

Interphase layer theory and application in the mechanics of composite materials

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Abstract In the present research work the interphase layer model is developed as a continuum media with local cohesion and adhesion effects. By the model it was found that these effects can help to understand/predict macro/micro mechanics of the material, if the boundary conditions and phase effects are modeled across the length scales. This paper describes the kinematics of continuum media, the formulation of governing equations (fundamentals) and the statement of boundary conditions for multi-scale modeling of the material. An approach and the model has been validated to predict some basic mechanical properties of a polymeric matrix reinforced with nanoscale particles/fibres/tubes (including carbon nanotubes) as a function of size and also dispersion of nanoparticles. Presented mathematical model of an interphase layer allows estimating an interaction around and nearby interfaces of nanoparticle and material matrix. Using these approaches the prediction methodology and modeling tools have been developed by numerical simulations and analysis of the mechanical properties across the length scales. Results of the work will provide a platform for the development and understanding of nanoparticle-reinforced materials that are light-weight, vibration and shock resistant.

Introduction

Special properties of hyperfine structures (micro and nano-particles, nano-tubes) as well as mechanical properties of new materials manufactured on the basis of such structures are of great theoretical and practical interest. Non-classical mechanical phenomena and behavior of nanoparticle-reinforced composite materials are unknown in full measure by now and require further investigations. For a nanocomposite to be designed into a structure, some kind of optimisation/modelling is usually required to estimate its performance in normal operation conditions. The availability of suitable models can greatly help in this process. In the paper [31] the variant of the nanoscale continuum theory was elaborated on the bases of the notion of interatomic potentials of materials in the framework of the continuum mechanics. This continuum theory allowed to describe internal interactions on the level of nanometers and was used for the developing of constitutive models for SNWT-reinforced polymer composites. Similar variants of the nanoscale continuum theories [30, 41] were elaborated on the basis of the equivalent-continuum modeling technique and in view of discrete nature of atomic interactions.

The study of consistent multiscale continuum model is important from both fundamental and applied viewpoints. The developed model higher-order continuum theory can be used to fill up the gap between approaches for the gradient elasticity [1, 2, 15] and gradient plasticity [12, 13, 14]. Applications of the model may include the modeling of ultra dispersed composite materials, foamy solids, dynamics of interfaces and surface effects, crackling, cavitation and turbulence etc.

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Advanced model of continuum mediums with kept dislocations [20] may consider stress-strain fields across the length scales and the corresponding superficial phenomena [16, 17, 19, 21]. In these researches general mathematical statement of corresponding boundary-condition problem was determined by Lagrange's functional and corresponding Euler's equations based on the boundary conditions. An important aspect of the model is investigation of multi-scale cohesion and adhesion effects at the interfaces of nanoparticle-reinforced materials that are important for stress-strain relation between material phases. The model has been successfully applied to prediction/modeling of mechanical properties (Young modulus) of nanoparticle-reinforced polymeric composites as a function of nanoparticle's diameter and dispersion taking into account cohesion type interactions [16, 17] and both cohesion and adhesion superficial interactions. [19, 21]

One of the main goal of mechanics of composite materials is the definition of the effective mechanical properties using the homogenisation technique. The problem of calculating the effective characteristics of a composite consisting of a homogeneous matrix and small amount of ellipsoidal inclusions of different elastic modulus is, in principle, solved in framework of the classical theory of elasticity [24, 25, 30, 36]. The publications devoted to the study of effective characteristics of composites for the finite quantity of the concentration may be conventionally subdivided into the following groups: the method of averaged strain field (Mori-Tanaka method) of the matrix [24, 40], the self-consistent method of effective matrix [7, 25], the method based on the analysis of periodic structures [6, 26, 28, 33], and the method based on the hypothesis of three phases [32].

Note, that effect of reinforcement by nanoparticles, however, was not finally investigated and requires further computational tools. It was found, for example, that CNT reinforcement of polymer matrix at 0.5% volume rate may increase a modulus of elasticity by 40–60% [34, 35]. Model given by [35] cannot predict effective modulus of elasticity and explain the effect of substantial growth of mechanical properties of the material [34]. Therefore, some advanced model is required.

In the present paper to model of an interphase layer an advanced continuum model with field of kept dislocation is applied in mechanics of materials. This model considers the cohesion and adhesion local effects between nanoparticle and matrix as the length scale effects. It is worth noting that the local interface effects are particularly important at high defect

concentrations in the material and large size of surface-to-volume ratio that increase area of contact between nanoparticle and matrix. Using these approaches the prediction methodology and modeling tools have been developed by numerical simulations and analysis of the mechanical properties across the length scales. So, the generalized Eshelby solution is given and asymptotical averaging technique of homogenization is extended on the higher-order continuum theory of the mediums, which allow to take into account the specific properties of the interphase layer at modelling of the composites with micro- and nano-inclusions. An important aspect of the model is investigation of multi-scale effects at the interfaces of nanoparticle-reinforced materials that are important for stress-strain relation between material phases. An advantage of proposed approach is computationally effective methodology based on a fundamental theory of continuum mechanics.

Multiscale model of continuous media

According to the kinematics variation principle [5, 17, 18, 29], a functional of material's energy can be found and then a set of force interactions at the introduced kinematics relations is determined. Thus, the model is totally determined by the number of kinematics relations and therefore, it may consider some linear reversible stress-strain processes. We will define a defectless Papkovich medium as a medium with a continuous vector potential of the distortion tensor of deformation d_{ij}^0 :

$$d_{ij}^0 = \frac{\partial R_i^0}{\partial x_j}, \quad (1.1)$$

the displacement vector R_i^0 is continuous and the distortion tensor d_{in}^0 is a general solution of the homogeneous equation:

$$(\gamma_{in}^0 + \frac{1}{3}\theta^0\delta_{in} - \omega_k^0\mathfrak{A}_{ink})_m\mathfrak{A}_{nmj} = 0 \quad (1.2)$$

where the equation $\gamma_{in}^0 + \frac{1}{3}\theta^0\delta_{in}$ determines a symmetrical part of the tensor d_{ij}^0 , and the equation $\omega_k^0\mathfrak{A}_{ink}$ determines its non-symmetric part; δ_{ij} is the Kronecker delta; ω_k^0 is the vector of curls and it can be found as $\omega_k^0 = -\frac{1}{2}\frac{\partial R_i^0}{\partial x_j}\mathfrak{A}_{ijk}$, \mathfrak{A}_{ijk} is the permutation symbol, γ_{in}^0 is a deviator tensor or deviator strain; $\frac{1}{3}\theta^0\delta_{in}$ is a spherical tensor; and θ^0 is amplitude of the spherical tensor.

It is worth noting that the Eq. (1.1) states the kinematics relations between twelve degrees of freedom γ_{ij} ,

θ , ω_k and R_i of the model. In general case for base model we will consider the mediums with kept dislocation [20, 22]. In the case of defect-containing continuous medium it is characterized by the non-homogeneous Papkovitch equations as follows

$$(\gamma_{in} + \frac{1}{3}\theta\delta_{in} - \omega_k\mathfrak{A}_{ink})_{,m} \mathfrak{A}_{nmj} = \Xi_{ij} \tag{1.3}$$

where $(d_{in})_{,m} = (\gamma_{in} + \frac{1}{3}\theta\delta_{in} - \omega_k\mathfrak{A}_{ink})_{,m}$ is the general tensor of curvatures of the model.

Continuous tensor of “inconsistencies” of displacements Ξ_{ij} given in Eqs. (1.3) can be used as a tensor of dislocations density, see [9]. In the defectless homogeneous Papkovitch medium the distortion tensor d_{ij}^0 is integrable since it can be determined from the Eq. $d_{ij}^0 = \frac{\partial R_i^0}{\partial x_j}$ by means of integration over the displacement vector, and the integrability conditions (1.2) are fulfilled. On the contrary to that, for the Papkovitch–Cosserat medium with defects, the distortion tensor of deformation d_{ij} can be represented in the general case as a sum of two parts: the integrable part (d_{ij}^0), and the non-integrable part (d_{ij}^{Ξ}). In the case of non-defect homogeneous Papkovitch medium a distortion tensor is expressed by mathematical product of integration from the Eq. (1.3). The solution of the above Papkovitch Eq. (1.3) with respect to γ_{ij} , ω_k and θ can be expressed as the product of the following general solution of the homogeneous Eq. (1.2) for d_{ij}^0 ($d_{ij}^0 = \gamma_{ij}^0 + \frac{1}{3}\theta^0\delta_{ij} - \omega_k^0\mathfrak{A}_{ijk}$), and the partial solution of the non-homogeneous Papkovitch Eq. (1.3) to be given in the form as $d_{ij}^{\Xi} = d_{ij}^0 + d_{ij}^{\Xi}$, ($d_{ij}^{\Xi} = \gamma_{ij}^{\Xi} + \frac{1}{3}\theta^{\Xi}\delta_{ij} - \omega_k^{\Xi}\mathfrak{A}_{ijk}$). Partial solutions of non-homogeneous Papkovitch equation with respect to the distortion tensor d_{ij}^{Ξ} or with respect to factors of γ_{ij}^{Ξ} , ω_k^{Ξ} and θ^{Ξ} (that is the same way) can be considered as degrees of freedom that are independent displacements. The distortion tensor expressed by $d_{ij}^{\Xi} \equiv \gamma_{ij}^{\Xi} + \frac{1}{3}\theta^{\Xi}\delta_{ij} - \omega_k^{\Xi}\mathfrak{A}_{ijk}$ can be considered as “generalized displacements” (“plastic distortion” [9]). Since the “inconsistencies” tensor Ξ_{ij} can be incorporated into the “generalized displacements” by the following relations:

$$(\gamma_{in}^{\Xi} = \frac{1}{3}\theta^{\Xi}\delta_{in} - \omega_k^{\Xi}\mathfrak{A}_{ink})_{,m} \mathfrak{A}_{nmj} = \Xi_{ij} \tag{1.4}$$

it can be referred as a tensor of “generalized strains” for these “generalized displacements”.

Using the Cosserat terminology, it can be written that $\omega_k^0 = -\frac{1}{2}\frac{\partial R_i^0}{\partial x_j}\mathfrak{A}_{ijk}$ is the restricted curvature, and ω_k^{Ξ} is a free curvature or spin. By the same way, it

can be found that γ_{ij}^0 and θ^0 is restricted strains, γ_{ij}^{Ξ} and θ^{Ξ} is free strains. The following differential conservation law is valid for tensor $\Xi_{ij} : \frac{\partial \Xi_{ij}}{\partial x_j} = 0$. In other words, the flux of tensor Ξ_{ij} through the arbitrary surface stretched over the chosen planar contour is the invariant. Therefore, it can be chosen as a measure of dislocations. It is important to note that one of major features of the Papkovitch–Cosserat continuous media is that it is not possible to describe the birth or disappearance of dislocations in the framework of these media models because $\oint \Xi_{ij}n_j dF = 0$. Therefore, the defects associated with the conserved dislocation tensor Ξ_{ij} cannot be born or disappear.

In the works [16, 18, 29] the kinematical variational method of modeling is formulated. In concordance with it the kinematical connections of the medium are defined, the virtual work of internal forces is postulated as a virtual action of reaction force factors on the kinematical connections (1.1), (1.4) peculiar to the medium. This action is presented as a linear form of variations of its arguments and can be integrated for the conservative mediums. As a result the strain energy is determined. For the linear mediums the potential energy is being the quadratic form of one’s arguments. For the mediums with kept dislocations such kinematical connections are the Papkovitch’s inhomogeneous equations in use to free distortion, and Papkovitch’s homogeneous equations for the constrained distortion. The last ones can be integrated in the general form. The Cauchy’s asymmetrical correlations are the solution of the Papkovitch’s homogeneous equations for the constrained distortion. Thus, according to the kinematical variational principle the virtual action of the internal forces one should present in the following form:

$$\delta U = \iiint \left[\sigma_{ij}\delta \left(d_{ij}^0 - \frac{\partial R_i}{\partial x_j} \right) + m_{ij}\delta \left(\Xi_{ij} - \frac{\partial d_{in}^{\Xi}}{\partial x_m} \mathfrak{A}_{nmj} \right) \right] dV. \tag{1.5}$$

Here δU is the virtual work of the internal connections which is the linear form of its argument’s variations; σ_{ij} and m_{ij} are a tensors of a Lagrange multipliers, which in physical meaning are the reaction force factors, providing a fulfillment of the respective kinematical connections.

Let’s present δU in (1.5) as the linear form of one’s argument’s variations. Using the integration by parts we’ll get the following expression in the items, including the derivatives:

$$\begin{aligned} \delta U = & \iiint_G \left[\sigma_{ij} \delta d_{ij}^0 + \frac{\partial \sigma_{ij}}{\partial x_j} \delta R_i + m_{ij} \delta \Xi_{ij} \right. \\ & \left. + \frac{\partial m_{ij}}{\partial x_m} \mathcal{E}_{nmj} \delta d_{in}^{\Xi} \right] dV \\ & + \iint_{\partial G} \left[-\sigma_{ij} n_j \delta R_i - m_{ij} n_m \mathcal{E}_{nmj} \delta d_{in}^{\Xi} \right] dV' \end{aligned} \quad (1.6)$$

For mediums without the dissipation of energy the potential U exists, that the virtual action δU in (1.6) is the variation of this potential:

$$\begin{aligned} U = & \iiint_G U_G dV + \iint_{\partial G} \iint U_{\partial G} dV', \\ U_G = & U_G(d_{ij}^0; d_{ij}^{\Xi}; \Xi_{ij}), \quad U_{\partial G} = U_{\partial G}(d_{ij}^{\Xi}) \end{aligned} \quad (1.7)$$

Note, that we consider the generalized medium model with scale effects, which is not conflicted with classical theory and known experimental data's. Because the displacement vector was excluded from the list of arguments for the density of potential energy in the volume U_G and on the surface $U_{\partial G}$. Stating some physical linearity of the model, the density of potential energy U of the model (1.7) can be found in a bilinear quadratic form of its own arguments of the different tensor's dimensions. The constants in the bilinear quadratic form are, therefore, physical constants of the model and thus establish a generalized equation of the Hook's law (constitutive relations) for a Papkovitch–Cosserat's continuum model in the following form:

$$\sigma_{ij} = \frac{\partial U_G}{\partial d_{ij}^0}, \quad m_{ij} = \frac{\partial U_G}{\partial \Xi_{ij}}, \quad p_{ij} = \frac{\partial U_G}{\partial d_{ij}^{\Xi}}, \quad M_{ij} = \frac{\partial U_{\partial G}}{\partial d_{ij}^{\Xi}} = A_{ijnm} d_{nm}^{\Xi} \quad (1.8)$$

here σ_{ij} are stresses, m_{ij} are moment stresses in the valume, p_{ij} are dislocation stresses, M_{ij} are moment stresses on the surface.

One should interpret the formulas (1.8) as a generalized Green's formulas for the volume and surface force factors. These equations make possible to write the Lagrangian and find the Euler's equations.:

$$\begin{aligned} \delta L = & \iiint_G \left[\left(\frac{\partial \sigma_{ij}}{\partial x_j} + X_i \right) \delta R_i^0 - \left(\frac{\partial m_{in}^{\Xi}}{\partial x_m} \mathcal{E}_{nmj} + p_{ij} \right) \delta d_{ij}^{\Xi} \right] dV \\ & + \iint_{\partial G} \iint \left[(Y_i - \sigma_{ij} n_j) \delta R_i^0 - (M_{in} + m_{ij} n_m \mathcal{E}_{nmj}) \right. \\ & \left. \times \delta d_{ik}^{\Xi} (\delta_{kn} - n_k n_n) \right] dV' = 0 \end{aligned} \quad (1.9)$$

We used here the following equations $n_p n_q \mathcal{E}_{pqj} = 0$, which is result of convolution of the symmetrical tensor $n_p n_q$ with the antisymmetric pseudotensor \mathcal{E}_{pqj} . In result, the list of arguments is determined by six "plain" components of the free distortion tensor d_{im}^{Ξ} ($\delta_{pm} - n_p n_m$): $U_{\partial G} = U_{\partial G}(d_{ik}^{\Xi} (\delta_{kj} - n_k n_j))$ and Eq. (1.9) gives the correct variational formulation of the boundary problem for the mediums with kept dislocations. Note, that for the investigated medium model in every ordinary point of the surface we have nine boundary conditions. The analysis of the governing equations and the boundary problem as whole makes possible to prove that general order of the equations in respect to components of the displacement vector and the potentials for the components of the free distortion is equal to eighteen. So, the mathematical formulation of the investigated model is consistent, because nine boundary conditions for the boundary problem of eighteenth order there are (please compare with [23]. Generally for each of parts of the free distortion tensor d_{ij}^{Ξ} : θ^{Ξ} , ω_k^{Ξ} and γ_{in}^{Ξ} accordingly the their own specific scale effects are have place. These scale effects define the specific length of internal interactions. Let's make the common remark concerning structure of the solution of the problem (1.9). It can be proved that the governing equations of the boundary problem respect to the displacement vector R_i in general case can be written in the form of the product of two operators: L_{ij} and H_{ij} , $L_{ij}(H_{ij}(R_i))$, where $L_{ij}(\dots)$ is the classical Lamé operator $L_{ij}(\dots) = \mu \Delta(\dots) \delta_{ij} + (\mu + \lambda) \frac{\partial^2(\dots)}{\partial x_i \partial x_j}$, (μ , λ are the Lamé coefficients) and $M_{ij}(\dots)$ is more common operator, which can be considered as generalized operator of Helmgoltz type [20]. Operator $H_{ij}(\dots)$ defines the local effects for proposed particular variant of the gradient theory.

Formulation of the interphase layer model

Within the framework of the multiscale model, a theoretical model of an interphase layer is obtained as particular simplified case of the general model of the medium with kept dislocations (1.9). To construct the most simple gradient theory we assume that $\gamma_{in}^{\Xi} = 0$, and $\omega_k^{\Xi} = a_1 \omega_k$, $\theta^{\Xi} = b_1 \theta$, where θ and ω_k are corresponding constrained deformations, a_1 and b_1 are constants. Other words we assume that the lengths of the scale related with θ^{Ξ} and ω_k^{Ξ} are proportional. These assumptions lead to correct mathematical formulation for the mediums with specific local cohesion and adhesive interactions as particular model of the general Papkovitch–Cosserat's medium model with kept dislocations (1.9). After all the mathematical statement of the simplified variant of the interphase layer model is completely determined by the following equation for Lagrange functional and variation equation:

$$\delta L = \delta[\bar{A} - (U_G + U_{\partial G})],$$

$$L = \bar{A} - \frac{1}{2} \iiint_G \left[2\mu\gamma_{ij}\gamma_{ij} + \left(\frac{2\mu}{3} + \lambda\right)\theta^2 + 8\frac{\mu^2}{C}\xi_{ij}\xi_{ij} + \frac{(2\mu + \lambda)^2}{C}\theta_i\theta_i \right] dV - \frac{1}{2} \iint_{\partial G} \iint_{\partial G} [D_{ij}\dot{R}_i\dot{R}_j] dV' \quad (2.1)$$

where G is the volume of investigated body, ∂G is the boundary surface of the elastic body, \bar{A} is the work of external forces on the displacement vector R_i ; $\xi_{ij} = \frac{1}{2} \frac{\partial \omega_i}{\partial x_j} + \frac{1}{2} \frac{\partial \omega_j}{\partial x_i} = -\frac{1}{4} \frac{\partial^2 R_n}{\partial x_i \partial x_m} \Theta_{nmi} - \frac{1}{4} \frac{\partial^2 R_n}{\partial x_i \partial x_m} \Theta_{nmj}$; $\theta_i = \frac{\partial \theta}{\partial x_i} = \frac{\partial R_i}{\partial x_i \partial x_i}$; $\dot{R}_i = \frac{\partial R_i}{\partial x_j} n_j$; $D_{ij} = A n_i n_j + B(\delta_{ij} - n_i n_j)$; μ, λ are the Lamé coefficients; C is the physical constant that determine the cohesion interactions [17]; the coefficient B is responsible for the surface effects at each point of the surface within the tangential plane; the coefficient A is responsible for the interaction normal to the surface; $D_{ij}\dot{R}_i\dot{R}_j = A n_i n_j \dot{R}_i \dot{R}_j + B(\delta_{ij} - n_i n_j) \dot{R}_i \dot{R}_j$ is the surface energy density associated with changes of defect number due to deformation.

Stress state of the proposed model is define by the following equations for the stresses σ_{ij} and for the moments m_{ij} , (2.1):

$$\sigma_{ij} = \frac{\partial U_G}{\partial(\partial R_i^0 / \partial x_j)} = 2\mu\gamma_{ij} + \left(\frac{2\mu}{3} + \lambda\right)\theta\delta_{ij},$$

$$m_{ij} = \frac{\partial U_G}{\partial \Xi_{ij}} = 8\frac{\mu^2}{C}\xi_{ij} + \frac{(2\mu + \lambda)^2}{C}\theta_k \Theta_{ijk}. \quad (2.2)$$

On any surface with a normal vector n_i , vector of forces can be determined using Eq. (2.2) as follows:

$$P_i = \left\{ 2\mu\gamma_{ij} + \left(\frac{2\mu}{3} + \lambda\right)\theta\delta_{ij} + l_0^2 \left[2\mu\Delta\omega_n \Theta_{ijn} - \frac{(2\mu + \lambda)^2}{\mu} \Delta\theta\delta_{ij} \right] \right\} n_j + l_0^2 (\delta_{qj} - n_q n_j) \frac{\partial}{\partial x_q} \times \left[-2\mu \left(\frac{\partial \omega_k}{\partial x_p} + \frac{\partial \omega_p}{\partial x_k} \right) n_p \Theta_{ijk} + \frac{(2\mu + \lambda)^2}{\mu} \frac{\partial \theta}{\partial x_k} n_k \delta_{ij} \right] \quad (2.3)$$

and on the surface with a normal vector n_i , moment of vector is written in the following form:

$$M_i = l_0^2 \left[-2\mu(n_m n_j \Theta_{ijn} + n_n n_j \Theta_{ijm}) \frac{\partial \omega_n}{\partial x_m} + \frac{(2\mu + \lambda)^2}{\mu} \frac{\partial \theta}{\partial x_k} n_k n_i \right] \quad (2.4)$$

here Δ is the Laplace operator.

Based on the vector P_i , effective normal stresses in a direction of a normal vector n_p and effective shear stresses in the tangent plane are established. Obviously that $n_j(\delta_{ij} - n_i n_j) = 0$. Then the normal vector is expressed as: $\tilde{\sigma}_{ii} = T_i n_i$, and two components of tangent components of stresses are equal to: $P_i(\delta_{ij} - n_i n_j)$. Note that the stress state for proposed model of the interphase layer is described by the symmetrical stress tensor.

The assumptions introduced above ($\gamma_{in}^{\Xi} = 0$, and $\omega_k^{\Xi} = a_1 \omega_k$, $\theta^{\Xi} = b_1 \theta$, a_1 and b_1 are constants) allow to formulate the boundary problem for the mediums with specific local cohesion and adhesive interactions. Using Eq. (2.1) we can write:

$$\iiint_G \left\{ \left[L_{ij} \left[-\frac{l_0^2}{\mu} L_{ij}(\dots) + \delta_{ij}(\dots) \right] R_i + F_i \right] \delta R_i \right\} dV + \iint_{\partial G} \left[(M_i - D_{ij}\dot{R}_j) \delta \frac{\partial R_i}{\partial x_q} n_q dF + (T_i - P_i) \delta R_i \right] dV' = 0, \quad (2.5)$$

where $l_0^2 = \frac{\mu}{C}$, $L_{ij}(\dots)$ is the operator of the classical theory of elasticity, $-\frac{1}{C} L_{ij}(\dots) + \delta_{jk}(\dots)$ is operator defining the local cohesion type effects for proposed gradient theory; dV' is the boundary surface element, n_k is the normal vector of the boundary surface; F_i is the vector of density of the external loads over the material volume, T_i is the vector of density of the surface load; generalized forces M_i and P_i are defined on the surface ∂G by the Eqs. (2.3), (2.4).

Both of coefficients A, B in Eqs. (2.3), (2.4) correspond to the interactions of adhesion type. Surface effects describe the local effects that are concentrated near the material domain boundaries. To understand the physical sense let's define displacement of cohesion field. Let's name a vector of the cohesion displacement the following vector: $u_i = -\frac{1}{C} L_{ij}(R_j) = -\frac{1}{C} \left[(2\mu + \lambda) \frac{\partial^2 R_i}{\partial x_i \partial x_j} + \mu(\delta_{ij} \Delta R_j - \frac{\partial^2 R_i}{\partial x_i \partial x_j}) \right]$. Using general statement (1.9) we can receive the equations for a vector function u_i : $-CH_{ij}(u_j) + F_i = 0$, where $H_{ij}(\dots) = -\frac{1}{C} L_{ij}(\dots) + \delta_{jk}(\dots)$. Similarly we shall enter definition of a vector of classical displacements U_i . It is possible to change a sequence of action of operators. Then we shall receive the following definition of a vector U_i : $U_i = H_{ij}(R_j) = \left[-\frac{1}{C} L_{ij}(\dots) + (\dots)\delta_{ij} \right] R_j$. Obviously, the vector U_i is satisfies to the classical equations of balance: $L_{ij}(U_j) + F_i = 0$. Taking into account definitions for U_i and for u_i it is possible to present the general solution of the governing equations $L_{ij}(H_{ij}(R_i)) + F_i = 0$ as the following decomposition: $R_i = U_i - u_i$. Thus, the boundary value problem (2.4) represents the couple

boundary value problem for the classical solution and the solution for cohesion fields model. Boundary conditions in both cases are cross-linked and support each other. Thus, the boundary value problem represents a coupled boundary value problem for the classical solution U_i and a solution for cohesion field model u_i . However, the boundary value problem generally is not divided. It is worth noting that cohesion interactions are expressed by new physical parameter of model C . In recent researches [17] it was shown that this parameter is fracture factor and may be responsible for cohesion interactions. Estimation of numerical value of C parameter can be pursued by an analytic solution of an open crack at loading in normal direction. On the other hand, as it was shown in [16, 21], the parameters associated with cohesion and adhesion scale effects can be found as a result of solution of the identification problem using experimental data on effective mechanical properties of materials.

Contact boundary problem

Let’s consider the contact problem of two phases (matrix and inclusion) and analyze the boundary value problem (2.5). Assume that on the surface considered bodies the following relations have place $D_{ij} = 0$. In other words superficial effects of adhesion are neglected. Note that introduced assumption is not of fundamental importance but allow to simplify analysis and procedure of the solution construction. The Euler equation in variation Eq. (2.5) gives the following governing differential equation of fourth order for gradient continuum model of cohesion field:

$$-\frac{1}{C}LL_C(\vec{R}) + \vec{F} = 0, \quad L(\vec{R}) = \mu\nabla^2\vec{R} + (\mu + \lambda)\nabla\text{div}\vec{R},$$

$$L_C(\vec{R}) = L(\vec{R}) - C\vec{R}, \tag{3.1}$$

where $L(\vec{R}) \equiv L_{ij}(R_i) = \mu\nabla^2(R_i)\delta_{ij} + (\mu + \lambda)\frac{\partial^2(R_i)}{\partial x_i\partial x_j}$ is the differential operator of the linear theory of elasticity, i.e. operator of Lamé equation. We can write also four contact conditions on the border of inclusion-matrix for conjugation of the general field of displacements \vec{R} and general forces fields:

$$\left[\vec{R}\right] = \left[\frac{\partial\vec{R}}{\partial n}\right] = \left[\vec{M}_{(n)}(\vec{R})\right] = \left[\vec{P}(\vec{R})\right] = 0, \tag{3.2}$$

here $\left[\vec{R}\right] = \vec{R}_f - \vec{R}_m$ is the jump of the \vec{R} on the surface of inclusion and so one.

First two conditions (3.2) determine the continuity of the displacement field \vec{R} together with the first

derivatives near the border of inclusion-matrix, last two conditions are natural boundary conditions for variational Eq. (2.5), which are the continuity conditions for moments $\vec{M}_{(n)}(\vec{R})$ and surface forces $\vec{P}(\vec{R})$. From structure of the differential operator (3.1) follows, that the general field of displacements consists from two fields of displacement: \vec{U} and \vec{u} , $\vec{R} = \vec{U} - \vec{u}$. One displacement field \vec{U} is the classical field of displacements and satisfies the classical Lamé equation of the theory of elasticity: $L(\vec{U}) + \vec{F} = 0$. Another field of displacements \vec{u} is the cohesion field and satisfies the equation $L_C(\vec{R}) + \vec{F} = 0$, where $L_C(\vec{R}) \equiv -CH_{ij}(R_j) = L_{ij}(R_j) - C\delta_{ij}(R_j)$. These parts of the fields of displacements can be allocated from the general field of displacements with the help of Lamé operator:

$$\vec{U} = \vec{R} - \frac{1}{C}L(\vec{R}) = -\frac{1}{C}L_C(\vec{R}), \quad \vec{u} = -\frac{1}{C}L(\vec{R}). \tag{3.3}$$

Thus, the problem (3.1), (3.2) for the equation of the fourth order is equivalent to a problem of the coupled analysis for two equations of the second order determining the classical field of displacements \vec{U} and displacements of the cohesion field \vec{u} , conjugated among themselves through four conditions (3.2) on the boundary of inclusion-matrix. Cohesion moments working in three orthogonal directions, one of which is the external normal \vec{n} , and others two are any two tangential directions \vec{s} and $\vec{\tau}$, are defined by the following way:

$$\vec{M}_{(n)}(\vec{R}) = \left\{M_{ij}(\vec{R})n_j\right\}, \quad \vec{M}_{(s)}(\vec{R}) = \left\{M_{ij}(\vec{R})s_j\right\},$$

$$\vec{M}_{(\tau)}(\vec{R}) = \left\{M_{ij}(\vec{R})\tau_j\right\}, \tag{3.4}$$

here tensor $M_{ij}(\vec{R})$ defines by Eqs (2.4): $M_{ij}(\vec{R}) = \frac{(2\mu+\lambda)^2}{C}\frac{\partial\theta(\vec{R})}{\partial x_m}n_m\delta_{ij} - \frac{2\mu^2}{C}\left(\frac{\partial\omega_k(\vec{R})}{\partial x_m} + \frac{\partial\omega_m(\vec{R})}{\partial x_k}\right)n_m\mathfrak{A}_{ijk}$, and $\theta(\vec{R}) = \text{div}\vec{R}$, δ_{ij} is Kronecker delta, \mathfrak{A}_{ijk} is the permutation symbol.

Surface forces $\vec{P}(\vec{R})$ from the condition (3.2) can be defined through classical surface forces $\vec{p}(\vec{U}) = \{\sigma_{ij}(\vec{U})n_j\}$ and tangential cohesion moments by the following formulas:

$$P_i(\vec{R}) = p_i(\vec{U}) + \frac{\partial M_{i(s)}(\vec{R})}{\partial s} + \frac{\partial M_{i(\tau)}(\vec{R})}{\partial \tau}$$

$$= p_i(\vec{U}) + \frac{\partial M_{ij}(\vec{R})}{\partial x_p}(\delta_{pj} - n_p n_j)$$

$$= p_i(\vec{U}) + \frac{\partial}{\partial x_p} \left[\frac{(2\mu + \lambda)^2}{C} \frac{\partial\theta(\vec{R})}{\partial n} \delta_{ij} - \frac{2\mu^2}{C} \frac{\partial\omega_k(\vec{R})}{\partial x_m} \right. \\ \left. \times (n_m \mathfrak{A}_{ijk} + n_k \mathfrak{A}_{ijm}) \right] (\delta_{pj} - n_p n_j) \tag{3.5}$$

The Eqs. (3.5) are another form of representations of the surface forces (2.3), in which the classical part of surface forces are extracted in explicit form.

On the basis of the Eq. (3.1), (3.2) effective characteristics of a composite materials are calculated taking into account local effects. Hereinafter three approaches will be developed: (i) the integral Eshelby formula [8] will be received for matrix with isolated inclusion; (ii) the generalized Eshelby solution for isolated inclusion in matrix will be found and generalized Eshelby matrix will be established; (iii) the exact asymptotic average solution will be obtain on the base of the procedure of asymptotic homogenization [3] for composite materials with periodic structure in framework of the gradient model of interphase layer. For the solution of auxiliary problems arising here and for numerical simulation of the stress-state in framework of the model of interphase layer the block analytical-numerical method [37, 38, 39] is used. This method allows to calculate effectively auxiliary characteristics (components of stress tensor, energy in a cell, etc).

Integral Eshelby’s formula

To receive the integral Eshelby formula we will use the Eshelby procedure [8]. It may be proved, that for a problem (4.1), (4.2) has place the following integral relationship between integral in the volume G and integral on the surface ∂G for two arbitrary fields of displacements \vec{R} and \vec{R}_0 by analogue with the Green’s formula:

$$\frac{1}{C} \int_{\partial G} L L_C(\vec{R}) \vec{R}_0 dV = \int_{\partial G} \vec{P}(\vec{R}) \vec{R}_0 dV' + \int_{\partial G} \vec{M}_{(n)}(\vec{R}) \frac{\partial \vec{R}_0}{\partial n} dV' - 2E(\vec{R}, \vec{R}_0), \tag{4.1}$$

$$E(\vec{R}, \vec{R}_0) = \int_G \left[2\mu \varepsilon_{ij}(\vec{R}) \varepsilon_{ij}(\vec{R}_0) + \lambda \theta(\vec{R}) \theta(\vec{R}_0) + 8 \frac{\mu^2}{C} \xi_{ij}(\vec{R}) \xi_{ij}(\vec{R}_0) + \frac{(2\mu + \lambda)^2}{C} \theta_i(\vec{R}) \theta_i(\vec{R}_0) \right] dV,$$

where $\theta_i = \theta, \theta = \partial \theta / \partial x_i \varepsilon_{ij} = 1/2(R_{i,j} + R_{j,i}), \xi_{ij} = 1/2(\omega_{i,j} + \omega_{j,i})$.

The rule of Einstein about summation on repeating indexes is used. The integral relationship (4.1) is carried out also in area with inclusion because on boundary of inclusion-matrix the conjugation conditions (3.2) are satisfied. From this representation the generalized integral formula of Eshelby [10] is received. This formula is used for an estimation of the

strain energy in considered body with inclusion for the gradient interphase model.

Let consider the homogeneous ($\vec{F} = 0$) problem (3.1), (3.2) in domain G . The boundary ∂G is loaded by distributed surface forces $\vec{P}(\vec{R}) = \vec{P}_0$, and by the moments $\vec{M}_{(n)}(\vec{R}) = \vec{M}_{0(n)}$. Assume that displacement \vec{R} is the solution of such boundary problem. Let’s introduce parallel with \vec{R} also the field of displacements \vec{R}_0 in domain G for the same boundary problem without inclusion. Then the integral (4.1) for energy $E(G) = E(\vec{R}, \vec{R}_0)$ can be write in the following form:

$$E(G) = E_0(G) - \frac{1}{2} E'(G),$$

$$E'(G) = \int_{\partial G} \left[\vec{P}(\vec{R}_0) \vec{R}' + \vec{M}_{(n)}(\vec{R}_0) \frac{\partial \vec{R}'}{\partial n} \right] dV',$$

where dV' is the element of surface of the body G , $E_0(G) = E(\vec{R}_0, \vec{R}_0)$ is the energy for the homogeneous problem without inclusion, $E'(G)$ is the increment of energy in the body due to inclusion, which is the energy of interaction for two stress-strain states corresponding to two displacements fields \vec{R}_0 and $\vec{R}' = \vec{R} - \vec{R}_0$.

Applying Eq. (4.1) for a combination of fields \vec{R}_0 and $\vec{R}'(\vec{R}' = \vec{R} - \vec{R}_0)$ in the area outside of inclusion we can receive:

$$E'(G) = 2E(\vec{R}_0, \vec{R}') - 2E(\vec{R}', \vec{R}_0) + \int_{\Gamma} \left[\vec{P}(\vec{R}') \vec{R}_0 - \vec{P}(\vec{R}_0) \vec{R}' + \vec{M}_{(n)}(\vec{R}') \frac{\partial \vec{R}_0}{\partial n} - \vec{M}_{(n)}(\vec{R}_0) \frac{\partial \vec{R}'}{\partial n} \right] dV',$$

where Γ is the any surface around inclusion, in particular, it is the surface of inclusion (the normal vector on Γ is directed outside of inclusion).

Then, taking into account symmetry of the bilinear form $E(\vec{R}', \vec{R}_0)$ and using relation $\vec{R}' = \vec{R} - \vec{R}_0$ we receive an integral formulae for an estimation of energy increment due to change of the homogeneous cell on the cell with inclusion:

$$E(G) = E_0(G) - \frac{1}{2} E'(G), \tag{4.2}$$

$$E'(G) = \int_{\Gamma} \left[\vec{P}(\vec{R}) \vec{R}_0 - \vec{P}(\vec{R}_0) \vec{R} + \vec{M}_{(n)}(\vec{R}) \frac{\partial \vec{R}_0}{\partial n} - \vec{M}_{(n)}(\vec{R}_0) \frac{\partial \vec{R}}{\partial n} \right] dV'. \tag{4.3}$$

The cell with inclusion has the same as homogeneous cell loading conditions. Equations (4.2) (4.3) generalize corresponding integral Eshelby’s formula [8] on the gradient model of the interphase layer. In particular, if the field of displacements \vec{R}_0 corresponds to homogeneous deformations in which there is no cohesion component \vec{u}_0 , the integral for an estimation of energy becomes simpler because $\vec{R}_0 = \vec{U}_0$:

$$E'(G) = \int_{\Gamma} \left[\vec{P}(\vec{R})\vec{U}_0 + \vec{M}_{(n)}(\vec{R}) \frac{\partial \vec{U}_0}{\partial n} - \vec{p}(\vec{U}_0)\vec{R} \right] dV'. \tag{4.4}$$

It is proposed that the field of displacements, stresses (surface forces) and cohesion moments in Eqs. (4.2)–(4.4) can be calculated numerically using for example the special analytical-numerical method, which is developed in the present work. Then the Eqs. (4.2), (4.3) allow to find the approximate estimation of the effective moduli of matrix reinforced by inclusions and take into account local interphase layer. Indeed let’s consider for example the homogeneous loading of materials under tension. We can find the following approximated equation for effective Young modulus: $2\mu + \lambda|_{\text{eff}} = E_0 / (E_0 - E' / 2)$, where E_0 and E' are defined by Eqs. (4.2), (4.3) and can be calculated numerically.

Generalized Eshelby’s solution: Eshelby’s matrix

Let’s remind that Eshelby considered the deformation problem of isolated inclusion with matrix under homogeneous loading on the infinity in framework of the classical theory of elasticity. In case of single inclusion subjected to the action of a uniform field, the strains within the inclusion, $\varepsilon_{kl}^{\text{incl}}$, relate to the remote strain, ε_{kl}^0 , as follows [10, 11, 25]

$$\Delta\lambda_{ijkl}\varepsilon_{kl}^{\text{incl}} + \lambda_{ijkl}^0\varepsilon_{kl}^* = 0, \quad \varepsilon_{kl}^{\text{incl}} = \varepsilon_{kl}^0 + \varepsilon_{kl}^{\text{add}},$$

here λ^0 is tensor of moduli of elasticity for the matrix without inclusion, and $\Delta\lambda$ is matrix of jumps of moduli of the elasticity between inclusion and matrix. Strains $\varepsilon_{kl}^{\text{add}}$ are the additional, or “restrained” strains within the inclusion, ε_{kl}^* are the equivalent free strains. They are correlated by means of Eshelby’s tensor \hat{S}_{pqrs} as follows:

$$\varepsilon_{pq}^{\text{add}}(P) = \hat{S}_{pqrs}(P)\varepsilon_{rs}^*,$$

where $P = (x_1, x_2, x_3)$ is some point in the considered body, \hat{S}_{ijpq} is so-called Eshelby’s matrix.

The Eshelby matrix plays a fundamental role in mechanics of composites because gives the effective instrument for definition of effective averaging mechanical properties of composite materials [24, 25]. So, in compliance with the fundamental Eshelby’s method in case of dilute concentration of the inclusions we can find the effective mechanical properties of composite λ^{eff} (the matrix with inclusion) using the Eshelby’s matrix \hat{S}_{ijpq} :

$$\lambda^{\text{eff}} = \lambda^0 + \lambda^0 K \Omega \quad K = (\lambda^0 + \Delta\lambda\hat{S})^{-1} \quad \Delta\lambda = (\Delta\lambda^{-1}\lambda^0 + \hat{S})^{-1}$$

or

$$\lambda^{\text{eff}} = \lambda^0 + T\Delta\lambda\Omega \quad T = \lambda^0 (\lambda^0 + \Delta\lambda\hat{S})^{-1} = (I + \Delta\lambda\hat{S}\lambda^{0^{-1}})^{-1}$$

The expressions for the components of Eshelby’s tensor in case of isotropic matrix are known [10, 11, 25].

In our work we received the generalization of the Eshelby’s solution in framework of the nonclassical gradient model of materials for matrix and inclusion which allow to take into account the local scale effects concentrated near bounds of matrix/inclusions. It was established that the generalized matrix has the following form:

$$\tilde{S}_{ijpq}(P) = \hat{S}_{ijpq}(P) - S_{ijpq}(P), \tag{5.1}$$

where $\hat{S}_{ijpq}(P)$ is the classical Eshelby’s matrix and $S_{ijpq}(P)$ is an additional term due to cohesion field.

This generalization is based on the representation of fundamental solution of spatial problem (3.1), (3.2) in the form of difference of two fundamental solutions of classical and non-classical problems of elasticity:

$$\vec{R}_j(P, P') = \{R_{ij}\} = \vec{U}_j(P, P') - \vec{u}_j(P, P'), \tag{5.2}$$

$$\vec{U}_j(P, P') = \{U_{ij}\}, \quad U_{ij}(P, P') = \frac{1}{4\pi\mu} \frac{\delta_{ij}}{|P - P'|} - \frac{1}{16\pi\mu(1 - \nu)} \frac{\partial^2}{\partial x_i \partial x_j} (|P - P'|), \tag{5.3}$$

$$\vec{u}_j(P, P') = \{u_{ij}\}, \quad u_{ij}(P, P') = \frac{1}{4\pi\mu} \frac{\delta_{ij} e^{-\kappa_2 |P - P'|}}{|P - P'|} - \frac{1}{4\pi C} \frac{\partial^2}{\partial x_i \partial x_j} \left(\frac{e^{-\kappa_1 |P - P'|} - e^{-\kappa_2 |P - P'|}}{|P - P'|} \right), \tag{5.4}$$

where $\kappa_1 = \sqrt{C/2\mu + \lambda}$, $\kappa_2 = \sqrt{C/\mu}$, $P = (x_1, x_2, x_3)$ and $P' = (x'_1, x'_2, x'_3)$ two points in the space, $\vec{R}_j(P, P')$ is the vector of displacements, caused by the point force applied in point P' in x_j -direction (i.e. it is the generalization of the fundamental solution of a classical problem in elasticity theory, i.e. it is Somilliana tensor).

The Eq. (5.2) follows from structure of operator (3.1). Generalized Somilliana tensor (5.4) tends to classical tensor (5.3) when $C \rightarrow 0$. The isolated inclusion in infinity matrix (see Fig. 1) with common jump condition (3.2) and with requirement $\vec{R} \rightarrow \vec{U}_0$, $P \rightarrow \infty$ was considered. Here \vec{u}_0 is the displacement corresponding to uniform stress-strain state with constant stress deformation $\varepsilon_{pq}^{(0)}$.

We have been constructed solution of this problem on the base of (5.2)–(5.4) in the form of a simple layer potential with known density:

$$\begin{aligned} \vec{R}(P) &= \vec{U}_0(P) + \vec{R}^c(P), \quad \vec{R}^c = \{R_i^c\}, \\ R_i^c(P) &= \int_{\partial G} [\sigma_{jk}^{(0)}] n_k R_{ij}(P, P') dP', \end{aligned} \tag{5.5}$$

where $[\sigma_{jk}^{(0)}]$ are jumps of stress tensor on inclusion, $[\sigma_{ik}^{(0)}] = [\lambda] \varepsilon_{ii}^{(0)} \delta_{ik} + 2[\mu] \varepsilon_{ik}^{(0)}$, $\vec{R}^c(P)$ is the restricted displacements; in Eq. (5.5) integration carry out on the surface of inclusion ∂G , and G is area of inclusion; P is any point of volume (the point of matrix or inclusion); P' is varying point on the surface of inclusion.

In accordance with (5.2) displacements $\vec{R}^c(P)$ can be submitted as decomposition on the classical and cohesion components. It can be check up in compliance with properties of (5.5) that the restricted displacements $\vec{R}^c(P)$ and their normal derivatives are continuous, and also the cohesion moments $\vec{M}_{(n)}(\vec{R}^c)$ are continuous if $\nu_f = \nu_m$ and $l_f^0 = l_m^0$. Thus, first three conditions (3.2) are executed for considered case. It can be found that last condition just gives necessary jump $[\vec{p}(\vec{U}^c)] = -[\sigma_{ik}^{(0)}] n_k$ for surface forces of the constructed solution. After transformation formula (5.5) with the help of Ostrogradsky–Gauss theorem and after calculation restricted stress deformation $\varepsilon_{ij}^c(P)$ we obtain generalized Eshelby matrix $\tilde{S}_{ijpq}(P)$ in the form (5.1) with the following components:

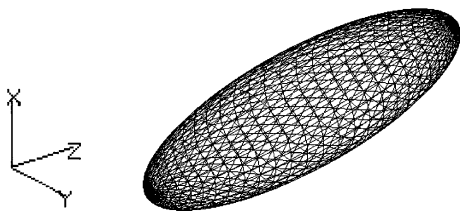


Fig. 1 Inclusion as spheroid in infinity matrix

$$\begin{aligned} \hat{S}_{ijpq}(P) &= \hat{T}_{ijkl}(P) C_{klpq}, \\ \hat{T}_{ijkl}(P) &= -\frac{\delta_{li} \hat{\varphi}_{,kj}(P) + \delta_{lj} \hat{\varphi}_{,ki}(P)}{8\pi\mu} + \frac{\hat{\psi}_{,ijkl}(P)}{16\pi\mu(1-\nu)}, \end{aligned} \tag{5.6}$$

$$\hat{\varphi}(P) = \int_G \frac{dP'}{|P - P'|}, \quad \hat{\psi}(P) = \int_G |P - P'| dP'; \tag{5.7}$$

$$\begin{aligned} S_{ijpq}(P) &= T_{ijkl}(P) C_{klpq}, \\ T_{ijkl}(P) &= -\frac{\delta_{li} \varphi_{,kj}(P) + \delta_{lj} \varphi_{,ki}(P)}{8\pi\mu} + \frac{\psi_{,ijkl}(P)}{4\pi C}, \end{aligned} \tag{5.8}$$

$$\begin{aligned} \varphi(P) &= \text{varphi}(P, \kappa_2) = \int_G \frac{e^{-\kappa_2|P - P'|}}{|P - P'|} dP', \\ \psi(P) &= \varphi(P, \kappa_2) - \varphi(P, \kappa_1). \end{aligned} \tag{5.9}$$

The matrix (5.6), corresponds to the classical solution and coincides with the matrix received by Eshelby in the work [10]. The new matrix S_{ijkq} (5.8) corresponds to the cohesion field. This matrix is the correction term to the Eshelby solution in the framework of considered model of cohesion type interphase layer.

Explicit analytical formulas (5.6)–(5.7) define behavior of the constructed solution in the matrix and in the inclusion. Using Eqs (5.6), (5.7) Eshelby has been investigated in detail the behavior of the classical part of the solution U , which has in particular asymptotic on infinity as A/r^2 . He has shown also, that the solution $\vec{U}^c(P)$ gives the homogeneous field of deformation inside inclusion of ellipsoid form.

The generalized solution (5.5) has another behavior inside inclusion. Homogeneous of deformation field inside inclusion is broken due to cohesion part of the solution (5.5). On the infinity solution saves the classical asymptotic A/r^2 , because the cohesion part is exponentially tends to zero when $P \rightarrow \infty$. Formulas (5.6)–(5.9) can be used for homogenization of composite materials within the framework of spatial model of moment cohesion.

Asymptotic homogenization for gradient model

In according with a technique of asymptotic homogenization of processes in periodic media [3], we consider the Eq. (3.1), (3.2) in the infinite media with periodic microinclusions (for example, of the spheroidal form, Figs. 2, 3). We introduce together with slow variables $x=(x_1, x_2, x_3)$ so-called fast variables $\zeta = \varepsilon^{-1}x$, where ε is the characteristic size of microinclusions (see Fig. 4), and we rewrite system of the Eqs. (3.1) in the matrix form, assuming that interphase layer lays into the cell:

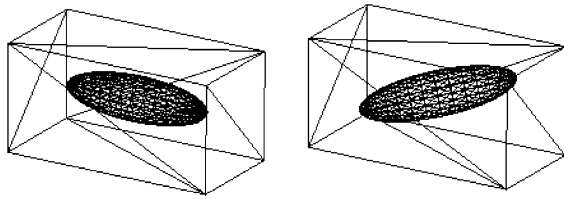


Fig. 2 A periodic cell with inclusion of the spheroidal form

$$-\frac{1}{C}LL_C(\zeta; \vec{R}) + \vec{F}(x) = 0,$$

$$L_C(\zeta; \vec{R}) \equiv \frac{\partial}{\partial x_k} \left(A_{kj}(\zeta) \frac{\partial \vec{R}}{\partial x_j} \right) - \varepsilon^{-2} C(\zeta) \vec{R} = 0, \quad (6.1)$$

where $A_{kj}(\zeta)$ is the matrix of Lamé coefficients $A_{kj}(\zeta) = \mu(\zeta)(\delta_{kq}\delta_{jp} + \delta_{kj}\delta_{pq}) + \lambda(\zeta)\delta_{kp}\delta_{jq}$, accepting constant value $\{\mu_f, \lambda_f\}$ in inclusion, and constant value $\{\mu_m, \lambda_m\}$ in the matrix of the composite material, $C(\zeta) = \mu(\zeta)/l_0^2(\zeta)$ is the cohesion field parameter, also accepting piecewise constant value, $l_0^2(\zeta)$ is the width of an interphase layer in the matrix and in inclusion.

Then we can construct the formal asymptotic decomposition of the solution (6.1) as a series on degrees of geometrical parameter ε , being the period of microinclusions translating:

$$\vec{R}(x, \zeta) = \sum_{l \geq 0} \sum_{i=(i_1 \dots i_l)} \varepsilon^l N_i(\zeta) D^i \vec{V}(x), \quad (6.2)$$

where $\vec{V}(x)$ is the slow function (i.e. solution of the homogenized operator), $N_i(\zeta)$ is the fast matrix functions being recurrent solution of a chain of problems on a cell of periodicity, i is the multi-index [3], $D^i \vec{V}(x)$ is the every possible derivatives of the order l on slow variables.

In decomposition (6.2) slow and fast variables are divided, matrix functions $N_i(\zeta)$ describe local behavior of the solution in the cell of periodicity, the vector function $\vec{V}(x)$ describes global behavior of the solution

and corresponds to the homogenized media with effective characteristics (i.e. it is satisfied the equation with constant coefficients). The equations for $N_i(\zeta)$ and the homogenized equation for $\vec{V}(x)$ is received by standard technique after substitution (6.2) in (6.1), applying a formula of differentiation of the complex function dependent on slow and fast variables, $D_x f(x, \zeta) = \frac{\partial f}{\partial x} + \varepsilon^{-1} \frac{\partial f}{\partial \zeta}$, and reducing of members with identical degrees ε^l in transformed formal asymptotic decomposition to zero. The most important are two first members in decomposition (6.2), because they describe a stress-strain state in the composite with account of microstructure and contain effective characteristics of homogenized media:

$$\vec{R}(x, \zeta) \approx \vec{V}(x) + \varepsilon \sum_l N_l(\zeta) \frac{\partial \vec{V}(x)}{\partial x_l},$$

$$\sum_{kj} \hat{A}_{kj} \frac{\partial^2 \vec{V}(x)}{\partial x_k \partial x_j} + \vec{F}(x) = 0. \quad (6.3)$$

here indexes l, k, j take on a values from 1 to 3.

The matrix coefficients \hat{A}_{kj} correspond to the homogenized elastic media (generally anisotropic) and are calculated through periodic matrix functions $N_l(\zeta)$ under the formula of averaging on a cell of periodicity G [3]:

$$\hat{A}_{kj} = \left\langle A_{kj}(\zeta) + \sum_l A_{kl}(\zeta) \left(\frac{\partial N_j(\zeta)}{\partial \zeta_l} - \frac{1}{C} \frac{\partial H_j(\zeta)}{\partial \zeta_l} \right) \right\rangle, \quad (6.4)$$

$$H_j = L(N_j), \quad \langle f(\zeta) \rangle = \frac{1}{\text{mes}(G)} \int_G f(\zeta) d\zeta. \quad (6.5)$$

Matrix functions of fast variables $N_j(\zeta)$ are determined from the equations on the cell of periodicity with contact conjugate conditions (3.2) on boundary of inclusions:

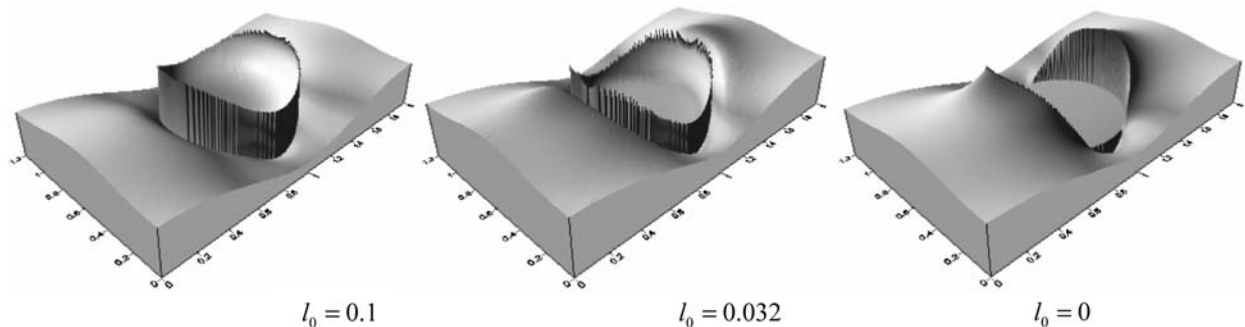


Fig. 3 Distribution of the energy density of in the cell at different value of cohesion parameter

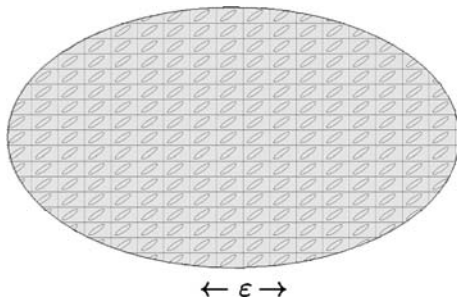


Fig. 4 A composite material with periodic microinclusions

$$\begin{aligned}
 LL_C(N_j + \zeta_j E) = 0, \quad [N_j] &= \left[\frac{\partial N_j}{\partial n} \right] = [M_{(n)}(N_j)] \\
 &= [P(N_j + \zeta_j E)] = 0, \quad (6.6)
 \end{aligned}$$

where E is the unique matrix, \vec{n} is the vector of an external normal to a surface of inclusion. The auxiliary problem (6.6) is reduced to a homogeneous problem of moment cohesion (3.1) in the cell of periodicity with inclusion and with conditions of periodic jump along directions ζ_1, ζ_2 or ζ_3 .

Eqs. (6.3)–(6.6) gives closed generalized solution of the homogenization problem in framework of the asymptotical homogenization method [6].

Let's introduce the vector functions \vec{R}_{kj} , which are column vectors of the matrix functions $N_j + \zeta_j E = \{\vec{R}_{kj}\}$. then these functions according to (6.6) satisfy to the homogeneous Eq. (3.1), (3.2) inside the cell of periodicity G with inclusion. They will consist from two component $\vec{R}_{kj} = \vec{U}_{kj} - \vec{u}_{kj}$, first of which satisfies to homogeneous Lamé equation, and the second to the equation of cohesion field, and on the boundary of a parallelepiped G both of them satisfy to conditions of periodic jump of the following kind:

$$\begin{aligned}
 \vec{U}_{kj}(\zeta + \vec{e}_i L_i) &= \vec{U}_{kj}(\zeta), \quad i \neq j, \\
 \vec{U}_{kj}(\zeta + \vec{e}_j L_j) &= \vec{U}_{kj}(\zeta) + \vec{e}_k L_j; \\
 \vec{u}_{kj}(\zeta + \vec{e}_i L_i) &= \vec{u}_{kj}(\zeta). \quad (6.7)
 \end{aligned}$$

Because everyone of component \vec{U}_{kj} and \vec{u}_{kj} satisfy separately to the second order equation, then boundary conditions (6.7) together with conditions (3.2) on border of inclusions uniquely define function \vec{U}_{kj} , and function \vec{u}_{kj} accurate to an any constant. Result, the boundary problem (6.6) reduced to set of nine connected boundary problems respect to vector functions \vec{R}_{kj} . This problem can be solved numerically. In present work corresponding problem is solved for particular plane problem with the aid of the special analytical-numerical method.

Block analytical-numerical method of numerical modeling for gradient interphase layer

Here the block-analytical method of the boundary problem is developed for gradient model of an interphase layer. Special form of the solution is proposed using the auxiliary vector potentials satisfying Helmholtz or Laplace equations. These potentials are generalizations of known Neuber–Papkovich’s representations [27]. General scheme of the analytical-numerical method assumes splitting initial domain $\vec{G} = \cup \vec{B}_k$ into system crossed only on the boundary, $B_k \cap B_l = \emptyset, k \neq l$, simply connected sub-domains called blocks. Specific systems of functions and generalized Taylor series are used for obtaining of the solutions in the each of blocks. The appropriate theorems determining an analytical basis of a method are formulated.

We can uniquely represent any solution of the non-uniform equation $L_C(\vec{u}) = \vec{F}$ by two coordinated among themselves vector potentials, satisfying to spatial Helmholtz equation [39]:

$$\nabla^2 \vec{f}(P) - \frac{C}{\mu} \vec{f}(P) = \vec{F}(P), \quad \nabla^2 \vec{f}^*(P) - \frac{C}{2\mu + \lambda} \vec{f}^*(P) = \vec{F}(P). \quad (7.1)$$

We shall name these potentials as coordinated potentials in some point P_0 of the inside area if in this point any derivatives on variables $w = \zeta_1 + i\zeta_2$ and $z = \zeta_3$ coincide:

$$\frac{\partial^m \vec{f}(P_0)}{\partial w^m \partial z^{n-m}} = \frac{\partial^m \vec{f}^*(P_0)}{\partial w^m \partial z^{n-m}}, \quad \frac{\partial}{\partial w} = \frac{1}{2} \left(\frac{\partial}{\partial \zeta_1} - i \frac{\partial}{\partial \zeta_2} \right), \quad 0 \leq m \leq n \quad (7.2)$$

The condition (3.2) uniquely determines potential \vec{f}^* on the given potential \vec{f} , and the contrary. The following theorem defines the common view of the solution.

Theorem 1 Any solution of the equation $L_C(\vec{u}) = \vec{F}$ can be uniquely submitted as

$$\vec{u}(P) = \frac{1}{\mu} \vec{f}(P) + \frac{1}{C} \nabla \text{div} [\vec{f}^*(P) - \vec{f}(P)] \quad (7.3)$$

through two vector potentials \vec{f} and \vec{f}^* , satisfying Helmholtz Eq. (7.1), and coordinated among themselves by the condition (7.2).

Direct substitution (7.3) into the equation $L_C(\vec{u}) + \vec{F} = 0$ results in identity after transformation formula to a form:

$$L\vec{u} - C\vec{u} = \left[\nabla^2 \vec{f} - \frac{C}{\mu} \vec{f} \right] - \frac{2\mu + \lambda}{C} \nabla \operatorname{div} \left(\left[\nabla^2 \vec{f} - \frac{C}{\mu} \vec{f} \right] - \left[\nabla^2 \vec{f}^* - \frac{C}{2\mu + \lambda} \vec{f}^* \right] \right).$$

The theorem 1 asserts, that any solution of the $L_C(\vec{u}) + \vec{F} = 0$ can be submitted in the form (7.3) and coordinated conditions (7.2) provide uniqueness of relation (7.3).

It can be proved that for $C \rightarrow 0, \vec{F} = 0$ the right-hand side of Eq. (7.3) gives the famous Neuber–Papkovich representation for solutions of homogeneous equation of the classical theory of elasticity:

$$\vec{U}(P) = \frac{1}{\mu} \vec{f}_0(P) - \frac{1}{4\mu(1-\nu)} \nabla \left[\vec{r} \vec{f}_0(P) \right], \tag{7.4}$$

where $\vec{r} = \vec{P}_0 \vec{P}$ is the radius-vector in the point P from the point P_0, \vec{f}_0 is the harmonic vector, $\vec{r} \vec{f}_0$ is the scalar product of two vectors.

Thus, the solution of the problem on a cell of periodicity (6.6), (6.7) is reduced to a finding of vector potentials $\vec{f}_0(P)$ and $\vec{f}(P)$, satisfying Laplace and Helmholtz equations. The additional potential $\vec{f}^*(P)$ uniquely determines by conditions (7.2). These representations are used in the block analytical-numerical method applied for the solution of spatial problems of moment cohesion on the cell of periodicity.

Let’s discuss briefly the construction of solution in each of blocks. Inside blocks the solution of the homogeneous Eq. (7.1) is represented as series on system of special functions Φ_n^m [38], similar to the polynomials having singularity in infinity point and identically satisfying the homogeneous Eq. (7.1):

$$\Phi(P) = \sum_{n=0}^{\infty} \sum_{m=0}^n \left[a_{nm} \Phi_n^m(P - P_0) + b_{nm} \bar{\Phi}_n^m(P - P_0) \right] \tag{7.5}$$

$$\Phi_n^m(P) = \Phi_n^m(P, \kappa) = \sum_{p=0}^{\lfloor \frac{n-m}{2} \rfloor} \frac{I_{m+p}(\kappa r)}{p!} \left(\frac{r}{2\kappa} \right)^p e^{im\phi} \times \frac{d^{2p}}{dz^{2p}} (A_m z^{n-m}), \quad A_m = (2/\kappa)^m m!, \tag{7.6}$$

where $I_m(t)$ is the modified Bessel function of first kind [4], $re^{i\phi} = \zeta_1 + i\zeta_2, \kappa^2$ is the coefficient of the Helmholtz equation.

The representation (7.5) is analogue of Taylor series for solution of the Eq. (7.1), and its coefficients can be calculated with the help of differentiation on variables

z and w . It is uneasy to be convinced in validity of differential recurrent relationships:

$$\frac{\partial \Phi_n^m}{\partial z} = (n - m) \Phi_{n-1}^m, \quad \frac{\partial \Phi_n^m}{\partial w} = m \Phi_{n-1}^{m-1}, \quad m \neq 0, \\ \frac{\partial \Phi_n^m}{\partial \bar{w}} = - \frac{(n - m)(n - m - 1) \Phi_{n-1}^{m+1} - \kappa^2 \Phi_{n+1}^{m+1}}{4(m + 1)}.$$

These relationships allow to differentiate analytically local representations (7.1) and to construct generalized Taylor series for solution of the Eq. (7.1). The following theorem determines the properties of the generalized Taylor series (7.6).

Theorem 2 (generalized Taylor series) Any solution of the Eq. (7.1) can be written in some vicinity of a point $P_0 \in G$ as converging series (7.5), (7.6), and coefficients a_{nm} and b_{nm} are calculated with the help of differentiation of the solution Φ in a point P_0

$$a_{nm} = \frac{1}{m!(n - m)!} \frac{\partial^n \Phi(P)}{\partial w^m \partial z^{n-m}}, \\ b_{nm} = \frac{1}{m!(n - m)!} \frac{\partial^n \Phi(P)}{\partial \bar{w}^m \partial z^{n-m}}, \quad b_{n0} = 0.$$

Theorems 1 and 2 are the theoretical basis of the block analytical-numerical method in application to the solution of the problem (6.6), (6.7).

The harmonic potential $\vec{f}_0^{(k)}$ is introduced for the classical component of field of displacements \vec{U}_k , and pair of local potentials $\vec{f}^{*(k)}$ and $\vec{f}^{(k)}$ are introduced for description of the field of displacements \vec{u}_k in the block B_k . Potentials $\vec{f}^{*(k)}$ and $\vec{f}^{(k)}$ are approximated by series (7.5) on system of special functions (7.6) with the same coefficients:

$$\vec{f}^{(k)}(P) = \operatorname{Re} \sum_{n=0}^{M_k} \sum_{m=0}^n \vec{A}_{nm}^{(k)} \Phi_n^m(P - P_0^{(k)}, \kappa_1), \\ \vec{f}^{*(k)}(P) = \operatorname{Re} \sum_{n=0}^{M_k} \sum_{m=0}^n \vec{A}_{nm}^{(k)} \Phi_n^m(P - P_0^{(k)}, \kappa_2), \tag{7.7}$$

where $P_0^{(k)}$ is the some point inside the block B_k , and κ_1 and κ_2 are the corresponding parameters of the Eq. (6.1): $\kappa_1 = \sqrt{C/\mu}, \kappa_2 = \sqrt{C/(2\mu + \lambda)}$.

Coordinated condition for potentials (7.2) are fulfilled automatically on the basis of the theorem 2, because series (7.7) have the same coefficients $\vec{A}_{nm}^{(k)}$, which are calculated with the help of differentiation on variables w and z in the point $P_0^{(k)}$. The harmonic potential $\vec{f}_0^{(k)}$ approximated by series (7.5), (7.6) at $\kappa = 0$, i.e. by series on system of the normalized spherical functions.

Conjugation of local representations in blocks with conditions (3.2) is carried out by means of set of functionals of the least squares method simultaneously sewing function and normal derivative on the boundary between blocks. For the blocks adjoining to surface of inclusion from the matrix and from the inclusion, these functionals according to (5.6) have the following view:

$$\begin{aligned} & \left\| \vec{R}_k - \vec{R}_j \right\|_{L_2(S_{kj})}^2 + \left\| \frac{\partial \vec{R}_k}{\partial n} - \frac{\partial \vec{R}_j}{\partial n} \right\|_{L_2(S_{kj})}^2 \\ & + \sum_l \left\| \frac{\partial \vec{U}_k}{\partial n} - \frac{\partial \vec{U}_l}{\partial n} \right\|_{L_2(S_{kl})}^2 + \sum_l \left\| \frac{\partial \vec{u}_k}{\partial n} - \frac{\partial \vec{u}_l}{\partial n} \right\|_{L_2(S_{kl})}^2 = \min, \\ & \left\| \vec{P}(\vec{R}_k) - \vec{P}(\vec{R}_j) \right\|_{L_2(S_{kj})}^2 + \left\| \vec{M}_{(n)}(\vec{R}_k) - \vec{M}_{(n)}(\vec{R}_j) \right\|_{L_2(S_{kj})}^2 \\ & + \sum_l \left\| \vec{U}_k - \vec{U}_l \right\|_{L_2(S_{kl})}^2 + \sum_l \left\| \vec{u}_k - \vec{u}_l \right\|_{L_2(S_{kl})}^2 = \min, \end{aligned}$$

here S_{kj} is the part of the surface of inclusion, delimiting blocks B_k and B_j , adjoining to boundary of inclusion, S_{kl} is the common part of boundary of blocks B_k and B_l , laying strictly inside inclusion or in a matrix. For blocks B_k and B_l , not having the common boundary with the inclusion, components with norm $\left\| \dots \right\|_{L_2(S_{kj})}^2$ are absent. For the blocks adjoining to border of the parallelepiped, these functionals according to conditions (5.7) have the following view:

$$\begin{aligned} & \left\| \vec{U}_k^+ - \vec{U}_j^- - L\vec{e}_i \right\|_{L_2(S_k)}^2 + \left\| \vec{u}_k^+ - \vec{u}_j^- \right\|_{L_2(S_{kl})}^2 \\ & + \sum_l \left\| \frac{\partial \vec{U}_k}{\partial n} - \frac{\partial \vec{U}_l}{\partial n} \right\|_{L_2(S_{kl})}^2 + \sum_l \left\| \frac{\partial \vec{u}_k}{\partial n} - \frac{\partial \vec{u}_l}{\partial n} \right\|_{L_2(S_{kl})}^2 = \min, \\ & \left\| \frac{\partial \vec{U}_j^+}{\partial n} - \frac{\partial \vec{U}_k^-}{\partial n} \right\|_{L_2(S_j)}^2 + \left\| \frac{\partial \vec{u}_j^+}{\partial n} - \frac{\partial \vec{u}_k^-}{\partial n} \right\|_{L_2(S_j)}^2 \\ & + \sum_l \left\| \vec{U}_k - \vec{U}_l \right\|_{L_2(S_{kl})}^2 + \sum_l \left\| \vec{u}_k - \vec{u}_l \right\|_{L_2(S_{kl})}^2 = \min, \end{aligned}$$

here S_k and S_j are boundaries of blocks B_k and B_j , adjoining to the parallel sides of the cell of periodicity and connected among themselves by a condition of parallel transition along the corresponding coordinate axis; \vec{u}_k^+ , \vec{u}_k^- and \vec{u}_j^+ , \vec{u}_j^- are corresponding values of local functions on boundaries S_k and S_j . It is supposed, that block structure of the cell is arranged in such manner, that the parallel sides of the cell are divided by

adjoining blocks so, that to each boundary S_k there will be a parallel boundary S_j .

The condition of minimization of the set of functionals above gives the block system of linear equations for calculation of unknown coefficients in decomposition (7.5).

The developed analytical-numerical method is used for solving of the homogenization problem (6.4)–(6.6). This method can be used also for estimation of the effective mechanical properties on the base of the integral Eshelby’s formuluss (4.2)–(4.4).

Numerical results

Comparative calculations on a rectangular cell with the sizes $L \times H$ are presented for the problem (3.1), (3.2) below, using the block analytical-numerical method. The problem of the unidirectional tension along the longitudinal axis for the cell with inclusion $0x_1$ was considered. In Figs. 3, 5, 6 numerical results are given for the cell with inclusion of the round form with the radius 0.4 located in the center of a rectangular matrix with the sizes $L = 2$ and $H = 1.2$. Values of Poisson coefficients and shear modules in a matrix and inclusion are $\nu_m = \nu_f = 0.3$, $\mu_f / \mu_m = 2$. Influence of the width of interphase layer l_0 on distribution of stresses and density of energy in the matrix and inclusion is investigated. Distributions of density of energy and normal stresses σ_{11} in the cell with circular inclusion at different value of cohesion parameter ($l_0 = 0.1, 0.032, 0$) are shown in Figs. 3 and 5. Comparison of the stress-strain state in the cell for the gradient model of the interphase layer and for the classical problem, ($l_0 \rightarrow 0$) is given.

We can see the effect of the redistribution of the energy between the matrix and inclusion in Fig. 3. For the classical problem the energy is basically concentrated in the matrix. Gradient model gives the concentration effect of the energy in the rigid inclusion.

It is shown, that at certain geometrical and mechanical parameters additional loading of a rigid phase takes place. Thus the phase with smaller rigidity unloads (Fig. 5). As a whole it results in redistribution of stress state in components of a composite. Redistribution of deformation energy together with significant contact zones in nano-composites also allow to explain the effect of increasing of effective modulus for the composites reinforced by rigid micro- and nano-inclusions. Effect of energy redistribution gives a basis for qualitative explanation of the increasing effect of the ultimate strain in materials (including metal alloys), if they are modified by introduction of rigid nanoinclusions.

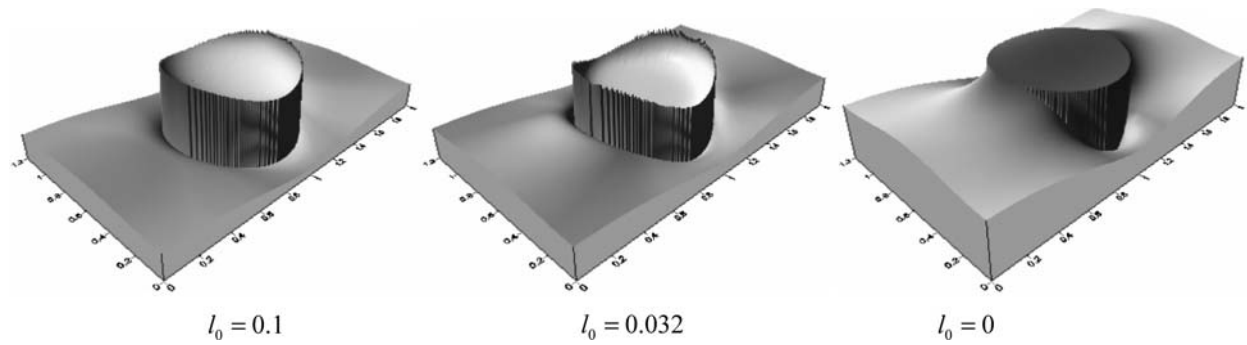


Fig. 5 Distribution of the normal stresses σ_{11}

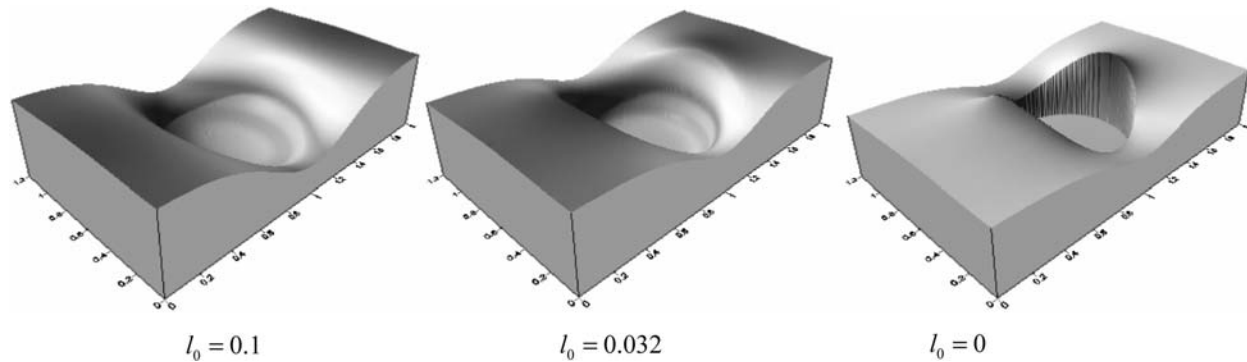


Fig. 6 Distribution of the dilatation function

Distribution of the dilatation function $\theta(\vec{R})$ is presented in Fig. 6 at the same values of the cohesion parameter. Effect of changing of the width of the interphase layer and also effect of smoothing of the solution near to the boundary of inclusion from parameter of the gradient model l_0 are observed in Fig. 6.

By the block analytical-numerical method have been calculated effective characteristics (6.4), (6.5) (with taking into account of not local effects) for a composite material with factor of volume fraction $\eta = \pi/16$ and with periodically repeating circular inclusions. The problem (6.6), (6.7) on unit square with circular inclusion of radius 0.25 was considered. This case corresponds to composite materials with factor of volume fraction $\eta = \pi/16$. Parameters of the matrix and inclusion are varied within the range: $0.1 < \mu_f/\mu_m < 15$, $v_f = v_m = 0.3$. The width of interphase layer was constant and equal $l_m = 0.06$ in the matrix, $l_f = 0.01$ in the inclusion. The matrix of effective coefficients \hat{A}_{kj} in this case corresponds to the orthotropic material with three homogenized elastic modulus. Comparative calculations of the effective modulus $\hat{A}_{1111} = \hat{E}$ and shear modulus $\hat{A}_{1122} = \hat{\mu}$, and corresponding coefficients \hat{E}_0 and $\hat{\mu}_0$ for the classical problem (without cohesion field) have been fulfilled. On Fig. 7 results of calcula-

tions are submitted. Results of homogenization at $\mu_f < \mu_m$ practically coincide with the classical case. Sufficient growth of homogenized Young modulus \hat{E} (up to $\approx 20\%$ at $\mu_f/\mu_m = 15$) is observed when $\mu_f > \mu_m$. At the same time we have the small growth of homogenized shear modulus $\hat{\mu}$ (on 9% at $\mu_f/\mu_m = 15$). So, e have effect of increasing of rigidity of the composite material for rigid inclusions $\mu_f/\mu_m=15$ due to the interphase layer. The shear effective modulus is changed slightly. More significant reinforcement effect

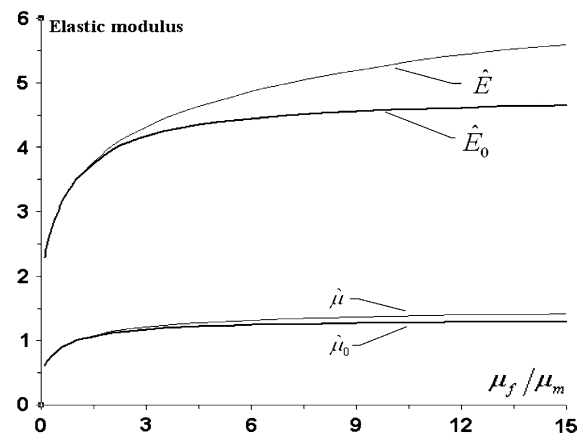


Fig. 7 Homogenized elastic modulus

can be achieved due to greater sizes of the interphase layers (l_0) and elongated form of spheroidal inclusions (geometrical factor).

Conclusions

Formal theoretical strain gradient model of the interphase layer with local cohesion and interfacial properties was proposed. Generalized Eshelby's solution and asymptotical averaging technique of homogenization were extended on the higher-order model. The effective the block-analytical method of the boundary problem was developed for gradient model of an interphase layer. Using these approaches the prediction methodology and modeling tools have been developed by numerical simulations and analysis of the stress-strain-stress and mechanical properties across the length scales.

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