Modeling of elastic properties of discretely reinforced composites with an implementation of R. Hill method and porous materials' deformation model

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Abstract. In the presented study a method of a calculation of effective elasticity modules of isotropic matrix composites with isolated spherical inclusions is proposed. The feature of the method is a calculation of a concentration of R.Hill model's average deformations coefficients through effective averaging volumes of deformation phases. In terms of quantity, those volumes are a ratio of a sum of deformations in a volume of a phase to a sum of deformation in a volume of a composite. Analytical relationships for a calculation of effective Young modulus and Poisson ratio of a composite are presented. The equation for a calculation of Young modulus is presented in a form of Voigt ratio. In contrast to Voigt model, instead of volume fractions of phases, fractions of effective averaging volumes are used. Effective averaging volumes can be found by means of solving boundary-value problem of elastic deformations of a representative cell of a two-phase composite using a basic discretization scheme and mathematical apparatus. For a solution, a boundary variant of porous composite with zero values of elastic constants of inclusions is implemented. Using experimental data for two-phase composites with different combinations of elasticity modules of phases, the proposed method's adequacy verification is conducted. The proposed model, in terms of Young modulus's calculation accuracy, is equal to fundamental models of Christensen (MCr) and Mori-Tanaka (MM-T). In comparison to MCr and MM-T, results of a calculation of Poisson ratio correlate with experimental data better. It was demonstrated, that formal zeroing of inclusion's elasticity modules in MCr and MM-T models does not allow to adequately describe elastic properties of porous materials. The proposed approach considers a boundary case of a composite with a porous matrix and, thus, covers a wider range of changes of components elastic constants.

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Introduction

During a design of objects made from composite materials, a problem of elastic properties' prediction of a composite using components' known qualities and their content. Nowadays, various methods of a calculation of composites' effective elasticity modules are developed [1-7]. However, an accurate description of properties of composites with unconditioned content of components, which elasticity modules seriously vary, is not always possible.

During a description of composites' properties, a procedure of statistical averaging is conducted and a material starts to be considered as continuum [1]. In continuum model, effective properties are determined by solving boundary-value problem of integral representative cell's elastic deformation. In a case of a contact of elastic bodies with different modules, a concentration of stresses and deformations occurs in an interphase boundary. A validity of continuum model depends on a method of an estimation of mode of deformation's (MD) heterogeneity of a cell during averaging process. In the method of R. Hill heterogeneity of MD is taken into account through concentration coefficients of average deformation phases [8]. However, accurate estimates of concentration coefficients are obtained only for a particular case when shear modules of isotropic phases are equal [8].

A problem of elastic properties' prediction is also characteristic for porous materials, which have a maximum possible difference of phase characteristics. Often, during a description of porous materials properties calculated relationships of two-phase composites are used, in which elastic constants of one of phases are equal to zero. However, results of such a calculation do not correlate with experimental data [9]. In that case, an opposite approach, in which, during a creation of deformation model of two-phase composite, a porous matrix's case will be taken into consideration in advance. In the presented paper an application of porous materials' deformation model in a calculation of effective elasticity modules of matrix composites using the method of R. Hill is discussed.

Materials and methods

Two-phase matrix composites with isolated inclusions are discussed. Each of phases and a composite in a whole are homogeneous and isotropic.

Effective elasticity modules' tensor C_{ijmn} of a two-phase composite is defined as follows [8]:

$$C_{ijnm} = c_1 C^1_{ijkl} K^1_{klmn} + c_2 C^2_{ijkl} K^2_{klmn} .$$

where K^k_{klmn} – concentration coefficients of average deformation of phase k (k = 1, 2); c_k – volumetric fractions of a composite's phases. Concentration coefficients K^k_{ijmn} are related with average deformations in phases $\langle \varepsilon_{ij} \rangle_{V_k}$ and in a composite $\langle \varepsilon_{ij} \rangle_V$ by the relationship:

$$\langle \varepsilon_{ij} \rangle_{V_k} = K^k_{ijmn} \langle \varepsilon_{nm} \rangle_V . \qquad (1)$$

Elastic properties of isotropic materials are characterized by two independent constants. As basic ones, accepting Young modulus and Poisson ratio. Effective Young modulus E of an isotropic composite can be determined as follows:

$$E = c_1 E_1 K_1 + c_2 E_2 K_2 , \qquad (2)$$

here E_1, E_2 – Young modules of isotropic phases; K_1, K_2 – concentration coefficients of average deformations of uniaxial tension ε_x, which are, according to (1), will be equal:

$$K_k = \frac{\langle \varepsilon_x \rangle_{V_k}}{\langle \varepsilon_x \rangle_V} ; \qquad (3)$$

where $\langle \varepsilon_x \rangle_{V_k}$ – average tensile deformations in volumes of phases V_k; $\langle \varepsilon_x \rangle_V$ – average tensile deformations in a volume of a composite V:

$$\langle \varepsilon_x \rangle_{V_k} = \frac{1}{V_k} \int_{V_k} \varepsilon'_x \, dV ;$$

$$\langle \varepsilon_x \rangle_V = \frac{1}{V} \int_V \varepsilon'_x \, dV . \qquad (4)$$

Concentration coefficients satisfy following ratios [8]:

$$c_1 K_1 + c_2 K_2 = 1 . \qquad (5)$$

Each phase in average deformation of a composite has its effective fraction and corresponding effective volume. Single-valuedness condition of total deformations in a volume of a phase results in a fact, that sum of average deformation of composite's tension $\langle \varepsilon_x \rangle_V$ in effective averaging volumes of phase $V_{\alpha k}$ will be equal to a sum of average tension deformations $\langle \varepsilon_x \rangle_k$ in volumes of phases V_k:

$$\langle \varepsilon_x \rangle_V V_{\alpha k} = \langle \varepsilon_x \rangle_{V_k} V_k . \qquad (6)$$

From (7) obtaining:

$$\langle \varepsilon_x \rangle_{V_k} = \frac{V_{\alpha k}}{V_k} \langle \varepsilon_x \rangle_V = \frac{\alpha_k}{c_k} \langle \varepsilon_x \rangle_V , \qquad (7)$$

where $\alpha_k = V_{\alpha k} / V$ – volume fraction of effective averaging volume of deformation of phase k. From a comparison of (3) and (7) it follows, that concentration coefficients K_k will be equal to:

$$K_k = \frac{\alpha_k}{c_k} . \qquad (8)$$

From (7), considering (4), obtaining:

$$\alpha_k = \frac{V_{\alpha k}}{V} = \int_{V_k} \varepsilon'_x \, dV \bigg/ \int_V \varepsilon'_x \, dV \qquad (9)$$

Thus, fractions of effective averaging volumes of deformations constitute a ratio of a sum of tensile deformations in a volume of a corresponding component to a sum of tensile deformations in a volume of a composite.

Considering (8), the ratio (5) takes the following form:

$$\alpha_1 + \alpha_2 = 1 . \qquad (10)$$

After a substitution of (8) into (2) obtaining:

$$E = \alpha_1 E_1 + \alpha_2 E_2 , \qquad (11)$$

The relationship (11), in terms of a structure, corresponds with known Voigt ratio. In contrast to Voigt model, in the proposed model, instead of volume fractions of phases, fractions of effective averaging volumes are used.

Effective Poisson ratio ν is equal to a ratio of an average transverse deformation $\langle \varepsilon_y \rangle_V$ to average longitudinal deformation $\langle \varepsilon_x \rangle_V$ of a composite:

$$\nu = -\frac{\langle \varepsilon_y \rangle_V}{\langle \varepsilon_x \rangle_V} .$$

By definition, deformations in effective averaging volumes are equal to corresponding average deformations of a composite:

$$\varepsilon_{x1} = \varepsilon_{x2} = \langle \varepsilon_x \rangle_V ; \qquad \varepsilon_{y1} = \varepsilon_{y2} = \langle \varepsilon_y \rangle_V . \qquad (12)$$

From (12) and (10) expressing average deformations through fractions of effective averaging volumes:

$$\langle \varepsilon_x \rangle_V = \varepsilon_{x1} \alpha_1 + \varepsilon_{x2} \alpha_2 ; \qquad \langle \varepsilon_y \rangle_V = \varepsilon_{y1} \alpha_{y1} + \varepsilon_{y2} \alpha_{y2}$$

and for Poisson ratio obtaining:

$$\nu = -\frac{\varepsilon_{y1} \alpha_{y1} + \varepsilon_{y2} \alpha_{y2}}{\varepsilon_{x1} \alpha_1 + \varepsilon_{x2} \alpha_2} , \qquad (13)$$

where α_{y1}, α_{y2} – fractions of effective averaging volumes of transversal deformations. Transverse ε_{ky} and longitudinal ε_{kx} deformations of phase k are related by Poisson law: $\varepsilon_{ky} = -\nu_k \varepsilon_{kx}$. Expressing ε_{kx}

through ε_{ky}, after transformations, considering (11) obtaining:

$$\nu = \frac{\nu_1 \nu_2}{\nu_1 \alpha_2 + \nu_2 \alpha_1}.$$

Using known values of Young modulus and Poisson ratio, shear modulus and triaxial compression modulus are calculated.

Effective averaging volumes of deformation

Relationships between effective averaging volumes of deformation and elasticity modules of phases and their content can be found by solving boundary-value problem of elastic deformation of representative cell of a two-phase composite. A representative cell is accepted in a form of cube with side *b* and spherical inclusion of radius *R*. Because of symmetry, 1/8 volume of the cell (fig.1) is considered.

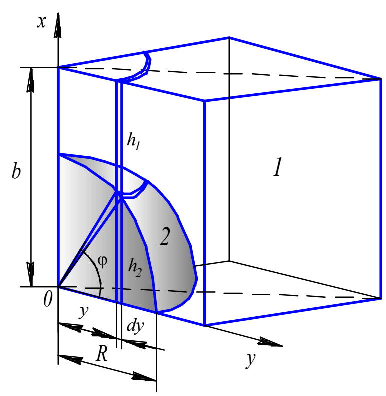

Fig.1. Representative cell of a composite

At a top face of the cell setting tension deformation ε_x. Accepting an approximation of homogeneous mode of deformation on the cell's faces. Then, faces of the cells will remain mutually parallel and will be justified to use flat cross-sections hypothesis. With a condition of homogeneity, total tension deformation $\varepsilon_{x\Sigma}$ in a cell with volume $V = b^3$ *is* equal to:

$$\varepsilon_{x\Sigma} = \int_V \varepsilon_x \, dV = \varepsilon_x b^3 \qquad (14)$$

In a framework of flat cross-section hypothesis volume V_{01} of matrix 1 around inclusion2 will deform uniformly, and tension deformation in that volume will be equal to ε_x. Finding total tension deformation in volume V_{01}:

$$\varepsilon^0_{x1\Sigma} = \varepsilon_x \cdot V_{01} = \varepsilon_x (b^3 - \frac{\pi}{4} R^2 b). \qquad (15)$$

Deformation of central area of the cell, which includes interphase boundary, is occurring non-uniformly. Dividing that area on *N* parallel connected elementary cylindrical cells with a thickness *dy*. Each cylindrical cell represents successively connected two-phase elements with a varied concentration of phases. Cells independently from each other are subjected to a specified tension deformation with value ε_x. Determining geometrical parameters of elementary cells:

- thickness of an elementary cell: $dy = R \sin\varphi \, d\varphi$;

- phases' concentration in an elementary cell:

$$c_1^{(n)} = \frac{h_1}{b} = 1 - \frac{R}{b}\sin\varphi; \qquad c_2^{(n)} = \frac{h_2}{b} = \frac{R}{b}\sin\varphi; \qquad (16)$$

- volume of phases in an elementary cell:

$$dV_1 = \frac{\pi}{2} R^2 b \, c_1^{(n)} \sin 2\varphi \, d\varphi;$$

$$dV_2 = \frac{\pi}{2} R^2 b \, c_2^{(n)} \sin 2\varphi \, d\varphi.$$

Finding total deformations in two-phase area of matrix 1

$$\varepsilon_{x1\Sigma} = \int \varepsilon_{x1} \cdot dV_1 = \frac{\pi R^2 b}{4} \int_0^{\pi/2} \varepsilon_{x1} c_1^{(n)} \sin 2\varphi \, d\varphi \qquad (17)$$

and inclusion 2:

$$\varepsilon_{x2\Sigma} = \int \varepsilon_{x2} \cdot dV_2 = \frac{\pi R^2 b}{4} \int_0^{\pi/2} \varepsilon_{x2} c_2^{(n)} \sin 2\varphi \, d\varphi. \qquad (18)$$

Fractions of effective averaging volumes of deformation α_k, according to (9) and considering (14), (15), (17), (18) will be equal to:

$$\alpha_1 = \frac{\varepsilon_{1\Sigma}}{\varepsilon_{x\Sigma}} = (1 - \frac{\pi R^2}{4b^2}) + \frac{\pi R^2}{4b^2 \varepsilon_x} \int_0^{\pi/2} \varepsilon_{x1} c_1^{(n)} \sin 2\varphi \, d\varphi;$$

$$\alpha_2 = \frac{\varepsilon_{2\Sigma}}{\varepsilon_{x\Sigma}} = \frac{\pi R^2}{4b^2 \varepsilon_x} \int_0^{\pi/2} \varepsilon_{x2} c_2^{(n)} \sin 2\varphi \, d\varphi. \qquad (19)$$

Ratio of sizes *R/b* can be found using a model of elastic deformation of porous materials. Presuming, that inclusion 2 is a pore. Then, Young modulus $E_2 = 0$ and from (11) obtaining:

$$E = \alpha_0 E_0, \qquad (20)$$

where α_0 – ratio of effective averaging volumes of a solid phase with elasticity modulus E_0. If inclusion 2 is a pore, then, in a case of a successive connection of elementary cells, deformation of matrix 1 in a central area is zero ($\varepsilon_{x1}^{(n)} = 0$), and effective averaging volume α_1 is equal to effective averaging volume of a solid phase of porous matrixα_{01}:

$$\alpha_1 = \alpha_{01} = 1 - \frac{\pi R^2}{4b^2}. \qquad (21)$$

Considering (21), relationships (20) take the following form:

$$\alpha_1 = \alpha_{01} + \frac{1-\alpha_{01}}{\varepsilon_x}\int_0^{\pi/2} \varepsilon_{x1} c_1^{(n)} \sin 2\varphi d\varphi;$$

$$\alpha_2 = \frac{1-\alpha_{01}}{\varepsilon_x}\int_0^{\pi/2} \varepsilon_{x2} c_2^{(n)} \sin 2\varphi d\varphi.$$

For a numerical integration, breaking angle π/2 into N parts and then obtaining relationships for a calculation of effective averaging volumes:

$$\alpha_1 = \alpha_{01} + \frac{\pi(1-\alpha_{01})}{2\varepsilon_x N}\sum_{n=1}^{N} \varepsilon_{x1}^{(n)} \cdot c_1^{(n)} \cdot \sin 2\varphi_n;$$

$$\alpha_2 = \frac{\pi(1-\alpha_{01})}{2\varepsilon_x N}\sum_{n=1}^{N} \varepsilon_{x2}^{(n)} \cdot c_2^{(n)} \cdot \sin 2\varphi_n, \qquad (22)$$

where $\varphi_n = \pi n / 2N$ - angle that defines a position of elementary cell n.

Ratio of characteristic sizes R/b in (16) for concentrations of phases in cell n expressing through volume fraction of inclusions c_2. Volume of body is proportional to 3rd power of a linear dimension and for c_2 obtaining:

$$c_2 = \frac{V_2}{V} \sim \left(\frac{R}{b}\right)^3.$$

Then, ratio R/b will be equal to:

$$\frac{R}{b} = \sqrt[3]{k c_2}, \qquad (23)$$

where k - constant, which is dependent on a type of packing of spherical inclusions.

The discussed structural model of a matrix composite is correct as long as inclusions are isolated and are not in contact with each other. Limiting fraction volume of isolated inclusions c_2^* corresponds to an occurrence of contacts and a formation of bounded packaging. In a case of a contact of spheres, R/b = 1 and volume fractions of inclusions c_2 will be equal to limiting: $c_2 = c_2^*$. From (23) for constant k obtaining:

$$k = 1/c_2^*. \qquad (24)$$

Considering (24), ratio R/b will be equal to:

$$\frac{R}{b} = \sqrt[3]{\frac{c_2}{c_2^*}}.$$

Limiting fraction volume of inclusions c_2^* is determined by spheres packaging characteristics. In a case of composites production by mixing of components, a formation of statistically loose packaging is the most possible scenario. Preliminary calculations also showed that a better correlation with experimental data is achieved for a model with statistically loose packaging, when c_2^*= 0.601 [10]. With the accepted assumption about a structure of a composite, relationships (16) will take following form:

$$c_1^{(n)} = 1 - \sqrt[3]{1{,}66 c_2} \cdot \sin\varphi_n; \quad c_2^{(n)} = \sqrt[3]{1{,}66 c_2} \cdot \sin\varphi_n.$$

Phases' deformation $\varepsilon_{xk}^{(n)}$ in (22) are obtained by solving uniaxial elastic tension problem of elementary cell with a designated value of deformation ε_x. From a condition of equality of stresses in components of tensioned cell n $\sigma_{x1}^{(n)} = \sigma_{x2}^{(n)}$ and an equation for a relationship of phases' deformation, obtaining:

$$\varepsilon_x = \varepsilon_{x1}^{(n)} \cdot c_{1x}^{(n)} + \varepsilon_{x2}^{(n)} \cdot c_{2x}^{(n)}$$

desired deformations are determined $\varepsilon_{xk}^{(n)}$:

$$\varepsilon_{x1}^{(n)} = \frac{\varepsilon_x E_2}{c_{1x}^{(n)} E_2 + c_{2x}^{(n)} E_1}; \qquad \varepsilon_{x2}^{(n)} = \frac{\varepsilon_x E_1}{c_{1x}^{(n)} E_2 + c_{2x}^{(n)} E_1}.$$

Accuracy of a calculation using the proposed method depends on number of elementary cells N. Studies on a convergence of numerical solutions have shown that increase of N over 100 virtually doesn't influence results of a calculation, so, N = 100 can be accepted.

Connecting obtained relationships with elastic characteristics of porous materials. Shear modules μ and triaxial compression modules K are the most oftenly determined. Similarly with (20) for shear module of porous material obtaining:

$$\mu = \alpha_{s0} \cdot \mu_0,$$

where μ_0 – shear modulus of solid phase; α_{s0} – effective averaging volume of a solid phase in a case of shear. Elastic properties of powders and sintered porous materials can be described with high accuracy using following relationships [11]:

$$\alpha_{s0} = \rho^n \frac{\rho - \rho_0}{1-\rho_0}; \qquad n = \frac{2-\rho-\rho_0}{1-\rho_0}, \qquad (25)$$

where ρ- relative density; ρ_0 – initial (bulk) relative density of a powder.

Expressing a fraction of effective averaging volume in tensionα_0 through a fraction of effective averaging volume in shear α_{s0}. For that using a relationship for macroscopic module of triaxial compression K for a porous material [11]

$$K = \frac{4}{3}\mu_0 \frac{(1+\nu_0)\alpha_{s0}}{2(1-2\nu_0)+(1+\nu_0)(1-\alpha_{s0})}$$

and equations for relationships of Young modulus Jung with shear and triaxial compression modules:

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

After simple transformations obtaining:

$$\alpha_0 = \frac{6\alpha_{s0}}{6 + (1+\nu_0)(1-\alpha_{s0})},$$

where ν_0 – Poisson ratio for a solid phase of a porous body. For a composite a role of a solid phase is performed by matrix 1. Function α_{01} for a calculation of effective averaging volumes α_k is obtained by a replacement of relative density ρ in (25) for a volume fraction of matrix c_1.For a composite with isolated inclusions it should be presumed that c_{10} = 0, and (25) is expressed as follows:

$$\alpha_{s0} = c_1^{3-c_1}.$$

Results and discussion

Verification of an adequacy of the proposed method was performed using experimental data for elastic properties of two-phase composites. For the comparison the most accurate models of elastic properties of isotropic composites were considered: three phase model of Christensen (MCr) and model Mori-Tanaka (MM-T). Calculated relationships of MCr model are listed in [1, 2], for model MM – in [4]. Compositions of two-phase composites and elastic constants of their components are presented in the table. 1. The first component of a composite serves as a matrix 1, the second component – as inclusion 2.

Table 1. Elastic constants of components

Composite	Component	Young modulus, GPa	Poisson ratio
NiAl-Al_2O_3 [12]	NiAl Al_2O_3	E_1 = 186 E_2 = 401	ν_1 = 0.31 ν_2 = 0.24
Al-SiC [13]	Al SiC	E_1 = 70 E_2 = 450	ν_1 = 0.34 ν_2 = 0.22
Co-WC [13]	Co WC	E_1 = 207 E_2 = 700	ν_1 = 0.31 ν_2 = 0.19
W-glass [14])	W Glass	E_1 = 355 E_2 = 81	ν_1 = 0.20 ν_2 = 0.24

Calculations are limited by maximum volume fraction matrix composites inclusions, which is $c_2^* = 0{,}601$. In a case, when inclusions' content is more than c_2^*, it is necessary to use a model with interpenetrating components.

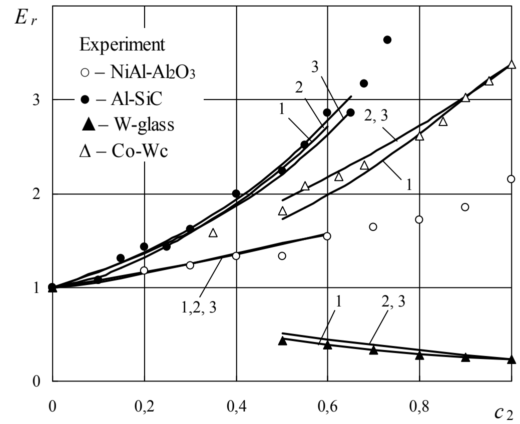

Fig.2. Relationships between reduced Young modulus of composites and their fraction volume of inclusions:
1 – The proposed model; 2 – MCr model; 3 – MM-T model.

Calculated relationships of Young modulus of a composite E, reduced to Young modulus of matrix E_1:$E_r = E/E_1$, are presented in fig.2. Results of calculations for all models are in a good correlation with the experimental data. A calculation using MCr and MM-T models leads to almost identical results. The proposed model, in terms of accuracy, is equal to fundamental MCr and MM-T models.

In fig.3 calculated data for Poisson ratio of WC-Co and Ni Al-Al_2O_3 composites with different volume content of inclusions – Co and Al_2O_3 is presented. In comparison with MCr and MM-T, results of a calculation correlate better with experimental data.

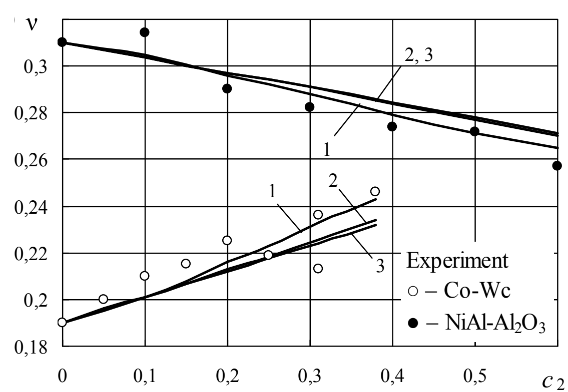

Fig.3. Relationships between Poisson ratio of composites and their fraction volume of inclusions:
1 – The proposed model; 2 – MCr model; 3 – MM-T model.

The maximum difference of elastic modules of phases is being realized in a case of porous materials, when one of phases (pores) has zero elastic constants. A valid description of elastic properties of porous materials indirectly indicates a universal nature of the model. In fig.4 calculated relationships between porosity θ effective Young modulus E and Young modulus of a solid phase E_0 for sintered iron is presented. In calculations with an implementation of the proposed model, relationships (20) and (25) were used. Bulk relative density argue ρ_0 in (25) was ρ_0=0.227 [15]. In a case of calculations with MCr and MM-T models, zero values of elastic constants of inclusions were accepted.

An implementation of MCr and MM-T models leads to a substantial overstatement of calculated values of porous iron's Young modulus. These models, as well as all of known continuum models of composites' effective properties, are obtained using an object with nonzero elastic modules of components. Our calculations (fig.4) and the results of the work [9] show, that formal zeroing of elasticity modules of inclusions does not you to adequately describe elastic properties of porous materials. The proposed model considers a case of a composite with porous matrix. Therefore, results of a calculation correlate well with experimental data. As a result, the proposed approach covers a wider range of changes of components' elastic constants.

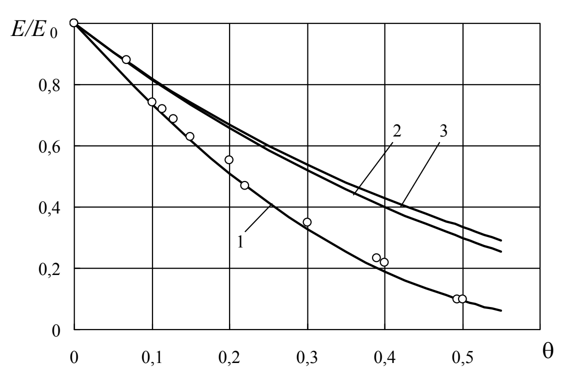

Fig.4. Relationships between relative Young modulus of sintered iron and porosity:
1 – The proposed model; 2 – MCr model; 3 – MM-T model. ○ – experiment [15].

Thus, in spite of an approximate method of a solution of boundary-value problem of elastic deformation of a representative cell, obtained calculated relationships allow to describe with a sufficient accuracy, elastic properties of matrix composites in a case of a different combination of elasticity modules and an unconditioned content of isolated inclusion.

Conclusion

On the basis of elastic deformation model of porous materials a method for a calculation of effective elastic constants of matrix composites with isolated inclusion is developed. The feature of the method is a calculation of a concentration of R.Hill model's average deformations coefficients through effective averaging volumes of deformation phases. In terms of quantity, effective averaging volumes of deformations constitute a ratio of a sum of deformations in a volume of a corresponding component to a sum of deformations in a volume of a composite. In the proposed method instead of analytical equations, a numerical solution of boundary-value problem of elastic deformation of two-phase composites' representative, using a basic discretization scheme and calculating algorithm. That complicates the calculation procedure. However, only by a change of inclusion's shape, the proposed model allows to carry out an evaluation of effective properties of matrix composites with non-spherical shape of inclusions.

For isotropic matrix composites, results of a calculation of effective elastic Young modulus and Poisson ratio are in good correlation with experimental data in a case of different combinations material constants and an unconditioned volume concentration of isolated inclusions. In contrast to the known continuum models, the proposed model takes into account a case of a composite with porous matrix and covers a wider range of changes of components elastic constants.

Further development of the approach, which was discussed in the presented paper, consists of modeling of elastic properties of isotropic wire-frame composites with interpenetrating components.

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