Nanomechanical modeling of the nanostructures and dispersed composites

S. Lurie[a] *, P. Belov[a], D. Volkov-Bogorodsky[b] and N. Tuchkova[a]

[a] *Dorodnicyn Computer Center of RAS, Vavilova str., 40, GSP-1, Moscow 119991, Russia*

[b] *Institute of Applied Mechanics of RAS, Leninskij prospect, 32-A, Moscow 117334, Russia*

Abstract

Nanoparticles, hyperthin films, nanotubes and composite materials obtained on the base of such nanostructures exhibit very attractive mechanical properties and are great interest to researchers from continuum mechanics. In this paper, we intend to develop the multiscale continuum model of solids to explain the uncommon properties of the thin structures and the composite materials with thin structures associated with special type local interactions between nanoparticles and matrix. We have used the variation approach assuming that the internal interactions are determined by general character of kinematical connections. This approach allows introducing the system of internal interactions of various types consequently, which correspond to various types of kinematic restrictions in the considered mediums. The model of Cosserat's pseudocontinuum with both nonfree deformations, which depend on the other generalized coordinates and free deformations and rotations (continuous field of defects) but with symmetric stress tensor was proposed. The particular model is considered, which according to the authors view may serve as base for investigations of the scale effects due to cohesion interactions. Description of the cohesion field near top of cracks and composite materials with inclusions are considered in this research.

Keywords: Multiscale effects, Cosserat's pseudocontinuum, Cohesion interactions, Cracks, Composite materials

1. Introduction

Unusual inherent properties of the hyperthin structures (nano-particles, nano-tubes) as well as mechanical properties of the new materials obtained on the base of such nano-structures are of a great concern and need to be explained. In particular, composite materials strengthen with such inclusions are of a great interest. Mechanical properties of such materials are explained mainly by uncommon inherent properties of the thin structures, and peculiarities of the interactions between the nano-particles and the matrix at their contact. These local interactions are concentrated near tops of cracks, phase interfaces and have the multiscale nature. In the recent works [1, 2] the variant of the nanoscale continuum theory is elaborated based on the introducing of the interatomic potentials of materials in framework of continuum mechanics. This continuum theory allows to describe the internal interactions at the nanometer scale. Other approach based on the higher order continuum theories of elasticity and Cosserat's pseudocontinuums theory will proposed in this paper to construct the continuum theory with scale effects. Further the models with scale effects are developed on the base of the variational formalism. Basically, it is accepted that new approaches should be involved for modeling multiscale effects in materials. Note that similar approaches were developed in the recent works [3–5] which have allowed to account the size dependence of plastic deformation at micron- and submicron- length scales.

It is suggested to use the correct consistent models built according to mathematically approved mechanical models to describe the properties of the thin structure and composites on their

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E-mail address: lurie@ccas.ru

base. Let us formulate the requirements to such models, restricting ourselves with the linear models:

1. The model have to describe the behavior of the deformed media taking into accounts the scale effects. Therefore, among the physical parameters of the model there should be constants of various dimensions.

2. The total potential energy of deformation, written for the model as a function of the fixed number of arguments have to depend not only on the volume density of potential energy, but also on the surface density of potential energy. This surface density is thought not to be reduced to some volumetric energy. This requirement is due to the necessity of accounting for the surface effects and scale effects determined by the phase interfaces.

3. The model have to be consistent and correct, i.e. the equations of equilibrium for the media and the boundary conditions have to correspond to a variational statement of the problem.

4. The generalized model taking into accounts the scale effects may not contradict the classical model, and have to include it as a limiting case. Hence, the presentation of the solution in the fundamental system may be in the form of decomposition, including the term, corresponding to the classical solution.

A new "kinematic" variation formalism approach is applied to develop the mathematical formulation [6, 7]. This approach allows introducing the system of internal interactions of various types consequently, which correspond to various types of kinematics restrains in the considered media.

2. The model of generalized Cosserat's medium

Let's assume, that the Papkovich's relations are not satisfied, i.e. are non-homogeneous

$$\frac{\partial}{\partial x_j}\left(\gamma_{in}+\frac{1}{3}\,\theta\delta_{in}-\omega_k\mathcal{E}_{ink}\right)\mathcal{E}_{nmj}=\Xi_{ij}. \qquad (1)$$

Here, as usually it is supposed to conduct summation over repeated indexes, γ_{ij} are components of the deviator of strain, θ — volumetric strain, ω_k — vector of elastic rotation, $\mathcal{E}_{ijk}$ — components of Levi–Chevita's tensor. Right part of the Papkovich's relations (1) determine by the incompatibility tensor Ξ_{ij}. The solution of (1) may be presented as

$$\gamma_{ij}+\frac{1}{3}\,\theta\delta_{ij}-\omega_k\mathcal{E}_{ijk}=d^0_{ij}+d^{\Xi}_{ij},$$

where d^0_{ij} is general solution of homogeneous Papkovich's relations (1)

$$d^0_{ij}=\frac{\partial R_i}{\partial x_j}=\gamma^0_{ij}+\frac{1}{3}\,\theta^0\delta_{ij}-\omega^0_k\mathcal{E}_{ijk},$$

where d^{Ξ}_{ij} is particular solution of non-homogeneous Papkovich's relations (1)

$$d^{\Xi}_{ij}=\gamma^{\Xi}_{ij}+\frac{1}{3}\,\theta^{\Xi}\delta_{ij}-\omega^{\Xi}_k\mathcal{E}_{ijk}.$$

Following to a "kinematic" variation principle, we shall write the possible work of the interior forces on corresponding kinematic restrains [6]:

$$\begin{aligned}\bar{\delta}U=&\iiint\Big\{\sigma_{ij}\delta\Big(\gamma^0_{ij}+\frac{1}{3}\,\theta^0\delta_{ij}-\omega^0_k\mathcal{E}_{ijk}-\frac{\partial R_i}{\partial x_j}\Big)\\&+m_{ij}\delta\Big[\Xi_{ij}-\frac{\partial}{\partial x_m}\\&\times\Big(\gamma^{\Xi}_{in}+\frac{1}{3}\,\theta^{\Xi}\delta_{in}-\omega^{\Xi}_k\mathcal{E}_{ink}\Big)\,\mathcal{E}_{nmj}\Big]\Big\}\,dV.\end{aligned}$$

Integrating by parts the last relation (2), leads:

$$\begin{aligned}\bar{\delta}U=&\iiint\Big[\frac{\partial\sigma_{ij}}{\partial x_j}\,\delta R_i+\sigma_{ij}\delta\gamma^0_{ij}+\frac{1}{3}\,\sigma_{ij}\delta_{ij}\delta\theta^0\\&-\sigma_{ij}\mathcal{E}_{ijk}\delta\omega^0_k+m_{ij}\delta\Xi_{ij}+\Big(\frac{1}{2}\,\frac{\partial m_{in}}{\partial x_m}\,\mathcal{E}_{jmn}\end{aligned}$$

$$+\frac{1}{2}\frac{\partial m_{jn}}{\partial x_m}\mathcal{E}_{imn}-\frac{1}{3}\frac{\partial m_{kn}}{\partial x_m}\mathcal{E}_{kmn}\delta_{ij}\Big)\,\delta\gamma^{\Xi}_{ij}$$

$$+\frac{1}{3}\frac{\partial m_{nj}}{\partial x_m}\mathcal{E}_{nmj}\delta\theta^{\Xi}$$

$$-\frac{\partial m_{ij}}{\partial x_m}\mathcal{E}_{nmj}\mathcal{E}_{ink}\delta\omega^{\Xi}_k\Big]\,dV$$

$$+\oiint\Big[-\sigma_{ij}n_j\delta R_i-m_{in}n_m\mathcal{E}_{jmn}\delta$$

$$\times\Big(\gamma^{\Xi}_{ij}+\frac{1}{3}\theta^{\Xi}\delta_{ij}-\omega^{\Xi}_k\mathcal{E}_{ijk}\Big)\Big]\,dF, \qquad (2)$$

where n_i is normal vector to the surface of the considered body. The obtained variation form (2) allows to establish the lists of arguments of volumetric and surface parts of a potential energy. Firstly, let's present the tensor of the incompatibility Ξ as expansion on a deviator tensor, sphere tensor and antisymmetric tensor:

$$\Xi_{ij}=\xi_{ij}+\frac{1}{3}\xi\delta_{ij}-\xi_k\mathcal{E}_{ijk},$$

$$\xi_{ij}=\frac{1}{2}(\Xi_{ij}+\Xi_{ji})-\frac{1}{3}\Xi_{pp}\delta_{ij}$$

$$=\frac{1}{2}\Big(\frac{\partial\gamma^{\Xi}_{in}}{\partial x_m}\mathcal{E}_{nmj}+\frac{\partial\gamma^{\Xi}_{jn}}{\partial x_m}\mathcal{E}_{nmi}\Big)$$

$$+\Big(\frac{1}{2}\frac{\partial\omega^{\Xi}_i}{\partial x_j}+\frac{1}{2}\frac{\partial\omega^{\Xi}_j}{\partial x_i}-\frac{1}{3}\frac{\partial\omega^{\Xi}_k}{\partial x_k}\delta_{ij}\Big), \qquad (3)$$

$$\xi=\Xi_{ij}\delta_{ij}=-2\frac{\partial\omega^{\Xi}_k}{\partial x_k},$$

$$\xi_k=-\frac{1}{2}\Xi_{ij}\mathcal{E}_{ijk}$$

$$=-\frac{\partial\gamma^{\Xi}_{kq}}{\partial x_q}+\frac{1}{3}\frac{\partial\theta^{\Xi}}{\partial x_k}+\frac{1}{2}\frac{\partial\omega^{\Xi}_n}{\partial x_m}\mathcal{E}_{nmk}.$$

We will write the tensor and vector magnitudes in a surface integral in the last variational equation as expansion on the normal component to surface and tangent component to a surface. With this purpose we introduce the following kinematic factors in a tangential direction and orthogonal direction to a surface:

$$\begin{aligned}
\widehat{\gamma}^{\Xi}_{pq}&=\gamma^{\Xi}_{pq}(\delta_{iq}-n_in_q)(\delta_{np}-n_nn_p),\\
\widehat{\omega}^{\Xi}_k&=\omega^{\Xi}_k(\delta_{kq}-n_kn_q),\\
\widehat{R}_k&=R_q(\delta_{kq}-n_kn_q),\\
\widehat{\gamma}^{\Xi}_k&=\gamma^{\Xi}_{pq}n_q(\delta_{np}-n_nn_p),\\
\omega^{\Xi}&=\omega^{\Xi}_qn_q,\\
R&=R_qn_q,\\
\gamma^{\Xi}&=\gamma^{\Xi}_{pq}n_pn_q,
\end{aligned} \qquad (4)$$

possible to write following expansions:

$$\begin{aligned}
\omega^{\Xi}_k&=\widehat{\omega}^{\Xi}_k+\omega^{\Xi}n_k,\\
\gamma^{\Xi}_{ij}&=\widehat{\gamma}^{\Xi}_{ij}+\widehat{\gamma}^{\Xi}_jn_i+\widehat{\gamma}^{\Xi}_in_j+\gamma^{\Xi}n_in_j,\\
R_k&=\widehat{R}_k+Rn_k.
\end{aligned} \qquad (5)$$

Expression for a tensor of a free distortion will be written as

$$\begin{aligned}
d^{\Xi}_{ij}&=\gamma^{\Xi}_{ij}+\frac{1}{3}\theta^{\Xi}\delta_{ij}-\omega^{\Xi}_k\mathcal{E}_{ijk}\\
&=\big(\widehat{\gamma}^{\Xi}_{ij}+\widehat{\gamma}^{\Xi}_jn_i+\widehat{\gamma}^{\Xi}_in_j+\gamma^{\Xi}n_in_j\big)\\
&\quad+\frac{1}{3}\theta^{\Xi}\delta_{ij}-\big(\widehat{\omega}^{\Xi}_k+\omega^{\Xi}n_k\big)\mathcal{E}_{ijk}.
\end{aligned} \qquad (6)$$

Taking into account the entered table of symbols (3)–(6) and assuming that the variation linear form is integrable (there is a potential energy), we can establish the list of arguments of volumetric and surface parts of a potential energy:

$$\begin{aligned}
U_V&=U_V\big(\gamma^0_{ij};\,\gamma^{\Xi}_{ij};\,\xi_{ij};\,R_k;\,\omega^0_k;\,\omega^{\Xi}_k;\,\xi_k;\,\theta^0;\,\theta^{\Xi};\,\xi\big),\\
U_F&=U_F\big(\widehat{\gamma}^{\Xi}_{ij};\,\widehat{\gamma}^{\Xi}_k;\,\omega^{\Xi}_k;\,\widehat{R}_k;\,\omega^{\Xi};\,\theta^{\Xi};\,R\big).
\end{aligned} \qquad (7)$$

Taking into account a physical linearity of stated model (i.e. quadratic form of a Lagrangian), we shall present a Lagrangian of considered model as quadratic form of the arguments of volumetric and surface parts of a potential energy. Coefficients in this form define the set of physical constants of model. In result we can find the generalized equations of a Hooke's law (constitutive relations) for common model of a Papkovich–Cosserat's continuum for the stresses σ_{ij}, for the moment stresses m_{ij}, for generalized of the cohesion forces σ_k and for a tensor of cohesion stresses in volume p_{ij}

$$\sigma_{ij} = \frac{\partial U_V}{\partial(\partial R_i/\partial x_j)}, \qquad m_{ij} = \frac{\partial U_V}{\partial \Xi_{ij}},$$

$$\sigma_k = \frac{\partial U_V}{\partial R_k}, \qquad p_{ij} = \frac{\partial U_V}{\partial d^{\Xi}_{ij}}.$$

The generalized equations of a Hooke's law for couple model of a Papkovich–Cosserat's medium on a surface of area also can be written:

$$\widehat{\tau}^{\Xi}_{ij} = \frac{\partial U_F}{\partial \gamma^{\Xi}_{ij}}, \qquad \widehat{\tau}^{\Xi}_{k} = \frac{\partial U_F}{\partial \widehat{\gamma}^{\Xi}_{k}}, \qquad \widehat{m}_k = \frac{\partial U_F}{\partial \widehat{\omega}^{\Xi}_{k}},$$

$$f_k = \frac{\partial U_F}{\partial \widehat{R}_k}, \qquad m^{\Xi} = \frac{\partial U_F}{\partial \omega^{\Xi}}, \qquad \sigma^{\Xi} = \frac{\partial U_F}{\partial \theta^{\Xi}},$$

$$f = \frac{\partial U_F}{\partial R}.$$

The coefficients in the linear forms in the right parts of constitutive equations are physical constants of model. Among them constants μ, λ are Lame's coefficients. As a result we can write the Lagrangian and establish the Euler's equations and natural boundary conditions:

$$\begin{aligned}
\delta L = \iiint \Big[\Big(\frac{\partial \sigma_{ij}}{\partial x_j} - \sigma_i + X_i \Big) \delta R_i \\
- \Big(\frac{\partial m^{\Xi}_{in}}{\partial x_m} \mathcal{E}_{nmj} + p_{ij} \Big) \delta d^{\Xi}_{ij} \Big] dV \\
+ \oiint \Big[(Y_i - \sigma_{ij} n_j - f_i)\, \delta \widehat{R}_i \\
+ (Y_i n_i - \sigma_{ij} n_i n_j - f)\, \delta R \\
+ (m_{in} n_m \mathcal{E}_{nmj} - \widehat{\tau}^{\Xi}_{ij})\, \delta \widehat{\gamma}^{\Xi}_{ij} \\
+ (m_{in} n_i n_m \mathcal{E}_{nmk} - \widehat{\tau}^{\Xi}_{k})\, \delta \widehat{\gamma}^{\Xi}_{k} \\
- (m_{in} n_m \mathcal{E}_{nmj} \mathcal{E}_{ijk} + \widehat{m}_k)\, \delta \widehat{m}^{\Xi}_{k} \\
- (m_{in} n_m n_k \mathcal{E}_{ijk} \mathcal{E}_{nmj} + m^{\Xi})\, \delta \omega^{\Xi} \qquad (8) \\
+ \Big(\frac{1}{3} m_{in} \delta_{ij} n_m \mathcal{E}_{nmj} - \sigma^{\Xi} \Big) \delta \theta^{\Xi} \Big] dF = 0.
\end{aligned}$$

Thus, the mathematical statement of a problem for Papkovich's–Cosserat's continuum is formulated, in which the unhomogenious Papkovich's relations (1) are introduced. The boundary value problem for generalized model is constructed.

3. Cohesion field model

Here on the basis of (8) the new model of the moment cohesion is offered. Let us make a following preliminary note. The successive analysis of Papkovich's–Cosserat's continuum allows to formulate the following statements:

- For the Papkovich's–Cosserat's continuum (8) with free deformations the appropriate particular concrete model of a Koiter's medium can be established;
- It can be proved exactly that the free strains can be algebraically written in the explicit form through some linear differential operators of the second order from vector of displacements.

The formulated statements give some formal foundation for simplification of model. Really, according to the statements the vector of free rotations ω^{Ξ}_k, for example, is determined in the following form:

$$\omega^{\Xi}_k = aR_k + b\omega_k + c\, \frac{\partial \theta}{\partial x_k} + d\, \frac{\partial \omega_n}{\partial x_m} \mathcal{E}_{nmk},$$

where a, b, c, d are some constants. The similar expansions can be established and for θ^{Ξ}, γ^{Ξ}_{ij}.

For offered most simple model of the "moment" cohesion we shall take in the expansion for free rotational displacements only one item: $\omega^{\Xi}_k = a_1 \omega_k$. In equations for θ^{Ξ} and γ^{Ξ}_{ij} we propose similarly to accept: $\theta^{\Xi} = b_1 \theta$, $\gamma^{\Xi}_{ij} = 0$. Here a_1 and b_1 are some rational functions of modules of common model (8). After such simplifications we shall accept an extraly following system of simplifying positions:

- Is considered further, the density of a volumetric potential energy U_V has not cross terms, i.e. is written in a canonical form;

- The denseness of a surface potential energy is equal zero;
- The model of the continuum with a symmetric stress tensor is studied;
- The "moment Poisson's constant" is equal zero (coefficient in the term generated by the vectors of curvatures $\xi_k\xi_k$ in U_V is equal zero);
- The coefficients, which have stayed after these simplifications in common model are selected so that the operator of the governing equation of model could be submitted as product of an operator of the classical theory of elasticity and operator, defining scale effect.

In result we shall receive the following expression for Lagrangian:

$$L = A - \frac{1}{2}\iiint \Big[2\mu\gamma_{ij}\gamma_{ij} + \Big(\frac{2\mu}{3} + \lambda\Big)\,\theta^2 + 8\,\frac{\mu^2}{C}\,\xi_{ij}\xi_{ij} + \frac{(2\mu+\lambda)^2}{C}\,\theta_i\theta_i\Big]\,dV.$$

Here $\theta_i = \dfrac{\partial\theta}{\partial x_i}$ and

$$\xi_{ij} = -\frac{1}{2}\,\frac{\partial^2 R_n}{\partial x_i\,\partial x_m}\,\mathcal{E}_{mnj} - \frac{1}{2}\,\frac{\partial^2 R_n}{\partial x_j\,\partial x_m}\,\mathcal{E}_{mni}.$$

The variational equation of considered cohesion fields model for body with smooth surface can be written as:

$$\begin{aligned}
&\iiint \Big[(2\mu+\lambda)\,\frac{\partial\theta}{\partial x_i} + 2\mu\,\frac{\partial\omega_n}{\partial x_m}\,\mathcal{E}_{nmi} - \frac{2\mu^2}{C}\,\Delta\,\frac{\partial\omega_n}{\partial x_m}\,\mathcal{E}_{nmi} - \frac{(2\mu+\lambda)^2}{C}\,\Delta\,\frac{\partial\theta}{\partial x_i} + P_i^V\Big]\,\delta R_i\,dV\\
&-\oiint \Big\{-\frac{2\mu^2}{C}\,(n_m n_j\mathcal{E}_{ijn} + n_n n_j\mathcal{E}_{ijm})\,\frac{\partial\omega_n}{\partial x_m} + \frac{(2\mu+\lambda)^2}{C}\,\frac{\partial\theta}{\partial x_k}\,n_k n_i\Big\}\,\delta\,\frac{\partial R_i}{\partial x_q}\,n_q\,dF\\
&+\oiint \Big\{P_i^F - \Big[2\mu\gamma_{ij} + \Big(\frac{2\mu}{3} + \lambda\Big)\,\theta\delta_{ij} + \frac{2\mu^2}{C}\,\Delta\omega_n\mathcal{E}_{ijn} - \frac{(2\mu+\lambda)^2}{C}\,\Delta\theta\delta_{ij}\Big]\,n_j\\
&\quad + (\delta_{qj} - n_q n_j)\,\frac{\partial}{\partial x_q} \times \Big[-\frac{2\mu^2}{C}\,\Big(\frac{\partial\omega_k}{\partial x_p} + \frac{\partial\omega_p}{\partial x_k}\Big)n_p\mathcal{E}_{ijk} + \frac{(2\mu+\lambda)^2}{C}\,\frac{\partial\theta}{\partial x_k}\,n_k\delta_{ij}\Big]\Big\}\,\delta R_i\,dF = 0. \qquad (9)
\end{aligned}$$

Here P_i^V is vector of density of external loads in the body's volume and P_i^F is vector of density of external loads in the body's surface. Let's consider governing equation for model (9). We shall enter the "classical" operator of balance:

$$L_{ij}(\ldots) = (\mu+\lambda)\,\frac{\partial^2(\ldots)}{\partial x_i\,\partial x_j} + \mu\delta_{ij}\Delta(\ldots). \qquad (10)$$

It is easy to be convinced of validity of the following equality:

$$\Delta\theta = \frac{1}{(2\mu+\lambda)}\,\frac{\partial(\ldots)}{\partial x_i}\,L_{ij}(R_j),$$

$$\Delta\omega_k = -\frac{1}{2\mu}\,\frac{\partial(\ldots)}{\partial x_q}\,L_{pj}(R_j)\,\mathcal{E}_{pqk}.$$

Taking into account last equations and (10), the governing equation in (9) can be rewriting in displacements as:

$$\Big[-\frac{1}{C}\,L_{ij}(\ldots) + (\ldots)\,\delta_{ij}\Big]\,L_{jk}(R_k) + P_i^V = 0. \qquad (11)$$

Here R_k is displacements vector. The offered model contains only one new physical constant C in comparison with the classical theory of elasticity. We can define displacement of cohesion field. Let's name a vector of the displacement of cohesion fields (cohesion displacement) the following vector:

$$u_i = -\frac{1}{C}\,L_{ij}(R_j)$$

$$= -\frac{1}{C}\Big[(\mu+\lambda)\,\frac{\partial^2 R_j}{\partial x_i\,\partial x_j} + \mu\delta_{ij}\Delta R_j\Big]. \qquad (12)$$

Using (12) we receive the equations for a vector function u_i:

$$H_{ij}(u_j) + P_i^V = 0,$$

where

$$H_{ij}(\ldots) = L_{ij}(\ldots) - C(\ldots)\,\delta_{ij}.$$

Similarly we shall enter definition of a vector of classical displacements U_i which is satisfies to the classical equations of balance: $L_{ij}(U_j) + P_i^V = 0$. In the equation (11) it is possible to change a sequence of action of operators. Then we shall receive

$$U_i = \Big[-\frac{1}{C}\,L_{ij}(\ldots) + (\ldots)\,\delta_{ij}\Big]\,R_j$$

and

$$R_i = U_i - u_i. \qquad (13)$$

Thus, the boundary value problem (9) represents the couple boundary value problem for the classical solution and the solution for cohesion fields model. The boundary value problem generally is not divided.

Let's introduce the orts system X_i, Y_i, Z_i and consider the plane problem of the "moment" cohesion. Assume that there are no projections of loads in the ort to direction Z_i: $P_i^V Z_i = 0$ and $P_i^F Z_i = 0$. Similarly, in a vector of the displacements there is no projection on the ort Z_i: $R_j Z_j = 0$: $r_i = R_j(\delta_{ij} - Z_i Z_j)$ and $r_i Z_i = 0$. We assume also, that the vector of displacements r_i is function of two coordinates, i.e. does not depend on coordinate z, $z = x_j Z_j$: $\dfrac{\partial r_i}{\partial x_j}\,Z_j = 0$.

Thus, it is supposed, that the vector is determined in plane area Ω with border G. The variational equation (14) then is reduced to the following kind:

$$\iint\Big\{\Big[-\frac{1}{C}\,L_{ij}(\ldots) + (\ldots)\,\delta_{ij}\Big]\,L_{jk}(r_k) + P_i^V\Big\}\,\delta r_i\,dx\,dy - \oint\limits_{n_i Z_i = 0}\frac{\mu^2}{C}\Big(\ddot r_s - \frac{\partial \dot r_n}{\partial s}\Big)\,\delta\dot r_s\,ds$$

$$- \oint\limits_{n_i Z_i = 0}\frac{(2\mu+\lambda)^2}{C}\Big(\ddot r_n - \frac{\partial \dot r_s}{\partial s}\Big)\,\delta\dot r_n\,ds$$

$$+ \oint\limits_{n_i Z_i = 0}\Big\{P_s^F - \Big[\mu\dot r_s + \mu\,\frac{\partial r_n}{\partial s} - \frac{\mu^2}{C}\,\nabla^2\Big(\dot r_s - \frac{\partial r_n}{\partial s}\Big)\Big] + \frac{(2\mu+\lambda)^2}{C}\Big(\frac{\partial^2 \dot r_s}{\partial s^2} + \frac{\partial \ddot r_n}{\partial s}\Big)\Big\}\,\delta r_s\,dF$$

$$+ \oint\limits_{n_i Z_i = 0}\Big\{P_n^F - \Big[(2\mu+\lambda)\,\dot r_n + \lambda\,\frac{\partial r_s}{\partial s} - \frac{(2\mu+\lambda)^2}{C}\,\nabla^2\Big(\frac{\partial r_s}{\partial s} + \dot r_n\Big)\Big] - \frac{\mu^2}{C}\Big(\frac{\partial \ddot r_s}{\partial s} - \frac{\partial^2 \dot r_n}{\partial s^2}\Big)\Big\}\,\delta r_n\,dF = 0, \qquad (14)$$

where $\dot r_{n,s} = \partial r_{n,s}/\partial n$, $r_i = r_s s_i + r_n n_i$, n_i is normal to the boundary G, $n_i s_i = 0$. Further the formulation of the plane problem in such statement will be used for the disperse composite modeling by numerical methods.

4. Examples

The model of cohesion field (9) will be used for the description of the deformations in materials in view of the scale effects associated with the cohesion interactions. Firstly, we attempt to estimate the new physical parameter C. It will be shown that parameter C is concerned with the famous parameters of the fracture mechanics. Then, the solutions for a compound material will be received. On example one-dimensional biplane problems, the approached estimation of influence of new scale effects, connected with bounds of other solid phases on effective characteristics of a material will be given. At last, within the framework of two-dimensional biplane problems numerical — analytical modeling of the characteristic cell of material of the rectangular form, containing two components (matrix and inclusion) will be given. It is shown account of the cohesion interactions can give the significant influence on accommodation properties of a matrix in dependence on the form and the sizes of inclusion.

4.1. Problem of the normal opening crack

Let's consider the problem of the normal opening crack. This problem was solved within the framework of double plane statement [6]. Let's consider now the same problem from a point of view of couple model of cohesion interactions also within the framework of double plane statement. The asymptotic solution near end of a crack can be written as

$$\nu(r,\varphi) = -2\,\frac{\sigma_a}{aE}\,(1-e^{-ar})(ar)^{1/2}\cos\left(\frac{\varphi}{2}\right),$$

$$\sigma = \sigma_a\,\frac{1-e^{-ar}}{(ar)^{1/2}}\,\sin\left(\frac{\varphi}{2}\right),$$

where $a^2 = \frac{C}{E}$, E is modulus of elasticity.

The written down solution describes the nonsingularity field of the stresses near top of the crack. This solution has the classical asymptotic behavior on the infinity [8]. It can be prove, that solution is a common solution of the equation of the cohesion field model within the framework of double plane statement and can be submitted as the sum of solutions of the harmonic equation and Helmholtz's equation. It can be shown that the boundary conditions for the problem under consideration are satisfied. Let's show, that constant of model C is interlinked to known parameters of a fracture mechanics.

Let's define distance r_0, on which stress as the function r accepts a maximum value. A requirement $\frac{\partial\sigma}{\partial(ar)} = 0$ gives the following equation for definition ar_0: $e^{ar_0} = 1+2ar_0$. This equation has the unique real root: $q = ar_0 = 1.256431$. Hence, we can write:

$$C = q^2\,\frac{E}{r_0^2} = 1.578619\,\frac{E}{r_0^2}.$$

Let's find the connection between amplitudes of displacements and stresses in a point where the stresses reach a maximum value. The magnitude of transverse displacements in this point we can define as magnitude of the crack open displacement. We can write

$$\nu(r_0,\,0) = -2\frac{\sigma_a}{aE}\,(1-e^{-ar_0})(ar_0)^{1/2} = -\delta_a,$$

where δ_a is the crack open displacement. Then, for amplitude of the stresses we can receive the following equation:

$$\sigma_a = E\,\frac{a\delta_a(1+2q)}{4q^{3/2}} = 0.623581\,Ea\delta_a.$$

Let us consider equation (23). Assuming that maximum of stresses is reached in the point $r = r_0$, $\varphi = \pi$, we can find:

$$\sigma_a = \sigma_{\max}\,\frac{(1+2q)}{2q^{1/2}} = 1.566974\,\sigma_{\max}.$$

Taking into account the previous equation we can write: $\sigma_{\max} = 0.397952\,Ea\delta_a$. Assume that crack open displacement δ_a reaches to critical value δ_c, when stresses $\sigma_{\max}$ reach to magnitude of theoretical strength σ_c. Thus, we can introduce the definition of the critical value of crack open displacement: $\delta_c = \frac{\sigma_c/E}{0.397952a}$. Then, we can write:

$$a^2 = \frac{C}{E} = \left(\frac{\sigma_c/E}{0.397952}\right)^2\frac{1}{\delta_c^2}.$$

Using of the last equation leads to the following formula for constant C:

$$C = \left(\frac{1/2\pi}{0.397952}\right)^2\frac{E}{\delta_c^2} = 0.159948\,\frac{E}{\delta_c^2}.$$

Note, that we used here the estimation of the value σ_c/E from [9]: $\sigma_c/E = 1/2\pi$. It is possible to define the value r_0 is the length of Barenblat's zone [8] through the critical value of crack open displacement δ_c: $r_0 = 3.141588\delta_c$. At last, the additional modulus C can be defined through specific surface energy γ. We must use the famous definition for value γ we can get: $2\gamma = \sigma_c\delta_c = \frac{E}{2\pi}\,\delta_c$. In result, we established that new physical constant of the model C is determined through based constants of fracture mechanics:

$C = 0.007345\,\dfrac{E^3}{\gamma^2}$ (specific surface energy γ);

$C = 1.578619\,\dfrac{E}{r_0^2}$ (magnitude of the Barenblatt's zone — r_0);

$C = 0.159948\,\dfrac{E}{\delta_c^2}$ (critical value of crack open displacement — δ_c).

4.2. The estimation of properties of periodic structure

Let's consider the compound beam loaded on edge at $x = 0$. Other edge of the beam at $x = x_2$ is loaded by external force P. The beam consists of two parts: in the first part ($0 \le x < x_1$) the material properties are determined by the modulus of elasticity E_M and the cohesive modulus C_M, in the second part ($x_1 < x \le x_2$) — modulus E_D, and the cohesive module C_D. Contact is carried out on the line $x = x_1$. The equation of balance should be solved for each fragment separately. All values of the first fragment we shall marked by index M (matrix), the second fragment by index D (defect). The solution of the written boundary value problems has the following view:

$$r^M(x) = \frac{P}{E^M F}\left[x - x_f e^{-a_M(x_1-x)}\right],$$

$$r^D(x) = \frac{P}{E^M F}\,x_1 + \frac{P}{E^D F}\,(x - x_1) + \frac{P}{E^D F}\,x_f\left[1 - e^{-a_D(x-x_1)} - \frac{E^D}{E^M}\right],$$

where

$$a_m = \sqrt{\frac{C_M}{E_M}}, \qquad a_D = \sqrt{\frac{C_D}{E_D}}$$

are the values which associated with the characteristic sizes of cohesion fields. In the last formulas for solutions the following notation is entered: $x_f = \dfrac{(E^D - E^M)}{E^D a_M + E^M a_D)}$. The value x_f has dimension of length and is the characteristic of length "interphase" of cohesion zones on the boundary of contact of various phases (matrix–inclusion). It is important to note that this value is determined only through properties of phases. Let's enter definition of thickness of an "interphase" layer as x_f. The potential energy for a matrix and inclusion (defect) are accordingly:

$$\begin{pmatrix} U^M \\ U^D \end{pmatrix} = \frac{P^2}{2F}\begin{pmatrix} 1/E^M \\ 1/E^D \end{pmatrix} \times \left[\begin{pmatrix} x_1 \\ x_2 - x_1 \end{pmatrix} \mp 2x_f + x_f^2 \begin{pmatrix} a_M \\ a_D \end{pmatrix}\right].$$

The first item in the written equations corresponds to classical representations of energy of deformation of the matrix and inclusion. Last two items correspond to the contribution of the cohesion the fields concentrated near boundary of contact of phases. We can formulate the following conclusions:

1. Redistribution of potential energy of deformation from less rigid fraction to the more rigid fraction takes place. In comparison with classical representation the matrix is unloaded, and an arming element (or defect) are loaded in addition. The effect of strengthening takes place.

2. For disperse composites the contribution to energy of deformation from a "volumetric" share of scale effects of cohesion fields grows under the square-law. For comparison, for a classical part energy of deformation grows linearly from a volume fraction of the arming fragment.

The solution received above takes into account the effects associated with the cohesion interactions concentrated in a zone of contact of phases. Let's consider a compound beam, which consists from $N + 1$ a fragment of a matrix (with characteristics E_M, C_M) and N fragments of the reinforced material (with characteristics E_D, C_D). The beam is in conditions uniaxial loading. We will try to establish the approached estimation of effective rigidity for such the composite material on the basis of one-dimensional model of "moment cohesion" (9) within the framework of one-dimensional statement. Writing the energy of deformation of the beam after obvious transformations we can receive:

$$U = \frac{P^2}{2F}\left[\left(\frac{l_M}{E^M}+\frac{l_D}{E^D}\right) - 2\,\frac{(E^D-E^M)}{E^M E^D}\,N x_f\right].$$

Let's compare this equation for energy with the potential energy of deformation for equivalent homogeneous beam with the modulus E_0. With the definition of a volume fraction of defects $f = \frac{l_D}{(l_M + l_D)}$, we can receive the following equation for the effective module E_0

$$E_0 = \frac{E^M}{\left[1 - \frac{(E^D-E^M)}{E^D}\left(f + 2N\frac{x_f}{(l_M+l_D)}\right)\right]}.$$

The last formula shows, that the modulus of a composite is determined not only through the traditional parameter $\frac{(E^D-E^M)}{E^D}\,f$ appearing at use of algorithm of Reuss's averaging. In a denominator of the received formula there is the additional item reflecting dependence of rigidity from quantity of defects N and length of an interphase layer x_f: $\frac{(E^D-E^M)}{E^D}\,N\,\frac{2x_f}{(l_M+l_D)}$. This expression is connected to the account of the cohesion fields near boundaries of contact of phases (matrix–inclusion). We have significant influence on rigidity when the length interphase cohesion zones x_f becomes the same order, as length of separate inclusion l_0^D: $x_f \sim l_0^D$, $l_0^D = \frac{l_D}{N}$, where l_D is a volume fraction of inclusions. In result, the end formula for the effective module of the beam E_0 can be write as:

$$E_0 = \frac{E^M}{[1 - \frac{(E^D-E^M)}{E^D}\,f(1+\frac{2x_f}{l_0^D})]}.$$

The formula allows us to describe at a qualitative level effect of increase of rigidity of a composite reinforced by the nanoparticles. The following results can be formulated:

1. In area of zones of contact there is the interphase layer caused by cohesion interactions. The interphase layer can give appreciable influence on rigidity of a composite material. The degree of this influence is determined by extent of zones of contact by thickness of an interphase layer and its rigidity. If to assume, that $x_f \sim l_0^D$ it is easy to be convinced a volume fraction occupied with this layer, approximately twice exceeds a volume fraction of inclusion.

2. The account of cohesion interactions qualitatively allows to model known effect of increase of rigidity of a disperse composite at reduction of the size of inclusion. The given formula shows that at the same degree of reinforcing (f = const), rigidity of a composite material is increased with decreasing of average length of inclusion l_0^D.

4.3. Composite cell with elliptic inclusion

The problem of modeling of cell with inclusion as some element of composite material is considered. This problem corresponds to a so-called case of a double plane problem in which two components of displacements are equal to zero. The problem is reduced to system of two equations (for classical and cohesion field,constituting the solution of full problem), connected among themselves through a special jump condition on contour of an ellipse. The algorithm of dividing of initial domain on blocks [10, 11] was applied at realization of a block analytical-numerical method for a double plane problem for a plate with elliptic inclusion [12]. In this problem it is required to find function R satisfying the equation:

$$-\frac{1}{C_{f,m}}\,L L_C R_{f,m} = 0, \qquad L = L_C\big|_{C=0},$$

$$L_C = (2\mu+\lambda)\,\frac{\partial^2}{\partial x^2} + \mu\,\frac{\partial^2}{\partial y^2} - C_{f,m},$$

with conditions of jump junction of a special kind on contour of inclusion.

The solution of a problem was constructed in two stages from two functions, $R = U - u$. At the first stage the classic problem was solved ($LU = 0$) with boundary conditions on border of inclusion and a plate of the following kind:

$$[U] = 0, \qquad \left[\mu \frac{\partial U}{\partial n} + (\mu+\lambda) \frac{\partial U}{\partial x}\right] = 0,$$

$$U(\pm L, y) = \pm 1, \qquad 0 < y < H,$$

$$\frac{\partial U}{\partial n}(x, 0) = \frac{\partial U}{\partial n}(x, H) = 0, \qquad -L < x < L,$$

where $[U] = U_f - U_m$, $U_{f,m}$ are the displacements in inclusion and a matrix, μ, λ are material constants (Lame coefficients), C is parameter of cohesion field, L, H are accordingly semi-width and height of a plate. At the second stage displacement of cohesion field u as the solution of a non-classical problem was found ($L_C u = 0$) with boundary conditions of the following kind:

$$[u] = \frac{[\mu]}{\langle\mu\rangle}\langle u\rangle, \qquad \left[\frac{\partial u}{\partial n} - \frac{\partial U}{\partial n}\right] = 0,$$

$$u(\pm L, y) = 0, \qquad 0 < y < H,$$

$$\frac{\partial u}{\partial n}(x, 0) = \frac{\partial u}{\partial n}(x, H) = 0, \qquad -L < x < L,$$

where $\langle u\rangle = u_f + u_m$, $u_{f,m}$ are the displacements in inclusion and in a matrix, $C_{f,m}$ are cohesion parameters in inclusion and in a matrix, $\langle\mu\rangle = \mu_f + \mu_m$, $\mu_{f,m}$ are the shear modulus in inclusion and in a matrix.

In a double plane problem two components of stress tensor are distinct from zero:

$$\sigma_x = (2\mu+\lambda)\frac{\partial R}{\partial x}, \qquad \tau_{xy} = \mu \frac{\partial R}{\partial y}.$$

Investigation of a distribution of stresses σ_x was carried out in [12], depending on parameters C and μ, and also from geometrical parameters of an ellipse. The comparison of this solution with classical problem shows that character of distribution of a field of tension noticeably varies. If in classic problem concentration of a field is in a matrix, then in a full problem concentration of a field prevails in inclusion [12].

In this work the distribution of potential energy in matrix and inclusion is investigated. Energy in a plate, equal to half work of external forces, can be counted as integral:

$$E(G) = \frac{1}{2}\int\limits_{\partial G} (\sigma_x n_x + \tau_{xy} n_y)\, R\, ds$$
$$= \int\limits_{G} \frac{1}{2}\left[(2\mu+\lambda)\left(\frac{\partial R}{\partial x}\right)^2 + \mu\left(\frac{\partial R}{\partial y}\right)^2 - CuR\right] dx\, dy,$$

where $p_x = \sigma_x n_x + \tau_{xy} n_y$ — a component of a vector of surface forces, u — displacement of cohesion field (the solution of a problem of the second stage). It is of interest the value of accomodation of energy in inclusion $\eta = E_f/E_m$, it is equal to the ratio of energy in a matrix to energy in inclusion [13]. We shall note, that in the integral on area there is a value of local energy $\varepsilon(R)$. Calculations were fulfilled under following assumptions: $L = 1$, $H = 1.2$, $\nu_f = \nu_m = 0.3$, $E_f/E_m = 3$, $C_f/\mu_f = C_m/\mu_m = 100$; major axis of ellipse $a = 1.4\varepsilon$, minor axis of ellipse $b = 0.5\varepsilon$, where $\varepsilon = (0.9, 0.7, 0.5)$.

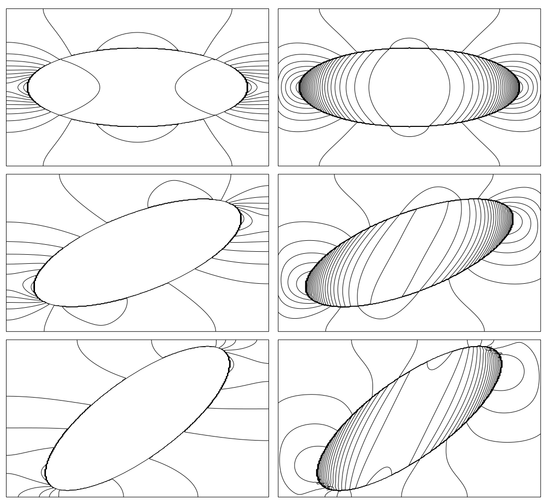

Figure 1. Examples of distribution of local energy $\varepsilon(U)$ and $\varepsilon(R)$ in a classic and full problem at partial turn of inclusion

Levels of energy distribution on Fig. 1 is presented with step $0.8\mu_m$, major axis of ellipse $a = 1.4\varepsilon$, minor axis of ellipse $b = 0.5\varepsilon$, where

$\varepsilon = 1.2$, angle θ between major axis and axis of ordinate is $\theta = (0°, 21°, 36°)$. On the Fig. 2 is presented distribution energy under full turn of inclusion: major axis of ellipse $a = 1.4\varepsilon$, minor axis of ellipse $b = 0.5\varepsilon$, where $\varepsilon = 0.7$, angle θ between major axis and axis of ordinate is changed between $10°$ and $90°$ with step $10°$. Numerical investigation shows that account of cohesion field (cohesion parameter C) leads to changing stress field and potential energy in the matrix and inclusions in composite. These effects allows to explain some unique properties of disperse composites with nanoinclusions. Figure 2 shows the distribution of the accommodation parameter η from the rotation of inclusions. Thus, for matrix

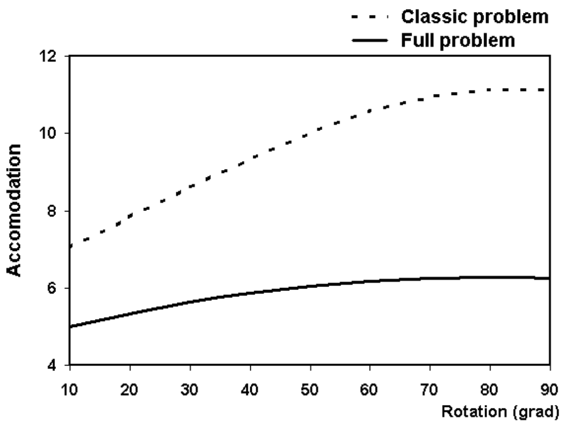

Figure 2. Dependence of accommodation η from rotation parameters of inclusion (full turn of inclusion) in a classic and full problem

with inclution in the considered cases taking cohesion interactions into accountleads to the effect of "unloading" of the matrix and to additional increase in the cell rigidity. It is shown, that accounting for the cohesion interactions results in reduction of concentration of deformation energy in the matrix in the vicinity of inclusions.

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