Available online at www.sciencedirect.com
SCIENCE DIRECT®
Composites: Part A xx (xxxx)1–8
composites Part A: applied science and manufacturing
www.elsevier.com/locate/compositesa

The application of the multiscale models for description of the dispersed composites

S.A. Lurie[a,b,*], P.A. Belov[a], N.P. Tuchkova[b]

[a]Institute of Applied Mechanics Russian Academy of Sciences, Leninskii pr. 32 a, 119991 Moscow, Russian Federation
[b]Dorodnicyn Computing Centre of the Russian Academy of Sciences, Vavilov st. 40, 119991 Moscow GSP-1, Russian Federation

Abstract

We studied composite materials reinforced by micro-particles. It is assumed that the following physical objects and appropriate local effects determine the specific properties of composites: cohesion fields and corresponding zones of internal interaction; adhesion interactions, which determine the peculiarity of interaction of contacting bodies. These effects are important and can define the mechanical properties of the mediums with developed interface surfaces. In this paper, we use the multiscale continuum model of solids to explain the specific properties of composite materials with thin structures associated with local interactions of special type between inclusions and a matrix.

Keywords: C. Micro-mechanics; A. Nano-structures; Multiscale continuum model; Filled composites; Effective properties

1. 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 and thus need to be explained. In the publication [1], 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 us to describe internal interactions on the level of nanometers and may be used to construct a model of deformation of carbon single-wall nanotubes (SWNT). Recently, in the paper [2], similar model was used for the developing of constitutive models for SNWT-reinforced polymer composites. This model is an outgrowth of the equivalent-continuum modeling technique and takes into account the discrete nature of atomic interactions for distances of nanometers. Other approach based on the higher-order continuum theory was developed in Ref. [3]; this approach takes into consideration the dependence of plastic deformation over the micron- and submicron-range. Recently, in the papers [4 and 5], the generalized continuum model with kept dislocations was developed. The mathematical statement of the model was given. This statement may be considered as the generalization of the Cosserat theory of pseudo-continuums. Generally, the model presented allows to describe local-cohesion interactions [4] and superficial effects [5].

Within the framework of the continuum theory presented, non-classical effects in the fracture mechanics, the theory of thin films, and the mechanics of filled composite materials were explained. In particular, the mathematical verification for the hypothesis of the cohesion field in fracture mechanics was proved [4]. The solution for a non-singular crack and the relationships between the non-classical parameter of the model and conventional parameters of the fracture mechanics were found. Therefore, in what follows, the effects associated with the non-classical constant will be named the cohesion effects.

In the theory of thin films, the following non-classical effects were explained [6,7]: (i) the increasing of a film rigidity with the reduction of its thickness; (ii) the delamination of a film out of the substrate of an indenter; (iii) the delamination of a substrate with thin rigid covering.

* Corresponding author. Address: Dorodnicyn Computing Centre of the Russian Academy of Sciences, Vavilov st. 40, 119991 Moscow GSP-1, Russian Federation. Fax: +7-95-135-6190

E-mail addresses: lurie@ccas.ru (S.A. Lurie), tuchkova@ccas.ru (N.P. Tuchkova).

1359-835X/$ - see front matter © 2004 Published by Elsevier Ltd.
doi:10.1016/j.compositesa.2004.06.014

In the mechanics of the filled composites, the hypothesis of an interphase layer was mathematically proved. The non-classical effect of reinforcing of composite materials was modeled in the case of the reduction of the size of inclusions at a constant inclusion volume fraction [4,5].

The phenomenon of strengthening of composite materials with nano-inclusions is also of great interest. It is known that the presence of small amount of nano-tubes results in the increase of the Young's modulus. This increase may be significant. It was reported that the presence of 0.5% (volumetric) of nano-tubes results in increase of the Young's modulus up to 40% [8]. The well-known solution [9] used for calculating effective properties of composite yields systematic error that result in underestimating the influence of the inclusions. The relative value of this error seems not to exceed 10%, but became more significant for small concentration of relatively short fibers. Despite this underestimating, the pure influence of nano-inclusions itself may not explain all cases of increase of elastic moduli of the composite [8]. Hence, it is necessary to take into account the influence of the third (intermediate) phase to the increase of elastic moduli.

Mechanical properties of composite materials can be explained mainly by uncommon inherent properties of the thin structures, and peculiarities of the interactions between the particles and the matrix at their contact. Influence of third phase to the effective properties of the composite has to be taken into accounts. The following problem may be formulated. Knowing mechanical and geometrical properties of all the phases, it is necessary to estimate the properties of the third phase and to calculate its effective properties. In the given work, for solving of the specified problem and prescription of composites reinforcement due to scale effects, it is proposed to use a variant of the model developed in Refs. [4 and 5]. It is proposed to consider the particular model at modeling and to take into account only interactions of cohesion type. The parameters of the model determining the account of non-classical effects in filled composites are defined from experimental data.

2. Mathematical statement and governing equations of model

It is assumed that the following physical objects and appropriate local effects may determine the uncommon properties of materials: cohesion fields and a zone of an internal interaction determined by them, which determine the peculiarity of the interaction of contacting bodies. It is suggested to use the correct consistent models built in accordance with the mathematically approved mechanical models [4,5]. Such models should satisfy the following requirements. (i) The models describe the behavior of the deformed media by taking into account the scale effects. Therefore, a set of the physical parameters of the models includes constants of various dimensions. (ii) The models of deformations are consistent and correct. The equilibrium equations coincide with the Euler equations and the boundary conditions follow from the natural boundary conditions. (iii) The generalized models of deformations taking into account the scale effects may not contradict to the classical models, and have to include them as a limiting case. Hence, the solution corresponding to the improved model in the form of decomposition into the fundamental system includes the terms corresponding to the classical solutions.

A new variant of the kinematic variational principle [4,5] was proposed to construct the governing equations and to formulate a mathematical statement for the consistent models, which are to satisfy the conditions mentioned earlier. The expression for the virtual work due to the internal forces is written, spectrum of the internal forces is to be determined by the undetermined Lagrange coefficients corresponding to the introduced kinematics restrains. The following system of the kinematical equations was considered as kinematical constrains: (i) the Cauchy relationships for distortion tensor; (ii) the conditions are known as the non-homogeneous Papkovich's equations. As a result, a model for a continuum with non-free deformations was obtained. Note that it is defects (dislocations) preserving continuum theory. Generally, this variation technique allows us to describe the scale effects of various types corresponding to exponential changeability and various nature of interaction.

Recall that the purpose of this work is the description of non-classical reinforcement effect for the filled composites with taking into consideration the interactions of local cohesion type at the bound of two phases. Thus, in this work, the interactions of superficial adhesion types [4] are not considered. Nevertheless, it is shown that cohesion interactions define properties of an interphase layer in the filled composites. To describe the cohesion interactions in materials in the framework of the general dislocations preserving continuum theory, the particular variant of the model of pseudo-continuum with symmetric stress tensor was proposed [5]. The variation statement of this model is based on the following variational equation for the Lagrange functional, L:

$$\delta L = 0, \quad L = A - \frac{1}{2}\iiint \left[2\mu\gamma_{ij}\gamma_{ij} + \left(\frac{2\mu}{3} + \lambda\right)\theta^2 + 8\frac{\mu^2}{C}\xi_{ij}\xi_{ij} + \frac{(2\mu+\lambda)^2}{C}\theta_i\theta_i \right] \mathrm{d}V \qquad (1)$$

Here, R_i are the components of the displacement vector, γ_{ij} and θ are the components of the deviator of strain and spherical deformation tensor, ω_k are the components of the rotation vector, $Э_{ijk}$ is the Levi-Civita tensor, δ_{ij} is the Kronecker delta,

$$\omega_k = -\frac{1}{2}\frac{\partial R_i}{\partial x_j}\ni_{ijk}, \quad \frac{\partial \omega_i}{\partial x_j} = \xi_{ij} + \frac{1}{3}\xi\delta_{ij} - \xi_k \ni_{ijk}, \quad \frac{\partial \theta}{\partial x_j} = \theta_j,$$

μ, λ are the Lame coefficient, and C is the physical constant that determine the cohesion interactions.

It is worth emphasizing that the model proposed contains only one new physical constant C as compared to the classical theory of elasticity. This constant has the dimensions that differ from the dimensions of the Lame coefficients, and differs from them on a square of length. In the work [5], it was shown that the constant C is related to conventional parameters of the fracture mechanics for a brittle material. In the given work, material mechanical and geometrical characteristics of an interphase layer will be defined with the help of this constant model for each of phases in a composite.

The considered variant of statement of the variational Eq. (1) gives us the following mathematical formulation of the continuum theory which takes into account the interactions of cohesion type [4]:

$$\iiint \left\{ L_{ij}\left[-\frac{l_0^2}{\mu} L_{ij}(\cdots) + \delta_{jk}(\cdots) \right] R_k + P_i^V \right\} \delta R_i \mathrm{d}V + \oiint \left[M_i \delta \frac{\partial R_i}{\partial x_q} n_q \mathrm{d}F + Y_i \delta R_i \right] \mathrm{d}F = 0. \quad (2)$$

Here, $l_0^2 = \mu/C$ and

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

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

Δ is the Laplace operator, P_i^V is the vector of density of the external loads over the body volume, P_i^F is the vector of density of the surface load, n_i are the components of the normal vector of the boundary surface F and $L_{ij}(\cdots)$ is the operator of the classical theory of elasticity, that is,

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

2. The approached estimation of elastic modulus of periodic structure

The problem of determination of properties of periodic structures is investigated within the framework of the statement of the cohesion field model. Let us consider the formal one-dimensional statement of the problem. Projections of the load and displacement vector are collinear to the longitudinal axis, X_i: $R_i = rX_i$. Then, the variational Eq. (2) is reduced to

$$\int_0^l EF\left(r'' - \frac{E}{C} r''''\right)\delta r \mathrm{d}x + \left\{ -EF\frac{E}{C}\ddot{r}\delta\dot{r} + \left[P - EF\left(\dot{r} - \frac{E}{C}\dddot{r}\right) \right]\delta r \right\} \Bigg|_{x=0}^{x=1} = 0 \quad (3)$$

Let us now consider a periodical structure, which consists from N fragments of the matrix (with the characteristics E_M and C_M) and N fragments of the reinforced material (with the characteristics E_D and C_D) and establish the estimation of the effective rigidity for this composite material. To do this, at the first stage, we shall construct the solution for each of phases of representative fragment of the composite. For a model one-dimensional problem (3) such solutions can be found easily in the analytical form. At the second stage, we can obtain the exact solution for a fragment consisting of two phases with regarding all the conditions of contact. At the boundary of contact of phases, the displacements are equal, the normal derivatives of displacements are equal, the classical stresses (static multipliers at the variation of displacements δr) are equal, and the 'moments' (static multipliers at a variation of rotations $\delta\dot{r}$) are also equal. Finally, knowing the solution for a compound fragment, we can arrive at the formula for its potential energy. We can also calculate the deformation energy of a composite material considering as a periodic structure in which an element of periodicity is the two-phase fragment. Comparing this relationship for energy with the deformation energy of the equivalent homogeneous fragment, we can find the effective Young's modulus of the equivalent fragment of material. In result, we can obtain the following equation for the effective modulus:

$$E_0 = \frac{1}{\left[\frac{1}{E^M}\frac{l_M}{(l_M+l_D)} + \frac{1}{E^D}\frac{l_D}{(l_M+l_D)} - 2E_f N \frac{x_f}{(l_M+l_D)} \right]}, \quad (4)$$

$$E_f = \frac{\left[E^D a_M \frac{(1+\mathrm{e}^{-2a_M l_M^0})}{(1-\mathrm{e}^{-2a_M l_M^0})} + E^M a_D \frac{(1+\mathrm{e}^{-2a_D l_D^0})}{(1-\mathrm{e}^{-2a_D l_D^0})} \right]}{\left[a_D \frac{(1+\mathrm{e}^{-2a_D l_D^0})}{(1-\mathrm{e}^{-2a_D l_D^0})} + a_M \frac{(1+\mathrm{e}^{-2a_M l_M^0})}{(1-\mathrm{e}^{-2a_M l_M^0})} \right]}, \quad (5)$$

$$x_f = \frac{(E^D - E^M)}{\left[E^D a_M \frac{(1+\mathrm{e}^{-2a_M l_M^0})}{(1-\mathrm{e}^{-2a_M l_M^0})} + E^M a_D \frac{(1+\mathrm{e}^{-2a_D l_D^0})}{(1-\mathrm{e}^{-2a_D l_D^0})} \right]},$$

$$a_M = \sqrt{\frac{C_M}{E_M}} \quad a_D = \sqrt{\frac{C_D}{E_D}}.$$

Here, the parameter N shows the number of contact boundaries of phases along each of the coordinate axes (the number of fragments of the reinforced material along each of axis); E_M, E_D, and E_0 are the Young moduli of the matrix, the inclusions, and the composite, respectively; f is the volume fraction of inclusions; l_D is the total length of the inclusions; l_D^0 is the characteristic diameter of an individual inclusion, l_M^0 is the length of the matrix between two nearest individual inclusions, E_f determines the Young's modulus of interphase layer, x_f is a specific parameter associated with the length of the interphase layer determined by the parameters of the cohesion field for the matrix and the inclusions; the parameters a_M and a_D determine the length of the cohesion interactions in the matrix and the inclusion, respectively.

Formula (4) is of general type. It allows us to estimate the modulus of elasticity of periodic structures in the framework of the unidirectional statement for an arbitrary value of volume fraction of the inclusions and for an arbitrary ratio between fractions of the matrix and the inclusions. It is important to note that Eqs. (4) and (5) show dependence of modulus of elasticity at distances of the order of the size of inclusions. Properties of an interphase layer and effective properties of a composite as a whole depend on the ration of the moduli of elasticity of the phases, on the dimensional parameters of the model associated with non-classical effects a_M and a_D, (or C_M and C_D), the volume fraction of inclusions f, and also depend on the size of inclusions l_D^0. Dimensional parameters of the model a_M and a_D define the properties of a given matrix and the properties of a given inclusion. These parameters are supposed to be determined as a result processing of experimental data for all the spectrum of the volume fractions of inclusions and diameters of inclusions.

For reliability, it is desirable to base the results on the results of experiment, which describe properties of a composite material with the fixed mechanical properties of phases, but for various volume fractions of inclusions and the various sizes of inclusions. In the work [10], such data are presented for two types of composites strengthened by glass particles with two various kinds of matrix: (1) epoxy resin; (2) unsaturated polyester. Having found the parameters a_M and a_D, found as a result of the processing of experimental data (the inverse problem), we can construct theoretical dependences for effective characteristics of the filled composites. If the model describes the behavior of a considered composite material adequately, the theoretical dependences obtained will give good agreement with the experimental data for all spectrums of changes of the volume fraction of inclusions and the sizes of inclusions. Thus, the theoretical dependences can be used for prediction of the properties composite materials with given characteristics of the matrix and inclusion if the volume fraction of inclusions and the size of inclusions are changed.

Furthermore, it worth noting that Eqs. (4) and (5) allow us to consider a special case when the size of inclusions and the size of a layer of the matrix separated the inclusions considerably exceeds lengths of corresponding cohesion zones: $a_M(x_1-x_0)\gg 1$ and $a_D(x_2-x_1)\gg 1$. In this case, the parameters of an interphase layer are defined with the aid of the following simple equations (instead of formulas (4) and (5)):

$$E_f = \frac{[E^D a_M + E^M a_D]}{[a_D + a_M]} \qquad x_f = \frac{(E^D - E^M)}{[E^D a_M + E^M a_D]} \tag{6}$$

Effective properties of a composite material can be defined using the following formula:

$$E_0 = \frac{E^M}{\left[1 - \frac{(E^D - E^M)}{E^D} f\left(1 + \frac{2x_f}{l_D^0}\right)\right]} \tag{7}$$

Eqs. (6) and (7) are simpler in comparison with Eqs. (4) and (5). In contrast to Eq. (4), it is possible to assume that the effective modulus of a material here is defined with the aid of only one additional independent parameter of the model x_f. This parameter varies independent of the volume fraction of inclusions. In this case, formulas (6) and (7) are thought to give us the micromechanical description of the filled composites with the small volume fraction of inclusions. Then, the general Eqs. (5) and (6) correspond to the nano-mechanical description of materials.

3. Identification problem

Let us consider the problem of determination of mathematical model parameters based on formula (5). From mathematical point of view, the problem of determination of parameters of a model such that theoretical data fit experimental data is an inverse problem. It is formulated as a variational problem: find a set of parameters that minimize some cost function. The model parameters α may be determined from minimization of a cost function Φ: $\min_{\alpha\in[0,\infty]} \Phi(\alpha)$. In the common case of nano-mechanical description, the set of the model parameters α is defined by the following values: a_D and a_M. The parameters of a composite material f, l_D^0, E_M, E_D should be known for a specific material. In particular, for the micromechanical description it is worth noting that the set of parameters of the model α is defined by one parameter x_f (6), (7). The length x_f of interphase cohesion zone is supposed to be an unknown constant parameter of the mathematical model.

Assume that we have the set of experimental points K with the coordinates $(E^e,f^e,R^e)_1,(E^e,f^e,R^e)_2,\ldots,(E^e,f^e,R^e)_K$, where $l_D^0=2R$ is the length of reinforcing element. The problem of identification of parameters of the mathematical model may be formulated as follows: find the set of parameters α such that the 'distance' between experimental set of points with the coordinates $(E^e,f^e,R^e)_K$, $K=1,2\ldots$, and the theoretical set of points $(E^t,f^e,R^e)_1$, $(E^t,f^e,R^e)_2,\ldots$ must be minimum. The 'distance' between experimental set of points and theoretical set of points is defined as the cost function $\Phi(\alpha)$. For solving the identification problem ('data assimilation problem'), we used the experimental data from the work [10]. The graphic data from Ref. [10] were processed with the help of special software and represented in numerical form convenient for solving the identification problem. The definition of a cost functional is important part of the problem of the model parameter identification. The influence of different cost functions on the model parameters were carried out for approximate description of composite structures. The comparative estimation of the following cost functions was carried out:

$$L_2 = \frac{1}{K}\sqrt{\sum_{i=1}^{K}[E^t - E_i^e]^2}, \quad \Phi = \sum_{i=1}^{K}\frac{1}{K}[E_i^t - E_i^e]^2,$$

$$\text{and } C_{\text{abs}} = \max_{1\le i\le K}|E^t - E_i^e|, \quad C_{\text{rel}} = \max_{1\le i\le K}\left|\frac{E^t - E_i^e}{E_i^e}\right|.$$

The large quantity of numerical results allowed us to get a conclusion that the best results may be obtained on the basis of the following cost function:

$$\Phi = \sum_{i=1}^{K}\frac{1}{K}[E_i^t - E_i^e]^2.$$

Taking into account the experimental data [10], the parameters of mathematical model were determined for two kinds of composite materials: (1) the composite material based on epoxy resin reinforced by glass fraction: $E_M = 3.41$ GPa, $E_D = 87.5$ GPa; (2) the composite material based on nonsaturated polyester reinforced by glass fraction: $E_M = 4.29$ GPa, $E_D = 87.5$ Gpa. A plot of the experimental data for two kinds of composites is shown in Fig. 1a and b. Lines correspond to various diameters of inclusions: $R^e = 138.50$ μm, $R^e = 89.40$ μm, $R^e = 62.30$ μm, $R^e = 61.40$ μm, $R^e = 31.90$ μm, $R^e = 28.50$ μm.

The minimization of function Φ was carried out numerically with the aid of the conjugate gradient technique [11]. The parameters the mathematical model a_D and a_M (for nano-mechanical approach) and x_f (for micromechanical approach) were determined for two kinds of composite materials. The following values of the model parameters were received for nano-mechanical description: (1) $a_D = 3.51\times10^{-2}$ μm^{-1}, $a_M = 1.0\times10^{-3}$ μm^{-1} for the composite material with epoxy resin and (2) $a_D = 2.19\times10^{-1}$ μm^{-1}, $a_M = 2.77\times10^{-3}$ μm^{-1} for the composite material with unsaturated polyester. To obtain micromechanical description, we also found the formal parameter x_f: (1) $x_f = 27.63$ μm, for the composite material with epoxy resin and (2) $x_f = 37.06$ μm for the composite material with unsaturated polyester. Having found the values of the model parameters for two types of composites, we obtain the theoretical dependences for the moduli of elasticity. The theoretical values of the effective Young's modulus of composites are plotted in Figs. 2 and 3 as functions of the volume fraction for various values of the diameters of inclusions. The curves corresponding to the exact nano-mechanical description are shown as dashed lines. For comparison, we represent in Figs. 2 and 3 the dependences, which correspond to the micromechanical description (solid lines). These dependences are true only for small values of a volume fraction of inclusions. In addition, the experimental data specified by asterisks are shown in these figures.

4. Results and discussion

In accordance with the results obtained and graphs represented in Figs. 2 and 3, we may make the following conclusions. The theoretical results obtained in the framework of general model and calculated by formulas (5) and (6) are in good agreement with experimental data over the whole range of values of volume fraction of inclusions and over the whole range of sizes of inclusions under consideration. This conclusion holds true for the both types of composite materials under consideration. A particular case of the general model, micro-mechanic description, may be obtained on the basis of formulas (6) and (7); the dependences obtained in this case are in good agreement with experiments for small values of the volume fraction of inclusions. Recall that formulas (4) and (5) are obtained on the basis of the exact solution in the framework of one-dimensional model that takes into consideration

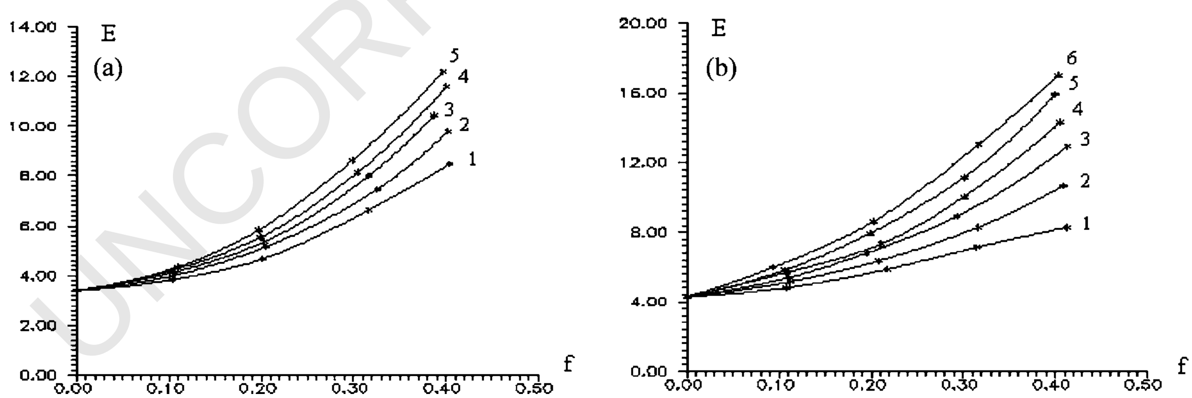

Fig. 1. Experimental date. Young's modulus (Gpa) as function of inclusion volume fraction f: (a) epoxy resin (1, $R^e = 138.50$ μm; 2, $R^e = 89.40$ μm; 3, $R^e = 62.30$ μm; 4, $R^e = 31.90$ μm; 5, $R^e = 28.50$ μm); (b) nonsaturated polyester (1, $R^e = 138.50$ μm; 2, $R^e = 89.40$ μm; 3, $R^e = 76.40$ μm; 4, $R^e = 62.30$ μm; 5, $R^e = 31.90$ μm; 6, $R^e = 28.50$ μm).

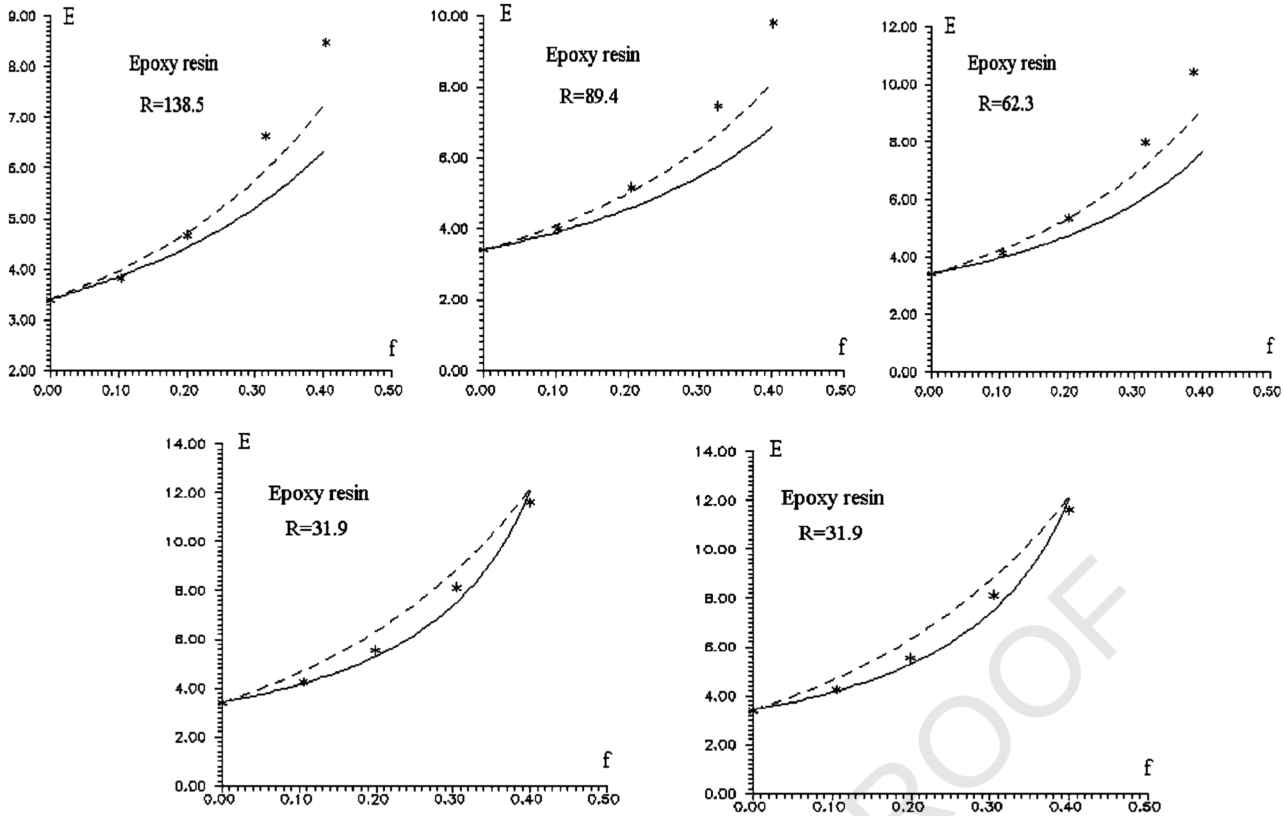

Fig. 2. Young's modulus (Gpa) of Epoxy resin reinforced by Glass inclusions as function of volume fraction *f*.

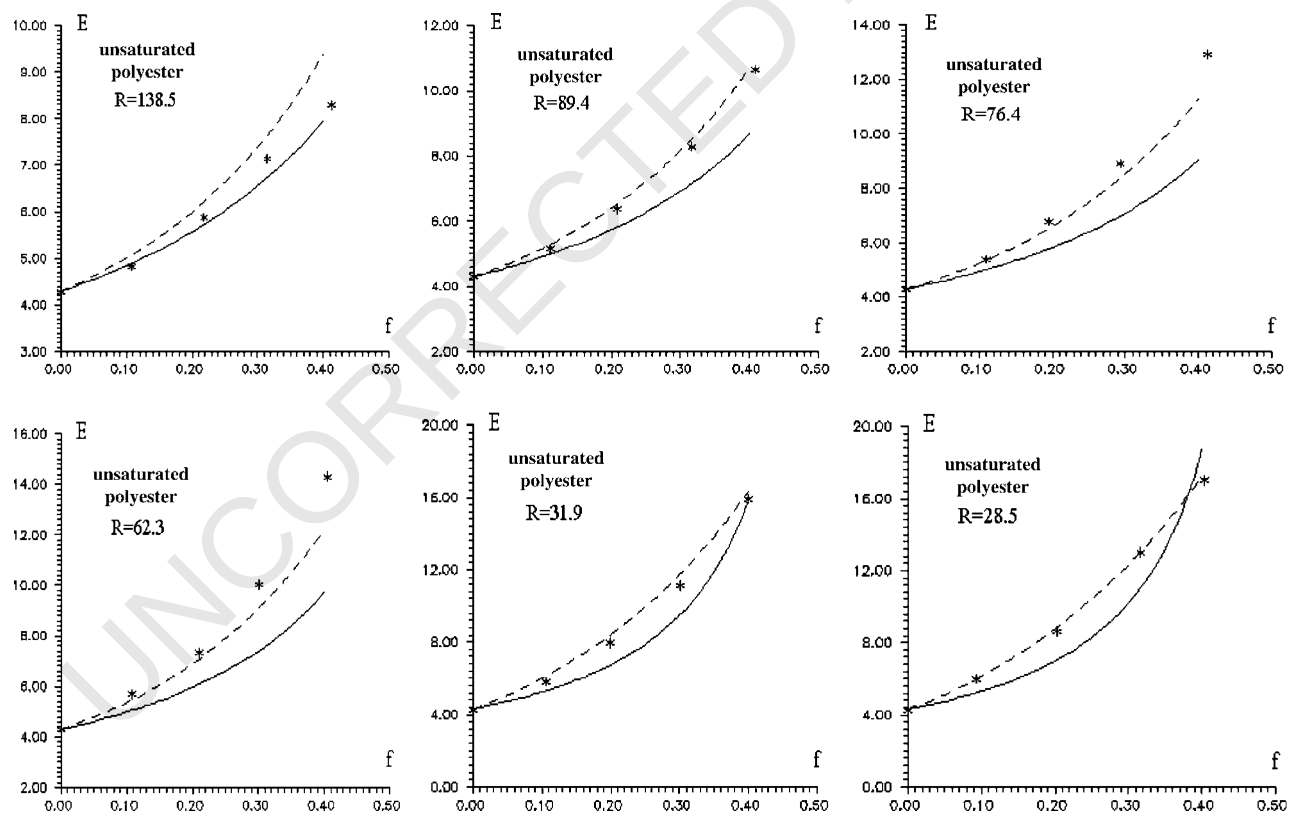

Fig. 3. Young's modulus (Gpa) of unsaturated polyester reinforced by Glass inclusions as function of volume fraction *f*.

inter-phase cohesive interactions. The adventure of this simple solution is that it may be represented analytically. It is obvious that this approach allows us to get not exact but approximate estimations of the effective characteristics in the framework of three-dimensional model proposed. Nevertheless, from the graphs shown in Figs. 2 and 3 we can see that these estimates are accurate enough. It is worth noting that, on the one hand, formulas (4) and (5) are obtained on the basis of one-dimensional statement but, on the other hand, they correspond to the exact solution and, consequently, these formulas are true over the whole range of values of volume fraction of inclusions. Considering the results obtained it should be also noted that the solution of the problem of identification allows us to get the values of the model parameters for the inter-phase layer a_D and a_M. It is established that $a_M < a_D$ for the both types of composite materials. Taking into consideration that the parameters a_D^{-1} and a_M^{-1} have the dimensions of length and, in fact, determine the length of the inter-phase cohesive layer in the matrix and in the inclusion, we can see that the values of these parameters obtained are in good agreement with the physical sense of the inter-phase layer. The inter-phase layer is generated in the each of phases in the neighborhood of the contacting zone; at that, the depth of the inter-phase layer in the matrix (the phase with smaller rigidity) is greater as compared to the depth of the inter-phase layer in the inclusion (the phase with greater rigidity).

Let us discuss the qualitative properties of the proposed model. Generally speaking, the problem of determination of the effective parameters of a composite composed of homogeneous matrix and small amount of inclusions is solved [12–15]. To take into account the finite quantity of the concentration, we may use one of the following methods: the Mori-Tanaka method (the method of equivalent inclusions) [15], the self-consistent method (the method of equivalent matrix) [16,17], and the method based on the analysis of periodic structures [18–21]. The publications devoted to the study of effective characteristics of composites may be conventionally subdivided into three groups: the method of effective inclusions, the method of effective matrix, and the method based on the hypothesis of three phases [22]. Let us now demonstrate that the model of inter-phase layer proposed in this work include all the three methods mentioned as its consequence. Let us consider one-dimensional statement for a two-phase structure. In this case, in accordance to the classical theory for a two-phase fragment, we can use the Reuss formula for determination of effective properties of a composite. In the case of two-phase material, the modification of this formula based on some additional hypotheses (the method of effective inclusions, the method of effective matrix) is in contrast with the theory of elasticity. The theory of cohesion layer is a non-classic generalization of the theory of elasticity. In the present work, employing the theory of cohesion layer, we obtain a formula (4) that is similar to the Reuss formula. Consider the relationship for generalized rigidity (4) (the generalization of the Reuss formula) and rewrite it as follows:

$$\frac{l}{E} = \frac{(l_M - 2Nx_f)}{E^M} + \frac{(l_D + 2Nx_f)}{E^D},$$

$$x_M = a_M^{-1}\mathrm{th}(a_M l_M/N), \quad x_M = a_D^{-1}\mathrm{th}(a_D l_D/N),$$

$$l = l_D + l_M,$$

$$x_f = x_D x_M (E^D - E^M)(E^D x_D + E^M x_M)^{-1},$$

$$E_f = (E^D x_D + E^M x_M)(x_D + x_M)^{-1}$$

The model of effective matrix, the model of effective inclusion, and the model of three phases can be obtained as a consequence of this formula. In accordance with the model of effective matrix, we get the following values of effective rigidity:

$$\frac{l}{E} = \frac{l_M}{E_*^M} + \frac{l_D}{E^D};$$

here, the effective modulus of the matrix E_*^M can be calculated from the relationship

$$\frac{1}{E_*^M} = \frac{1}{E^M} - \left(\frac{1}{E^M} - \frac{1}{E^D}\right)\frac{2x_f}{l_M/N}.$$

In accordance with the model of effective inclusion, the modulus of a composite can be determined by the formula

$$\frac{l}{E} = \frac{l_M}{E^M} + \frac{l_D}{E_*^D}$$

and the effective modulus of inclusion E_*^D can be determined by the formula

$$\frac{1}{E_*^D} = \frac{1}{E^D} - \left(\frac{1}{E^M} - \frac{1}{E^D}\right)\frac{2x_f}{l_D/N}.$$

In accordance with the model of three phases, the modulus of a composite can be determined by the formula

$$\frac{l}{E} = \frac{l_M^*}{E^M} + \frac{l_D^*}{E^D} + \frac{l_f}{E_f},$$

where the properties of the phases are determined by the moduli E^M, E^D, and E^f, respectively, and the lengths of the phases are $l_M^* = l_M - 2Nx_M$, $l_D^* = l_D - 2Nx_D$, and $l_f = 2N(x_M + x_D)$. Thus, using the model of inter-phase layer, we have an opportunity to provide some grounding in theory for the hypotheses discussed earlier.

5. Conclusion

Employing the non-classic generalized theory of elasticity, we propose the model of inter-phase layer that takes into account scale effects. We obtain the relationships for the effective rigidity of composite materials. It is shown that theoretical results are in good agreement with experimental data and thus may be used in the prognosis of the behavior of a composite in the wide range of values of concentration and diameters of particles. The model of inter-phase layer allows us predict the properties of filled composites both for the case of small concentration and for the case of large concentration, for arbitrary relations between rigid phases, for a wide range of sizes of inclusions (non-classic behavior). All the results may be obtained in the framework of unified approach with no additional hypotheses. Using this theory, we can determine the parameters of an inter-phase layer, its length, and the modulus of elasticity. At that, the parameters of the inter-phase layer are completely determined by classic and non-classic properties of the phases.

Acknowledgements

The work supported by the European Office of Aerospace Research and Development, Int. Grant (N2154p).

References

[1] Zhang P, Huang Y, Geubelle PH, Klein PA, Hwang KC. The elastic modulus of single-wall carbon nanotubes: a continuum analysis incorporating interatomic potentials. Int J Solids Struct 2002;39: 3893–906.

[2] Odegard GM, Gates TS, Nicolson LM, Wise K. Equivalent-continuum modeling with application to carbon nanotubes 2002. NASA, TM-2002-211454.

[3] Gao H, Huang Y, Nix WD, Hutvhinson JW. Mechanism-based strain gradient plasticity-I. Theory. J Mech Solids 1999;47:1239–63.

[4] Lurie S, Belov P, Volkov-Bogorodsky D, Tuchkova N. Nanomechanical modeling of the nanostructures and dispersed composites. Int J Comp Mater Sci 2003;28(3-4):529–39.

[5] Lurie S, Belov P, Volkov-Bogorodsky D. Multiscale modeling in the mechanics of materials: cohesion, interfacial interactions, inclusions and defects. In: Wendland LW, editor. Analysis and simulation of multifield problems, 12. Berlin: Springer; 2003, p. 101–10.

[6] Bodunov A, Belov P, Lurie S. Scale effects in the thin films. J Compos Mater Struct VIMI 2002;2:33–40.

[7] Belov P, Lurie S. On modeling of scale effects in thin structures. Mech Compos Mater Struct 2002;8:78–88.

[8] Thostenson ET, Ren Z, Chou TW. Advances in the science and technology of carbon nanotubes and their composites: a review. Compos Sci Technol 2001;61:1899–912.

[9] Tibbetts GG, McHugh JJ. Mechanical properties of vapor-grown carbon fiber composites with thermoplastic matrices. J Mater Res 1999;14:2871–80.

[10] Miva M. Influence of the diameters of particles on the modulus of elasticity of reinforced polymers. Kobunshi Ronbunshu 1978;35(2): 125–9.

[11] Grachov NI, Evtushenko YG. A library of programs for solving optimal control problems. J Comp Math Math Phys 1980;19:99–119.

[12] Mura T. Micromechanics of defects in solids. Boston, MA: Martinus Nijhoff Publishers; 1982.

[13] Li Tucker III CL, Lang E. Stiffness predictions for unidirectional short-fiber composites: review and evaluation. Comp Sci Technol 1999;59:655–71.

[14] Odegard GM, Gates TS. Constitutive modeling of nanotube/polymer composites with various nanotube orientation In: Proceedings Annual Conference on Experimental and Applied Mechanics, June, Milwaukee, WI 2002.

[15] Mori T, Tanaka K. Average stress in matrix and average elastic energy of materials with misfitting inclusions. Acta Metallurg 1973;21: 571–4.

[16] Wakashima K, Otsuka M, Umekawa S. Thermal expansion of heterogeneous solids containing align ellipsoidal inclusions. J Compos Mater 1974;8:391–404.

[17] Budiansky B. On the elastic moduli of some heterogeneous materials. J Mech Phys Solids 1965;13:223–7.

[18] Bensoussan A, Lions JL, Papanicolau G. Asymptotic analysis for periodic structures. Amsterdam 1978.

[19] Nemat-Nasser S, Iwakuma T, Hejazi M. On composite with periodic structure. Mech Mater 1982;1(3):239–67.

[20] Nunan KC, Keller JB. Effective elasticity tensor of a periodic composite. J Mech Phys Solids 1984;32(4):259–80.

[21] Sangini AS, Lu W. Elastic coefficients of composites containing spherical inclusions in a periodic array. J Mech Phys Solids 1987; 35(1):1–21.

[22] Riccardi A, Montheillet F. A generalized self-consistent method for solids containing randomly oriented spheroidal inclusions. Acta Mechanica 1999;133:39–56.