigma_c = \langle\sigma\rangle$, then the expression for the effective conductivity turns out to be identical to the solution obtained under the condition of limiting locality [24] when the correlation function of the physical properties of a microinhomogeneous medium is described by the Dirac δ-function.

Moreover, it agrees also with the solution obtained when using the hypothesis of strong isotropy [25], when it is considered that the pairwise correlation functions of the physical properties are determined only by the distances between points in the heterogeneous system and are independent of the orientation of the segment connecting them. Finally, this same result was also obtained by the method of conditional moments [26, 27] as well as by using perturbation theory [28]. The identity of the solutions obtained by the methods enumerated indicates the equivalence of the models and constraints utilized in their derivation. Therefore, these hypotheses are formal in nature and do not reflect all the specific singularities of the heterogeneous system.

The selection of $\sigma_c = \langle\sigma\rangle$ and $\sigma_c = \langle\sigma^{-1}\rangle^{-1}$ also permits setting up two boundaries for the effective conductivity

$$\langle \sigma \rangle - \frac{c_1c_2(\sigma_1 - \sigma_2)^2}{2\langle \sigma^{-1} \rangle^{-1} + c_1\sigma_2 + c_2\sigma_1} \leqslant \sigma^* \leqslant \langle \sigma \rangle - \frac{c_1c_2(\sigma_1 - \sigma_2)^2}{2\langle \sigma \rangle + c_1\sigma_2 + c_2\sigma_1},$$

that are included within the Hashin–Shtrikman boundary.

Attention is turned to the fact that the expressions presented above for the range of possible values of the conductivity turn out to be symmetric in the subscripts denoting the system phase components. It should consequently be expected that the value of the effective conductivity of an arbitrary two-phase statistical system lies within the boundaries set up by this relationship while the effective conductivity of a matrix system can emerge beyond the mentioned boundaries while remaining, however, within the Hashin–Shtrikman boundaries [29].

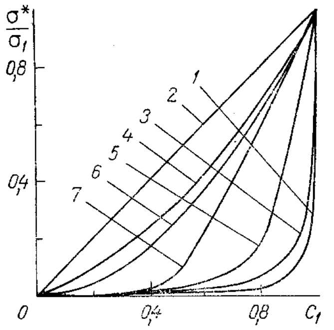

Fig. 1. Dependence of the effective conductivity on the concentration of the first phase c_1 for $\sigma_1/\sigma_2 = 100$ and different characteristics of the comparison body: 1) $\sigma_c = 0$; 2) $\sigma_c = \infty$; 3) $\sigma_c = \sigma_2$; 4) $\sigma_c = \sigma_1$; 5) $\sigma_c = \langle\sigma^{-1}\rangle^{-1}$; 6) $\sigma_c = \langle\sigma\rangle$; 7) $\sigma_c = \sigma^*$.

Finally setting $\sigma_c = \sigma^*$ into (5), we arrive, as should have been expected, at the self-consistent solution (3). It hence follows that for different geometric models of heterogeneous systems appropriate characteristics of the comparison body can be chosen for which the dependence (5) will describe their effective conductivity in the best manner in the whole range of phase component concentrations.

Presented as an illustration in the figure are dependences of the effective conductivity of a two-phase heterogeneous system on the bulk content of the first phase component set up in conformity with (5) for different characteristics of the comparison body. Attention is turned to the dependence of the conductivity on the bulk content of the first phase c_1 (curve 7) obtained for a statistical system with equally likely phase components ($\sigma_c = \sigma^*$). For a small bulk concentration of the first phase, when this equal-likelihood is not manifest, the computed values are close to the corresponding ones for a system of matrix type (curve 3). Conversely, as $c_1 \to 1$, when the first phase component evidently becomes a matrix one, the concentration dependence 7 approaches the curve 4.

In real cases when the object under discussion has a complex structure and it is difficult to refer it to any class of heterogeneous materials, the characteristic of the comparison medium can be utilized as an adjustment parameter by defining it by the value found experimentally for the effective conductivity in conformity with (5) for a fixed value of the concentration by using the expression

$$\sigma_c = \frac{\tilde{c}_1 \tilde{c}_2 (\sigma_1 - \sigma_2)^2}{2(\langle \sigma \rangle - \tilde{\sigma})} - \frac{1}{2} (\tilde{c}_1\sigma_2 + \tilde{c}_2\sigma_1).$$

Here $\tilde{\sigma}$ is the value determined experimentally for the specific conductivity, $\tilde{c}_1$ and $\tilde{c}_2$ are the bulk concentrations of the phase component corresponding to this value.

Generalization of the self-consistent field method can be realized by an analogous method in the case of two-dimensional systems (for instance, for fibrous or film structures). Then the relation between the local field in a circular inclusion and the macroscopic field acquires the form [4]

$$\mathbf{E}_i = \frac{2\sigma_c}{\sigma_c + \sigma_i} \langle \mathbf{E} \rangle .$$

Consequently, it is easy to obtain a solution analogous to that presented above

$$\sigma^* = \langle \sigma \rangle - \frac{c_1 c_2 (\sigma_1 - \sigma_2)^2}{\sigma_c + c_1\sigma_2 + c_2\sigma_1}.$$

This result agrees with that obtained by other methods in [17, 18].

NOTATION

$\mathbf{E}$, electrical field intensity vector; j, current density vector; σ_c, specific electrical conductivity of the comparison body; σ^*, effective electrical conductivity of the heterogeneous material; and c_i, bulk content of the i-th phase.

LITERATURE CITED

1. V. I. Odelevskii, Zh. Tekh. Fiz., 21, No. 6, 667-677 (1951).
2. G. N. Dul'nev and V. V. Novikov, Inzh.-Fiz. Zh., 41, No. 1, 172-194 (1981).
3. D. A. G. Bruggemann, Ann. Phys., 24, Ser. 5, No. 7, 636-650, Leipzig (1935).

4. L. D. Landau and E. M. Lifshits, Electrodynamics of Continuous Media [in Russian], Vol. VIII of the series "Theoretical Physics," Moscow (1982).
5. V. I. Odelevskii, Zh. Tekh. Fiz., 21, No. 6, 678-685 (1951).
6. E. K. Kondorskii, Dokl. Akad. Nauk SSSR, 80, No. 2, 197-200 (1951).
7. R. F. Landauer, J. Appl. Phys., 23, No. 7, 779-784 (1952).
8. D. A. Dreizin and A. M. Dykhne, Zh. Éksp. Teor. Fiz., 63, No. 1, 24-26 (1972).
9. Yu. A. Buevich, Zh. Prikl. Mekh. Tekh. Fiz., No. 4, 57-66 (1973).
10. Yu. A. Buevich and Yu. A. Korneev, Zh. Prikl. Mekh. Tekh. Fiz., No. 4, 79-87 (1974).
11. K. I. Polivanov, Ferromagnets [in Russian], Moscow (1957).
12. A. F. Chudnovskii, Thermophysical Characteristics of Disperse Materials [in Russian], Moscow (1962).
13. L. L. Vasil'ev and S. A. Tanaeva, Thermophysical Properties of Porous Materials [in Russian], Minsk (1971).
14. S. A. Tanaeva, L. S. Domorod, and L. B. Evseeva, Heat and Mass Transfer in Systems with Porous Elements [in Russian], Minsk (1981), pp. 114-120.
15. G. N. Dul'nev, Yu. P. Zarichnyak, D. M. Karpinos, et al., Teplofiz. Vys. Temp., 13, No. 6, 1189-1192 (1975).
16. N. M. Oleinik and V. P. Dushchenko, Teplofiz. Teplotekh., No. 30, 96-99, Kiev (1976).
17. T. D. Shermergor, Elasticity Theory of Microinhomogeneous Media [in Russian], Moscow (1977).
18. A. G. Fokin, Zh. Tekh. Fiz., 41, No. 6, 1073-1079 (1971).
19. A. G. Fokin, Zh. Tekh. Fiz., 43, No. 1, 71-77 (1973).
20. A. G. Fokin, Prikl. Mat. Mekh., 41, No. 6, 1095-1098 (1977).
21. A. M. Dykhne, Zh. Éksp. Teor. Fiz., 52, No. 1, 264-266 (1967).
22. Z. Hashin and S. Shtrikman, J. Appl. Phys., 33, No. 10, 3125 (1967).
23. J. C. Maxwell, Electricity and Magnetism, Vol. 1, Oxford (1892).
24. S. D. Volkov and V. P. Stavrov, Statistical Mechanics of Composite Materials [in Russian], Minsk (1978).
25. V. V. Bolotin and V. N. Moskalenko, Zh. Prikl. Mekh. Tekh. Fiz., No. 6, 7-13 (1967).
26. L. P. Khoroshun and B. P. Maslov, Methods of Automated Computation of Physicomechanical Constants of Materials [in Russian], Kiev (1980).
27. L. P. Khoroshun, Prikl. Mekh., 2, No. 9, 99-106 (1966).
28. M. I. Shvidler, Statistical Hydrodynamics of Porous Media [in Russian], Moscow (1985).
29. V. A. Berdichevskii, Variational Principles of the Mechanics of a Continuous Medium [in Russian], Moscow (1983).