ISSN 1067-8212, Russian Journal of Non-Ferrous Metals, 2016, Vol. 57, No. 3, pp. 251–255. © Allerton Press, Inc., 2016.
Original Russian Text © A.F. Fedotov, 2015, published in Izvestiya Vysshikh Uchebnykh Zavedenii. Poroshkovaya Metallurgiya i Funktsional'nye Pokrytiya, 2015, No. 1, pp. 32–37.

Prediction of Effective Elasticity Moduli of Porous Composite Materials

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Received March 17, 2014; in final form, April 16, 2014; accepted April 21, 2014

Abstract—A method for calculating the effective elasticity moduli of porous composite materials is committed. Its distinctive feature is in calculating the elasticity moduli of the composite solid phase through the effective volume averaging of component deformations. Analytical dependences for calculating effective deformation volume averaging of the solid phase and its components are presented. The results of a calculation of the macroscopic Young modulus of porous composites agrees well with the experimental data.

Keywords: porous composite, elastic moduli, averaging volume

DOI: 10.3103/S1067821216030056

INTRODUCTION

The development of modern branches of industry is in many aspects associated with the development and application of various composite materials, including porous ones. The reliable quantitative evaluation of physicomechanical properties, in particular, elastic ones, is one factor in yielding the operational reliability of constructional elements made of porous materials. When predicting macroscopic or effective properties of porous composites, two problems are solved sequentially. Initially, the effective properties of a multicomponent solid phase are determined. Then the effective properties of the porous material itself are calculated. Porous materials are considered two-phase composites with zero material constants of one phase.

The known methods of mechanics of microinhomogeneous media [1–4] do not allow us to describe the elastic properties of composites with an arbitrary content and strong distinction of elasticity moduli of components. This circumstance is especially attributed to porous materials, which have maximally possible distinction of component properties. The asymptotic averaging method [5] allows us to calculate the effective properties of composites at any difference in properties and any component geometry. However, the "pay" for accuracy is the complexity of the mathematical apparatus and performed constructions, and this method is available only for innumerous specialists. The numerical finite element method allows us to form a three-dimensional representative cell, which reflects an actual heterogeneous structure, and describe mechanical properties of the composite with a high accuracy. However, when forming the three-dimensional structural model and discretizing it, a complex software should be developed or commercial software complexes, for example Ansys, should be used.

The authors of [6, 7] developed a mathematically simple method of calculating the effective mechanical properties of isotropic composites. Its distinctive feature is in calculating the composite properties through the effective volume averaging of component deformations. The latter are determined from the solution of the boundary problem of deforming the representative cell of a two-phase composite with consideration for the deformation variant of the porous material. Thereby, the case of the limiting possible case of distinction of phase characteristics and maximal deformation concentration in composite components is taken into account. The authors of [6] found analytical dependences for calculating the effective shear and bulk compression moduli in the approximation of a plane phase interface. The results of calculation according to model [6] agree well with the experimental data.

In this study we consider the calculation by the effective volume-averaging method for elastic constants of porous composites.

ELASTIC CONSTANTS IN THE EFFECTIVE DEFORMATION VOLUME-AVERAGING METHOD

To calculate elastic constants of porous materials with a composite solid phase, the same dependences and relationships are used as for materials with the solid phase homogeneous in regards to the composition. Herewith, an equivalent homogeneous solid phase with effective properties is considered instead of the heterogeneous solid phase. We will determine effective elastic constants of the heterogeneous solid phase by the effective deformation volume-averaging method.

Elastic properties of isotropic materials are characterized by two independent constants. Let us accept the Young modulus and shear modulus as basic constants. Let us limit ourselves by the consideration of porous composites with a binary solid phase. Effective properties of composites with the number of components larger than two are found by the sequential reduction of a multicomponent composition to a binary one. The effective Young modulus (E_0) of a binary solid phase, which also consists of isotropic components, will be determined through concentration coefficients of average deformations as follows:

$$E_0 = c_1 E_1 K_{\varepsilon 1} + c_2 E_2 K_{\varepsilon 2}, \tag{1}$$

where E_1 and E_2 are the Young moduli of components, c_1 and c_2 are the volume fractions of components, and $K_{\varepsilon 1}$ and $K_{\varepsilon 2}$ are concentration coefficients of average deformations of uniaxial tension ε_x.

Concentration coefficients of average deformations represent the ratio of volume-average components (V_k) of tension deformations $\langle \varepsilon_x \rangle_{V_k}$ to average tension deformations $\langle \varepsilon_x \rangle_V$ in the composite volume (V):

$$K_{\varepsilon k} = \frac{\langle \varepsilon_x \rangle_{V_k}}{\langle \varepsilon_x \rangle_V}. \tag{2}$$

Here and below, lower index k is referred to various components ($k = 1, 2$).

Average deformations $\langle \varepsilon_x \rangle_{V_k}$ and $\langle \varepsilon_x \rangle_V$ are calculated by averaging microscopic deformations ε_x' over corresponding volumes:

$$\langle \varepsilon_x \rangle_{V_k} = \frac{1}{V_k} \int_{V_k} \varepsilon_x' dV, \quad \langle \varepsilon_x \rangle_V = \frac{1}{V} \int_V \varepsilon_x' dV. \tag{3}$$

Each component in average composite deformation $\langle \varepsilon_x \rangle_V$ has its own effective fraction and corresponding effective volume $V_{\alpha k}$. Then the summary deformation in composite volume V can be presented as the sum of average composite deformation $\langle \varepsilon_x \rangle_V$ in volumes $V_{\alpha k}$:

$$\langle \varepsilon_x \rangle_V V = \langle \varepsilon_x \rangle_V V_{\alpha 1} + \langle \varepsilon_x \rangle_V V_{\alpha 2}. \tag{4}$$

It follows from the single-valuedness condition of the deformation sum in the component volume that the sum of average composite tension deformation $\langle \varepsilon_x \rangle_V$ in effective averaging volumes of components $V_{\alpha k}$ will be equal to the sum of averaging tension deformations $\langle \varepsilon_x \rangle_{V_k}$ in volumes of components V_k:

$$\langle \varepsilon_x \rangle_V V_{\alpha k} = \langle \varepsilon_x \rangle_{V_k} V_k. \tag{5}$$

We derive from dependence (5) that

$$\langle \varepsilon_x \rangle_{V_k} = \frac{V_{\alpha k}}{V_k} \langle \varepsilon_x \rangle_V = \frac{\alpha_{\varepsilon k}}{c_k} \langle \varepsilon_x \rangle_V, \tag{6}$$

where $\alpha_{\varepsilon k} = V_{\alpha k}/V$ is the fraction of effective volume averaging of tension deformations of the kth component. It follows from the comparison of dependences (2) and (5) that concentration coefficients $K_{\varepsilon k}$ will be equal to

$$K_{\varepsilon k} = \alpha_{\varepsilon k}/c_k. \tag{7}$$

After substituting (7) into (1), we have

$$E_0 = \alpha_{\varepsilon 1} E_1 + \alpha_{\varepsilon 2} E_2. \tag{8}$$

By analogy with dependence (8) for the shear modulus of the solid phase, we can write

$$\mu_0 = \alpha_{\gamma 1} \mu_1 + \alpha_{\gamma 2} \mu_2, \tag{9}$$

where μ_1 and μ_2 are the shear moduli of components and $\alpha_{\gamma k}$ are the fractions of effective averaging volumes of shear deformations of the kth component. Fractions of effective deformation averaging volumes in (8) and (9) are associated by relationships [6]

$$\alpha_{\varepsilon 1} + \alpha_{\varepsilon 2} = 1, \quad \alpha_{\gamma 1} + \alpha_{\gamma 2} = 1. \tag{10}$$

Dependences (8) and (9) correspond in structure to the known Voigt relationship. In contrast to the Voigt model, fractions of effective averaging volumes are used in the proposed model instead of volume fractions of components. Quantitatively, fractions of effective deformation averaging volumes are the ratio of the sum of tension or shear deformations to the sum of tension or shear deformations in the composite volume [6].

A porous material represents a two-phase composite consisting of the solid phase and pores. Pores have zero elasticity moduli. Then, based on (8) and (9), we derive for the effective Young modulus (E) and shear modulus (μ) of the porous composite

$$E = \alpha_t E_0, \quad \mu = \alpha_s \mu_0, \tag{11}$$

where α_t and α_s are the fractions of effective averaging volumes of tension and shear deformations of the solid phase. Effective averaging volumes α_t and α_s are known in mechanics of porous materials as the functions of porosity or relative density. Further we will also call parameters α_t and α_s porosity functions.

When calculating elasticity moduli of the porous material, it is required to calculate the Poisson coefficient of the composite solid phase. The effective Poisson coefficient equals the ratio of the average transverse deformation $\langle \varepsilon_y \rangle_V$ to average transverse deformation $\langle \varepsilon_x \rangle_V$ of the composite solid phase:

$$\nu_0 = -\frac{\langle \varepsilon_y \rangle_V}{\langle \varepsilon_x \rangle_V}. \tag{12}$$

After averaging, longitudinal $\langle \varepsilon_x \rangle_V$ and transverse $\langle \varepsilon_y \rangle_V$ deformations are distributed over the solid phase bulk uniformly. According to the definition, deformations in effective averaging volumes are equal to corresponding average composite deformations:

$$\varepsilon_{x1} = \varepsilon_{x2} = \langle \varepsilon_x \rangle_V, \quad \varepsilon_{y1} = \varepsilon_{y2} = \langle \varepsilon_y \rangle_V. \tag{13}$$

Allowing for (13) and (10), let us express average deformations through the fractions of effective averaging volumes:

$$\langle \varepsilon_x \rangle_V = \varepsilon_{x1}\alpha_1 + \varepsilon_{x2}\alpha_2, \quad \langle \varepsilon_y \rangle_V = \varepsilon_{y1}\alpha_{y1} + \varepsilon_{y2}\alpha_{y2} \tag{14}$$

and derive for the Poisson coefficient

$$\nu_0 = -\frac{\varepsilon_{y1}\alpha_{y1} + \varepsilon_{y2}\alpha_{y2}}{\varepsilon_{x1}\alpha_{\varepsilon 1} + \varepsilon_{x2}\alpha_{\varepsilon 2}}, \tag{15}$$

where α_{y1} and α_{y2} are the fractions of effective averaging volumes of transverse deformations, for which condition (10) is also fulfilled. Transverse deformation ε_{yk} in (15) is associated with longitudinal deformation ε_{xk} by the Poisson law: $\varepsilon_{yk} = -\nu_k\varepsilon_{xk}$. Expressing ε_{xk} through ε_{yk}, after transformations allowing for relationships (10) and (13), we derive the following dependence for calculating the Poisson coefficient of the composite solid phase:

$$\nu_0 = \frac{\nu_1\nu_2}{\nu_1\alpha_{\varepsilon 2} + \nu_2\alpha_{\varepsilon 1}}. \tag{16}$$

EFFECTIVE AVERAGING VOLUMES AND POROSITY FUNCTION

Effective deformation averaging volumes are found from the solution of the boundary problem of elastic deformation of the representative composite cell. The following analytical dependences of effective deformation averaging volumes are found for the hypothetic case of the plane phase interface [6]:

$$\begin{aligned} \alpha_1 &= \alpha_{01} + (1 - \alpha_{01} - \alpha_{02}) \\ &\times \frac{E_2}{E_2 - E_1}\left(1 - \frac{E_1}{E_2 - E_1}\ln\frac{E_2}{E_1}\right), \\ \alpha_2 &= \alpha_{02} + (1 - \alpha_{01} - \alpha_{02}) \\ &\times \frac{E_1}{E_2 - E_1}\left(\frac{E_2}{E_2 - E_1}\ln\frac{E_2}{E_1} - 1\right). \end{aligned} \tag{17}$$

Here, α_{01} and α_{02} are effective deformation averaging volumes, or porosity functions of the conditionally solid phase of the composite [6]. When calculating the Young modulus, we consider effective averaging volumes of tension deformations: $\alpha_1 = \alpha_{\varepsilon 1}$, $\alpha_2 = \alpha_{\varepsilon 2}$. Porosity functions under tension are used as parameters α_{01} and α_{02}: $\alpha_{01} = \alpha_{t1}$, $\alpha_{02} = \alpha_{t2}$. When calculating the shear modulus, effective averaging volumes of shear deformations are determined: $\alpha_1 = \alpha_{\gamma 1}$, $\alpha_2 = \alpha_{\gamma 2}$. Porosity functions play the role of parameters α_{01} and α_{02} for the shear: $\alpha_{01} = \alpha_{s1}$, $\alpha_{02} = \alpha_{s2}$. Thus, effective deformation averaging volumes $\alpha_{\varepsilon k}$ and $\alpha_{\gamma k}$ are determined through porosity functions α_t and α_s.

Various porosity functions are presented in scientific publications for calculating the elasticity moduli of porous materials. Elastic properties of powers and sintered porous materials are described with high accuracy by a modified Bal'shin dependence [9, 10]:

$$\alpha_s = \rho^n\frac{\rho - \rho_0}{1 - \rho_0}, \quad n = \frac{2 - \rho - \rho_0}{1 - \rho_0}, \tag{18}$$

where ρ is the relative density and ρ_0 is the initial (apparent) density of powder. Relative density ρ is associated with porosity θ by relationship $\rho = 1 - \theta$.

Let us express the porosity function for tension (α_t) through the porosity function for shear (α_s). For this purpose, let us use the dependence for macroscopic bulk compression modulus K of a porous material [9, 10]:

$$K = \frac{4}{3}\mu_0\frac{(1 + \nu_0)\alpha_s}{2(1 - 2\nu_0) + (1 + \nu_0)(1 - \alpha_s)} \tag{19}$$

and equations connecting the Young modulus with shear and bulk compression moduli:

$$E_0 = \frac{9K_0\mu_0}{3K_0 + \mu_0}, \quad E = \frac{9K\mu}{3K + \mu}. \tag{20}$$

After transformations, we derive

$$\alpha_t = \frac{6\alpha_s}{6 + (1 + \nu_0)(1 - \alpha_s)}. \tag{21}$$

The porosity function for shear (α_s) is expressed through the porosity function for tension (α_t) as follows:

$$\alpha_s = \frac{(7 + \nu_0)\alpha_t}{6 + (1 + \nu_0)\alpha_t}. \tag{22}$$

In calculations we consider the volume fraction of components c_k of relative density ρ in dependence (17) of porosity functions α_{01} and α_{02} instead of relative density itself. The initial volume fraction of components is accepted equal zero: $c_{k0} = 0$.

Effective elasticity moduli of the porous composite are calculated as follows. Initially, effective deformation averaging volumes are calculated from dependences (17). When calculating the shear modulus, we accept in (17)

$$\begin{aligned} \alpha_1 &= \alpha_{\gamma 1}, \quad \alpha_{01} = \alpha_{t1} = c_1^{3-c_1}, \\ \alpha_2 &= \alpha_{\gamma 2}, \quad \alpha_{02} = \alpha_{t2} = c_2^{3-c_2}. \end{aligned} \tag{23}$$

When calculating the Young modulus, we consider parameters of tension deformation:

$$\begin{aligned} \alpha_1 &= \alpha_{\varepsilon 1}, \quad \alpha_{01} = \alpha_{s1} = \frac{6\alpha_{t1}}{6 + (1 + \nu_1)(1 - \alpha_{t1})}, \\ \alpha_2 &= \alpha_{\varepsilon 2}, \quad \alpha_{02} = \alpha_{s2} = \frac{6\alpha_{t2}}{6 + (1 + \nu_2)(1 - \alpha_{t2})}, \end{aligned} \tag{24}$$

where ν_1 and ν_2 are the Poisson coefficients of components of the composite solid phase.

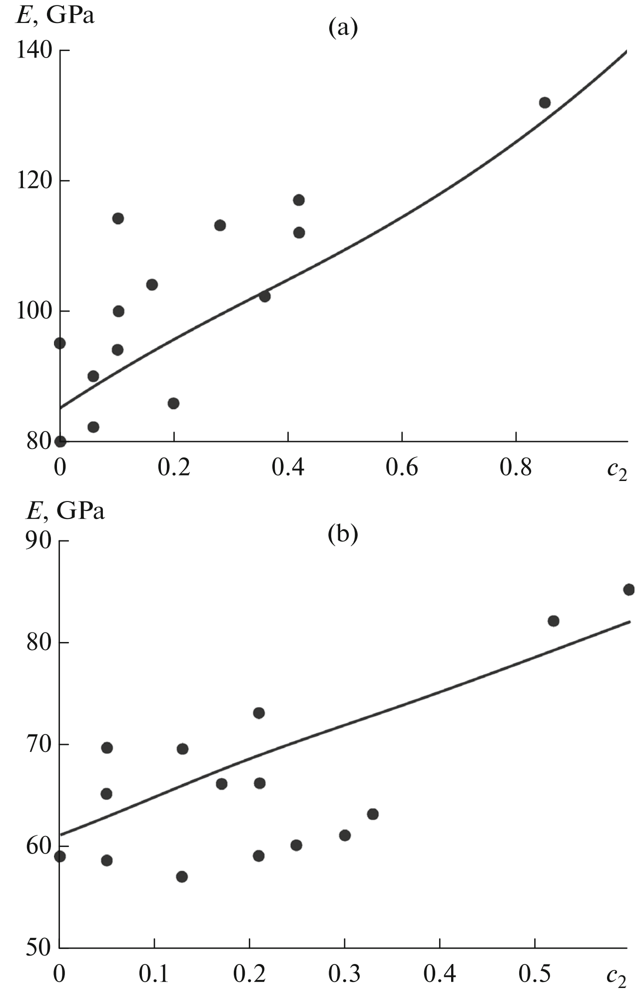

Fig. 1. Results of calculating the Young modulus for the Fe–Cu pseudoalloy at porosity (a) $\theta = 0.15$ and (b) 0.25. Points correspond to the experiment [11].

At known effective deformation averaging volumes, effective elasticity moduli of the composite solid phase E_0 and μ_0 are determined from dependences (8) and (9). Then target effective elasticity moduli of the porous composite are calculated from dependences (11). Relative density ρ is used in dependences (18) and (21) of porosity functions α_s and α_t, while the effective Poisson coefficient calculated from formula (16) is used in dependence (21).

TEST CALCULATIONS OF THE EFFECTIVE YOUNG MODULUS

We verified the accuracy of the proposed method using the experimental data of elastic properties of porous two-phase composites. It should be noted that the number of publications in which reliable results of experimental investigations into the influence of porosity on elastic constants of composites is very limited.

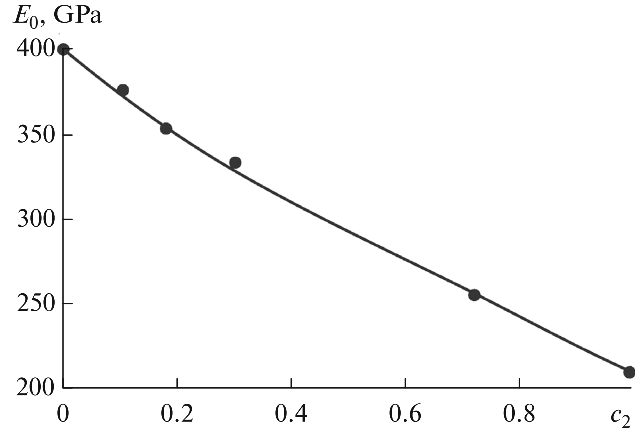

Fig. 2. Results of calculating the Young modulus for the Al_2O_3–ZrO_2 sintered composite. Points correspond to the experiment [14].

Figure 1 shows the calculated and experimental dependences of the Young modulus of the Fe–Cu porous pseudoalloy depending on the bulk iron content at porosity values $\theta = 0.15$ and 0.25. The experimental data are taken from [11] and have a very large spread of experimental points caused by the essential inhomogeneity of the sample structure. We accepted that component 1 is copper and component 2 is iron. We accepted the following Young moduli [12]: E_1 = 129 GPa and E_2 = 211 GPa, and the Poisson coefficients [13]: $\nu_1 = 0.28$ and $\nu_2 = 0.34$. Allowing for a large spread of the experimental data, the results of calculation show the quite acceptable accuracy (see Fig. 1).

The more exact experimental data were found in [14] for the Al_2O_3–ZrO_2 sintered two-phase composite. We accepted in calculations that component 1 is aluminum oxide Al_2O_3 and component 2 is zirconium dioxide ZrO_2. We accepted the following elastic constants [14]: E_1 = 400 GPa, $\nu_1 = 0.23$ for Al_2O_3 and E_2 = 210 GPa and $\nu_2 = 0.31$ for ZrO_2. We initially calculated the dependence of the effective Young modulus (E_0) of the Al_2O_3–ZrO_2 composite on the bulk content of zirconium dioxide (c_2). The results of calculations describe the experimental data with high accuracy (Fig. 2).

Then we calculated effective Young moduli of porous composites of the composition Al_2O_3–10.5 vol % ZrO_2 and Al_2O_3–72.6 vol % ZrO_2 with various degrees of porosity. The results of calculation also agree well the experimental data in this case (Fig. 3).

Thus, the proposed method and calculated dependences make it possible to describe elastic properties of both composite solid phase and porous composites rather exactly.

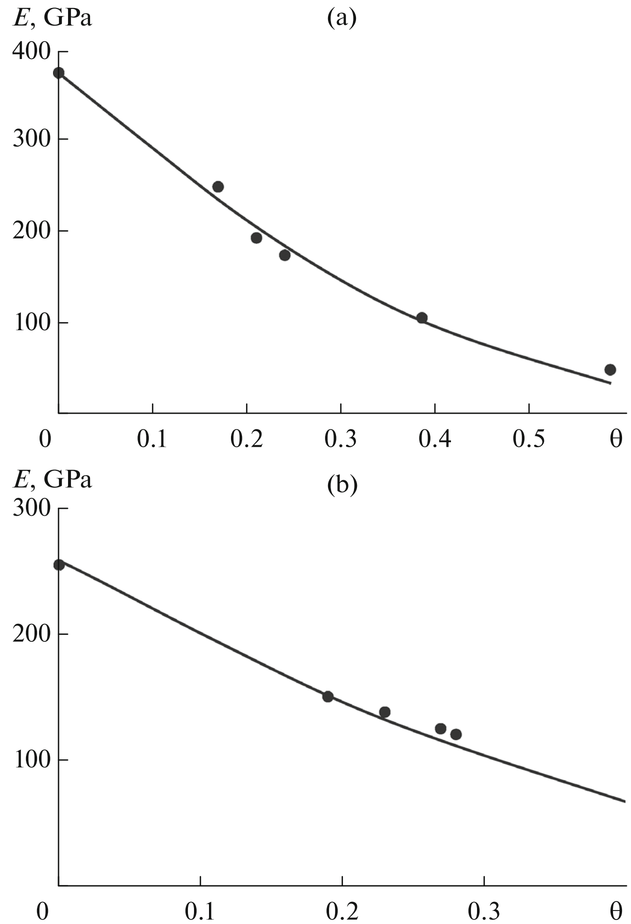

Fig. 3. Results of calculating the Young modulus for the (a) Al_2O_3–10.5 vol % ZrO_2 and (b) Al_2O_3–72.6 vol % ZrO_2 porous sintered composite. Points correspond to experiment [14].

CONCLUSIONS

To calculate macroscopic elastic moduli of porous composite materials, the same dependences as for porous materials with a solid phase homogeneous in regards to the composition can be used. Herewith, the heterogeneous solid phase is replaced by the equivalent homogeneous solid phase with effective elasticity moduli. Effective elasticity moduli of the composite solid phase can be calculated by the method of effective averaging volumes of component deformations. Calculated dependences of effective averaging volumes through porosity functions take into account the deforming variant of porous materials and, consequently, the maximally possible distinction in component properties of the porous material. The proposed dependences of porosity functions and effective deformation averaging volumes of allow us to describe the effective Young modulus of both the composite solid phase and porous composites adequately.

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Translated by N. Korovin