

Comparative Computer Modeling of Carbon-Polymer Composites with Carbon or Graphite Microfibers or Carbon Nanotubes

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Abstract: The basic approach is offered for problems of nanocomposites and their mechanical properties, which includes a short review of modern problems in nanomechanics of materials. The fibrous carbon-polymer composites with carbon or graphite microfibers or carbon nanotubes are especially discussed. The basic model of the linear or nonlinear elastically deforming micro- and nanocomposites is considered. Within the framework of this model, the comparative computer modeling is performed. The modeling permits to observe the features in prediction of values of basic mechanical constants. These results are utilized on next step of modeling – studying the peculiarities of wave propagation in particular fibrous micro- and nanocomposites under consideration.

Keyword: Micro- and nanomechanics of materials, basic approach, fibrous carbon-polymer composite, continuum models, mechanical properties, comparative analysis.

1 Description of the problems. Basic approach

When being invented not long ago [Wilson et al. (2002)], the atomic force and scanning electron microscopes allow to see the atoms and transform therefore during last two decades significantly the nanotechnology – from the field of futuristic sciences [Drexler (1990)] it was gone to the modern natural science (first of all, to physics and chemistry) [Harris (2000); Dresselhaus et al. (2001); Nalva (2000); Wilson et al. (2002)]. Ac-

tually the increasing number of scientists from the wide spectrum of natural sciences is turning the attention to the objects of nanolevel. The main practical (a practicalness becomes the predominating position of the scientific community) goal of such interest is the possibility of quick application of new knowledge about nanoobjects in diverse technologies; it is assumed in connection with which that the investigations can be referred to nanotechnologies. The leading world countries considered the development of nanotechnologies as being a great priority and have the special programs on nanotechnologies with very high level of finance. The majority of results are associated with studying the nanoformations physicists, chemists, and scholars from material science.

Attracting mechanics to investigations of nanomaterials is the necessary moment in development of nanotechnologies and nanomaterials and has the goal to provide the transition from nanomaterials to structural members made of nanomaterials. It must be note that even precision devices consist always of separate structural members. Probably, it can be assumed that nanomaterials as engineering materials have a perspective of application only in the form of nanocomposites in which nano-materials are used as the fillers.

Let us consider in this connection some problems of mechanics of nanocomposites. At that a matrix will be considered as made of polymeric materials what is generally accepted in the most part of publications on nanocomposites.

As it is noted in [Guz and Rushchitsky (2003)], in the general system of knowledge on materials, *the mechanics of nanocomposites* can be related to *the structural mechanics of materials*. Structural mechanics of materials is understood as that section of mechanics of materials in which the ba-

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sic relationships include the parameters characterizing the internal structure of materials. It is well-known that in majority of investigations on mechanics of materials, the information about internal structure is used only at the step when obtained results being interpreted.

In dependence on sizes of inhomogeneities in the internal structure of materials, the structural mechanics can be divided on *macromechanics*, *mesomechanics*, *micromechanics*, and *nanomechanics*. Taking into account the results of numerous publications the following classification of the *admissible range of changing the characteristic size of inhomogeneities in the internal structure of materials*.

macro: $10^{-2} - 10^{-5}$ m (from 1 cm till $10 \mu\text{m}$);
 meso: $10^{-3} - 10^{-8}$ m (from 1 mm till 10 nm);
 micro: $10^{-4} - 10^{-8}$ m (from $100 \mu\text{m}$ till 10 nm);
 nano: $10^{-7} - 10^{-9}$ m (from 100 nm till 1 nm).

was proposed in [Guz and Rushchitsky (2003)].

Schematically this classification is shown on Fig.1.

In conformity with classification (scale) under consideration equally with macro-, meso-, micro-, and nanomechanics the *micro-*, *meso-*, *micro-*, and *nanocomposites* can be considered. The proposed classification is conditional enough although also convenient enough in description of approaches and concrete results.

When constructing the foundations of mechanics of nanocomposites, there exist on author's opinion four spheres of basic problems: 1. Description of properties of nanoformations. 2. Description of properties of a matrix (a polymer binder). 3. Description of phenomena on interfaces of nanoformations and a matrix. 4. Determination of averaged properties of nanocomposites permitting the transition to mechanics of structural members. The terms *description* and *determination* are understood as the construction of mechanical models permitting to describe and to determine the mechanical phenomena and properties. Below in quite brief terms the mentioned four spheres of basic problems will be considered.

It is necessary to note that at present time the nu-

merous publications on mechanics of nanomaterials and nanocomposites exist. In this connection we will refer later to some reviews on these subjects only.

1.1 Description of properties of nanoformations

All nanoformations are constituted as the systems of atoms which interact with each other by forces of interatomic interaction. The carbon nanotubes (CNT) are the most prevailing and widely discussed in scientific investigations nanoformations; there are considered the single-walled (SWCNT) and multi-walled (MWCNT) carbon nanotubes. Fairly often the nanoformations are considered, fabrication of which is realized by mechanical joining up a few CNT; for example, so called nanowires. The ratio of a length of nanoformations to their diameter is changed within the wide range – from more than one thousand to the case when these sizes are comparative with each other. Thus the models both the infinitely long fibers and the separate granules can be applied.

In all cases the nanoformations are a discrete system consisting of separate atoms. At present, different theoretical and experimental methods for studying the nanoformations are evaluated and widely utilized. In theoretical methods, the Cauchy-Born approach [Born and Huang (1954)] is used when potentials of interatomic interaction of concrete structure (Tensoff-Brenner potential, Morse modified potential and so on) are getting. When such an approach being used, then as if averaging of properties is carried out and purely discrete medium consisting of separate atoms is changed on the continuum what is testified by the next situation. Following the application of this approach the information about Young modulus, Poisson ratio, density of material, geometrical sizes of nanoformations and so on – the parameters and coefficients characteristic for the continuum – is obtained. The mentioned procedure can be quite grounded called *the principle or process of continualization*. Probably, this term was for the first time used applied to nanoparticles in publication [Guz and Rushchitsky (2003)].

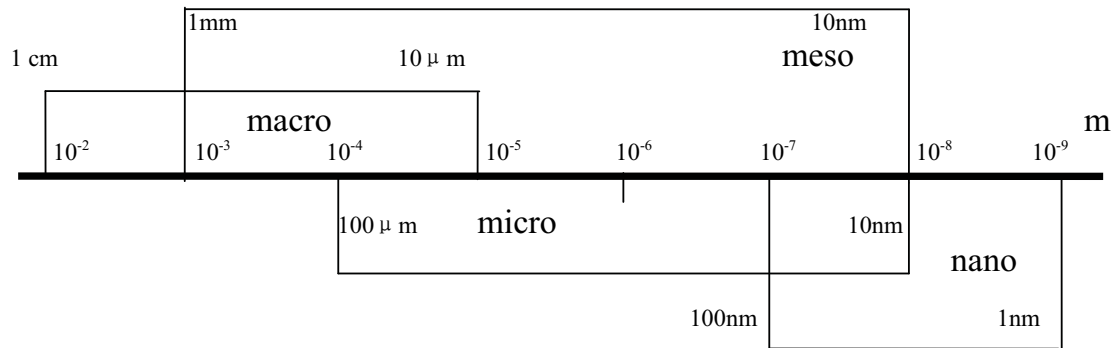


Figure 1: Scheme of belonging the structure of materials to the macro-, meso-, micro-, and nanoscales

A few experimental methods of determination of nanoformations properties exist. When they (methods of: thermal vibration, bending, tension et cetera) being utilized, then also the information on Young modulus, Poisson ratio and so on is obtained. Thus while the experimental methods being applied then also the information is obtained on parameters and coefficients, which are characteristic for continuum. So in this case the principle of continualization is as if applied.

It was obtained both in theoretical, and in experimental studies that for nanoformations (basically for SWCNT and MWCNT) the elastic deformations are characteristic. At that, the elastic deformations are running up to several tens percents under tension; the linear dependence between stresses and strains is remained up to the strain order 5-10 % . Under compression, the elastic deformations are observed up to reaching the values of strains with the order 5%. In existing publications, the mechanical properties of nanoformations are described in continuum approximation (after application of the continualization principle) mainly within the framework of the model of isotropic elastic body (isotropic elastic medium).

It should be noted also that for CNT the more adequate model is the model of transversally isotropic body with the isotropy axis coinciding with the CN?axis.

The review of results on experimental and theoretical determination of Young modulus for SWCNT and MWCNT is presented in [Zhang et al. (2004)]. The results on determination of Pois-

son ratio for zig-zag and armchair SWCNT are cited in [Xiao et al. (2005)]. Data on mechanical properties of nanoformations are cited also in review articles [Qian et al. (2002); Srivastava et al. (2003); Yakobson and Avouris (2001)], in separate chapters of collective mono-graphs [Dresselhaus et al. (ed) (2001); Harris (ed) (2000); Milne (ed) (2003); Nalwa (2000); Wilson et al. (2002)] and in a row of other publications.

From analysis of mentioned publications follows that the most common and relatively enough substantiated model for nanoformations (after application of continualization principle) is *the model of linear elastic isotropic body* with determination of all parameters corresponding to continuum concept.

Hereon by mentioned above comments as applied to description of properties of nanoformations we will restrict our self.

1.2 Description of properties of a matrix (a polymer binder)

When mechanics of nanocomposites being studied logically and consistently, then evidently it is necessary to consider the nanoformations and the matrix within the framework of kindred model representations.

It was noted above that the model of linear elastic isotropic body is applied for nanoformations on the final stage (in continuum approximation). In this connection, we will cite below some information on description of the polymer binder in continuum approximation too.

The large quantity of results for the matrix (the

polymer binder) in continuum approximation was obtained, when the fundamentals of micromechanics of microcomposites being created. This direction was actively discovered mainly in the second half of XX century. These results are expounded in numerous publications. For example, in collective multi-volume monographs [Broutman and Krock (ed) (1974-1975); Guz (ed) (1993-2003); Kelly and Zweben (ed) (2000); Milne et al. (ed) (2003)] and hand-books [Katz and Milewski (ed) (1978); Lubin (ed) (1982)] and a row of other publications. It can be therefore assumed that mentioned above results correspond in full measure to description of properties of the matrix (the polymer binder) in the case of nanocomposites with the polymer matrix also.

The analysis of cited publications show that the quite grounded model for the polymer matrix as applied to nanocomposites is *the model of linear isotropic elastic or viscoelastic body*. For temperate temperatures and relatively short-time action of the load the quite acceptable model for the polymer matrix is the model of linear isotropic elastic body.

Remark. Let us note that the linear dependence between stresses and strains in the polymer matrix can be kept up to the strain 1.5-2.5 % .

In mechanics of nanocomposites comparing, for example, with mechanics of microcomposites a fortiori with mechanics of composites of other structure, the additional situation arises as applied to polymer matrix. The point is that in nanocomposites comparing with microcomposites for one and the same volume fraction of fillers (for example, carbon nanotubes or graphite microfibrils) the significantly more interface between the matrix and fillers is formed. This can be explained by essential difference in sizes of inhomogeneities.

It is necessary to remember that in structural mechanics the notion of volume fraction of the matrix and fillers are introduced as applied to the representative volume or elementary cell and it doesn't depend naturally on absolute sizes of inhomogeneities.

The noted difference in interfaces is detecting when physical volumes of composites (for exam-

ple, micro- or nanosamples) being considered.

Let us consider this question at first with reference to unidirectional fibrous composites with fibers of circular cross-section. Let restrict the analysis by the case of long enough fibers, when the model "infinitely long fibers" is working. Then the analysis can be carried out in the plane of cross-section only (an elementary cell is marked out by the dotted line) as it is shown on Fig.2.

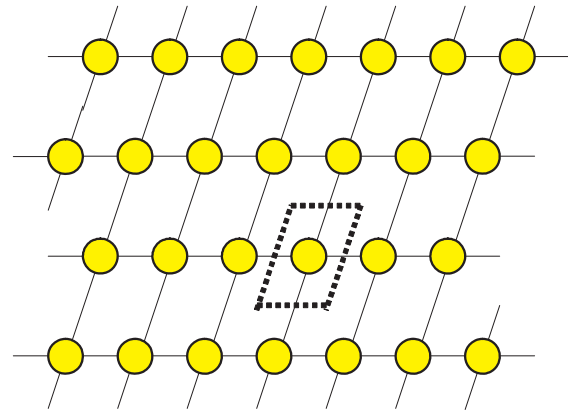


Figure 2: The plane of cross-section of unidirectional fibrous composite

Let us introduce the conventional notations for elementary cell or the representative volume: $v^{(f)}$ and $v^{(m)}$ – volumes of the material of fillers (fibers) and the matrix; $v = v^{(f)} + v^{(m)}$ – total volume; $c^{(f)}$ and $c^{(m)}$ – volume fractions of fillers and the matrix; s – area of interface with reference to the elementary cell. In this case the well-known expressions have a place

$$c^{(f)} = \frac{v^{(f)}}{v}, \quad c^{(m)} = \frac{v^{(m)}}{v}, \quad c^{(f)} + c^{(m)} = 1, \quad (1)$$

$$s = 2\pi r.$$

where r is the radius of fibers.

Let us consider the physical volume of composite, actually understanding it's as the sample of certain sizes. With the purpose of simplifying of expressions, let us choose the physical volume in the form of a circular cylinder and consider following the problem statement the plane of cross-section. In reference to the physical volume (the sample), the next notations can be in this case introduced: V - sample volume, D - sample surface,

S - total area of interfaces in the whole of sample, K - number of elementary cells in the sample volume, R - sample radius. Then the expressions are valid

$$S = Ks, \quad K = \frac{V}{v}, \quad D = 2\pi R, \quad V = \pi R^2. \quad (2)$$

It follows then from (1) and (2)

$$S = Ks = \frac{V}{v}s = s \frac{V}{v^{(f)}} c^{(f)}. \quad (3)$$

Taking into account the introduced notations and the form of the marked out elementary cell, the expression can be written

$$\frac{V}{v^{(f)}} = \left(\frac{R}{r}\right)^2. \quad (4)$$

From expressions (1)-(4) after some transformations the relationship for determination the value S (area of interfaces in the whole physical volume – sample) can be obtained in the following form

$$S = D \frac{R}{r} c^{(f)}. \quad (5)$$

Exactly the same expression follows from an analysis of the granular material with granules in the form of spheres. In this connection the next analysis seems to be general for typical unidirectional fibrous and granular composites.

Let us consider henceforward the physical volume (sample) one and the same sizes ($D = const$; $R = const$ in (5)) for micro- and nanocomposites. Let introduce the next notations:

r_N and $c_N^{(f)}$ – fiber radius and volume fraction of fibers for the nanocomposite; r_M and $c_M^{(f)}$ – fiber radius and volume fraction of fibers for the microcomposite; S_N and S_M – area of interfaces in the physical volume (sample) for nano- and macrocomposites. Taking into account the adopted notations and conditions, we obtain

$$S_N = D \frac{R}{r_N} c_N^{(f)}, \quad S_M = D \frac{R}{r_M} c_M^{(f)}. \quad (6)$$

According to Fig.1 for the lowest values r_N and r_M the next estimate can be assumed

$$10r_N \approx r_M. \quad (7)$$

It can be drawn the interesting conclusions from (6) and (7).

If the nano- and microcomposites with identical volume fraction of the fillers ($c_N^{(f)} = c_M^{(f)}$) are considered, then the relationship for areas of interfaces follows

$$S_N = \frac{r_M}{r_N} S_M, \quad S_N \approx 10S_M. \quad (8)$$

Thus in this case the increasing the area of interfaces in nanocomposites is observed on one order more than in microcomposites.

If the nano- and microcomposites with identical area of interfaces ($S_N = S_M$) are considered, then we obtain for volume fractions of the fillers

$$c_N^{(f)} = \frac{r_N}{r_M} c_M^{(f)}, \quad c_N^{(f)} \approx 10^{-1} c_M^{(f)}. \quad (9)$$

Thus in this case we obtain the essential (on the order) decreasing the fillers volume fraction in the nanocomposite as compared with the microcomposite.

The cited above estimates testify the urgency of developing the polymer matrix which will provide the effective adhesion in the case of significant increase of the interface area. Moreover these estimates testify the unreasonableness of studying the nanocomposites with high volume fraction of the fillers.

1.3 Description of phenomena on an interface of nanoformations and a matrix

In order to analyze the phenomena under consideration, it is convenient to introduce the notion of *geometrical interface* of nanoformations (as the filler) and the polymer matrix. The geometrical interface is understood as the surface, sizes and form of which are defined when the nanoformations being described in the continuum approximation.

When the nanoformations and the polymer matrix are united into the nanocomposite, the phenomena with involving the more deep mechanisms are occurring than it takes place, for example, in the case of microcomposites.

The point is that in the general case the nanoformations consist of the system of curvilinear layers; each of layers consists of the system of atoms

interacting with each other owing to forces of interatomic interaction.

In this connection, when the fillers and the matrix are united into the nanocomposite, then the interaction of atoms of the “extreme” layer of the atoms of nanoformations with nearest atoms of the polymer matrix (owing to forces of interatomic interaction) should evidently be displayed. In this way the consisting of interacting atoms of the nanoformations and the matrix thin intermediate layer is appearing. Studying the indicated phenomenon and determination of regularities which characterize the phenomenon seems to be the complicate and actual physical-chemical problem. Its solution can be realized by the representatives of corresponding scientific directions only.

When nevertheless the foundations of mechanics of nanocomposites being constructed, then for description of phenomena in the mentioned interface it will be expediently to use the traditional approaches of mechanics elaborated in the analysis of related problems. Traditionally in mechanics, the occurring in intermediate thin layers or on surfaces of thin bodies phenomena *are modeling by some boundary conditions*. At that *the boundary conditions “are carried” or “are taken to”* certain in some sense close but more simple surface.

Let us consider a few examples.

Example 1. In the classical theory of flow past a wing the boundary conditions on the wing surface “are taken on” the wing chord.

Example 2. In the theory of contact interaction of elastic bodies in the case when the stamp bottom has some deviation from the plane form, then the boundary conditions of contact interaction “are taken on” the plane boundary.

Example 3. In the problem of dynamical interaction of the liquid and elastic bodies (including thin-walled ones) the boundary conditions on the oscillating interface “are taken on” the fixed interface.

Taking into account the mentioned traditional in mechanics approaches and modeling the nanoformations and the matrix by continua, while the

foundations of mechanics of nano-composites being created, the next approach can be proposed, which corresponds to adopted in mechanics exactness.

It seems to be expedient the phenomena occurring at the thin intermediate layer between the filler and the matrix to model by certain boundary conditions of conjugation (interfacing) of two continua and take on or translate the mentioned conditions on the geometrical interface of the nanoformations and the matrix.

At that the establishment of concrete structure of the boundary conditions reflecting the phenomena in the interface is actually the problematical question, since physicists and chemists don't yet construct the quite substantiated theory of the mentioned phenomena.

Because of complexity of the problem on establishment of concrete structure of boundary conditions on geometrical boundary, the special topicality takes the development of two-sided estimates for given phenomena, which permit also to estimate the values of corresponding quantities under study.

From point of view of mechanics, the most “stiff” or perfect joining of two media (nanoformation – matrix) in continuum description corresponds to the conditions of full mechanical contact (continuity of displacement and stress vectors) on the interface. The most “mild” or imperfect joining of two media in continuum description corresponds to the conditions of “sliding” contact.

Thus *the study of nanocomposites for two indicated boundary conditions on the geometrical interface enables to obtain the two-sided estimates for quantities under study*, when different physical-chemical mechanisms being displayed in the interface.

It is necessary to emphasize that by using two mentioned boundary conditions the results in fracture mechanics of micro composites under compression were obtained when the start of the fracture process is defined by the phenomenon of stability loss into the internal structure of composite. Such type results were presented in the monograph [Guz (1990)] and in a row of other publica-

tions.

There is a need to note also that in mechanics of microcomposites the numerous problems exist, which are associated with necessity to ensure the corresponding adhesion strength on the interface. These problems are determined by different mechanisms in the intermediate layer. Nevertheless these mechanisms are not associated with manifestation of interatomic interaction forces in contrast to the nanocomposites where the influence of interatomic interaction forces in the intermediate layer can be essential.

1.4 Determination of averaged properties of nano-composites permitting the transition to mechanics of structural members

Cited above considerations on modeling the nanoformations, the matrix, and the conditions on interface can be used in studying the problems of statics, dynamics, stability, and fracture of nanocomposites within the framework of mechanics of nanocomposites with the polymer matrix. When such study being carried out, then the statement of problems and methods of solution can be used by analogy with corresponding approaches evaluated within the framework of mechanics of microcomposites (see, for example, the multi-volume collective (in 12 volumes) monograph [Guz (ed) (1993-2003)]. In such investigations, the model of piece-wise homogeneous medium and the model of medium with averaged properties can be applied traditionally.

When the study within the framework of mechanics of structural members made of nanocomposites being carried out, then apparently the most promising and may be the uniquely possible approach will be that one as the nanocomposite (piece-wise homogeneous material) is changed on the homogeneous material with averaged properties. In accordance with such an approach in problems of mechanics of structural members made of nanocomposites *the principle of homogenization* is applied preliminary or *the procedure of homogenization* is carried out, and the nano-composite is considered now as the homogeneous material with averaged properties.

It is to all appearance expediently to distinguish

two approaches to determination of averaged properties of nanocomposites: the first one – determination of reduced (averaged) properties within the framework of the model of anisotropic elastic homogeneous body; the second one – determination of averaged values of parameters appearing in more complicated structural models, for example, the model of mixture of materials.

As applied to nanocomposites when the reduced constants being determined within the framework of the first approach, then the statements of problems and the methods of investigations, which were elaborated for granular, fibrous, and layered microcomposites of determined and random structures, can be utilized. Such types of the statements of problems and the methods of investigations are expounded in numerous publications, for example, in corresponding volumes of collective multivolume monograph [Guz (ed) (1993-2003)].

It is necessary to note that in this case the values of averaged constants are asymptotically exact and follow under definite conditions from the strong results obtained within the framework of the three-dimensional theory.

With reference to the theory of wave propagation the cited conditions correspond to the situation, when the ratio of geometrical parameter characterizing the internal structure of nanocomposite to the wave length tends to zero, that is the situation as if corresponds to the long-wave approximation.

As applied to nanocomposites when the reduced constants being determined within the framework of the second approach, then should be noted that the theory of mixtures uses for determination of interaction of components the approximate approaches (as compared with the exact approach of the piece-wise homogeneous medium approach). Nevertheless the obtained basic relationships of the theory of mixtures permit to investigate in the theory of wave propagation in nanocomposites not only in the long-wave approximation, but for more wide range of wave lengths. Results on constructing different models of the theory of mixtures and investigation of a row of corresponding problems are presented in numerous publications. The basic relationships of the theory of

mixtures are offered, for example, in the monograph [Rushchitsky (1991)] and the review [Rushchitsky (1999)], where the basic publications on constructing the theory are also presented.

Let us note that above some comments as applied to the theory of wave propagation in nanocomposites are considered,

as an example only, when the analysis of the problem of determination of averaged properties in the process of homogenization being carried out. The similar situation is taken place in other problems of statics, dynamics, stability, and fracture of nanocomposites.

Remark. Above the terms “*principle, process, or concept of continualization*” and “*principle, process, or concept of homogenization*” are often used. Let us note in this connection that the principle, process, or concept of continualization consists in the substitution of the discrete system by some continuous one with determination of corresponding averaged properties within the framework of the continuous system. Analogously, the principle, process, or concept of homogenization consists in the substitution of the piece-wise homogeneous continuous system by some homogeneous continuous system with determination of corresponding averaged properties within the framework of the homogeneous continuous system.

Thus, principles, processes, or concepts of continualization and homogenization are utilizing for constructing the foundation of mechanics of nanocomposites with the polymer matrix and at the same time are differing in principle.

1.5 Basic approach

We will understand the basic approach as the aggregate of concepts, models and statements of problems, development of methods of investigation and obtaining the basic results, which are adequate to phenomena under consideration.

The produced above discussion and corresponding considerations testify to the next basic approach is quite ordinary when the foundations of mechanics of nanocomposites with polymer matrix are constructing.

The approach consists of four parts.

1. Modeling the nanoformations by the linear isotropic homogeneous body with averaged values of elastic constants obtained with utilization of the concept of continualization from results taking into account the action of forces of inter-atomic interaction.
2. Modeling the polymer matrix (binder) by the linear isotropic homogeneous elastic or viscoelastic body. Similar modeling was traditionally used when the foundations of mechanics of microcomposites were constructed. For temperate temperatures and comparatively short-time loading the polymer matrix can be modeled as applied to nanocomposites by the linearly elastic isotropic homogeneous body.
3. Modeling the interaction of the nanoformations and the matrix (in the thin intermediate layer with allowance for forces of inter-atomic interaction) by certain boundary conditions when these conditions being transferred on the geometrical interface. Application of the boundary conditions of the full (perfect) contact (continuity of displacement and stress vectors) and the boundary conditions of sliding contact for two-sided estimates of quantities under study.
4. Determination of averaged values of elastic constants for nanocomposites with utilization of different methods of homogenization what ensure the transition to mechanics of structural elements made of nanocomposites.

Thus, while the basic approach under discussion being realized, then investigations of different problems of statics, dynamics, stability, and fracture of mechanics of materials (nanocomposites) and mechanics of structural elements (made of nanocomposites) can be carried out.

In studying the problems of mechanics of nanocomposites, the model of piece-wise homogeneous medium (after realization of the concept of *continualization* for nano-formations) and

the model of homogeneous anisotropic body with averaged values of elastic constants (after realization of the concept of *continualization* for nanoformations and next realization of the concept of *homogenization* for obtained piece-wise homogeneous medium) is applicable.

In studying the problems of mechanics of structural elements made of nanocomposites the application of the model of homogeneous anisotropic body with averaged values of elastic constants (after realization of the concept of *continualization* for nanoformations and next realization of the concept of *homogenization* for obtained piece-wise homogeneous medium) is preferable.

There is no doubt that the analysis of multi-layered structural elements is important for mechanics of structural elements made of nanocomposites (for example, for constructing the models and theories of multi-layered rods, plates, and shells).

Nevertheless for each separate structural element (for each layer, for example) the model of homogeneous anisotropic body with averaged values of elastic constants (after realization of the concept of *continualization* for nanoformations and next realization of the concept of *homogenization* for obtained piece-wise homogeneous medium) is used.

Let us restrict ourselves in the undertaken discussion of constructing the foundations of mechanics of nanocomposites by the stated above in quite brief terms information.

Within the considered approach a number of new results are obtained. They are presented in publications of authors [Guz A.N. (2006); Guz A.N., Rodger and Guz I.A. (2005); Guz A.N. and Rushchitsky (2003); Guz I.A. and Rushchitsky (2004a,b,c)] and in a number of other publications; the related problems are considered in [Rushchitsky et al (2005); Rushchitsky (2005a,b,c)]. It is necessary to note that at present the row of review articles associated with different problems of mechanics of nanocomposites are already published; for example, [Buryachenko et al (2005); Lau and Hui (2002); Srivastava, Wei and Chao (2003); Thostenson, Chunyu and Chou

(2005)] and a row of other publications. Among review publications, it seems to be expedient to mark out the article [Thostenson, Chunyu and Chou (2005)] with significant title “Nanocomposites in context”, what is in harmony with the title “Composites in context” of well-known review [Kelly (1985)], published 20 years ago in the same journal *Composites Science and Technology*. Authors, when being analyzed the mechanics of nanocomposites, are noted also the mentioned above link.

Further in the paper some results of modeling of mechanical behavior of fibrous carbon-polymer composites with fillers in the form of carbon or graphite microfibers or carbon nanotubes are presented and discussed.

2 Basic structural models

As one of the first publications in the field of modeling the composite materials the Voigt publication of 1887 is considered, where the idea was advanced to evaluate of physical parameters with averaging the physical parameters of inhomogeneous material over the volume and orientation. In 1929 Reuss proposed the averaging of inverse tensors of physical properties of composites. Later in 1964 Hill showed that the evaluated by Voigt approach value gives the upper estimate whereas the evaluated by Reuss approach value gives the lower estimate. For example, the Young modulus of a granular composite with Young moduli of fibers and matrix $E^{(f)}$, $E^{(m)}$ and corresponding volume fractions $c^{(f)}$, $c^{(m)}$ are equal by Voigt $E^V = c^{(f)}E^{(f)} + c^{(m)}E^{(m)}$ and by Reuss $\frac{1}{E^R} = \frac{c^{(f)}}{E^{(f)}} + \frac{c^{(m)}}{E^{(m)}}$. Then Voigt-Reuss bracket is as follows

$$E^R \leq E^{eff} \leq E^V. \quad (10)$$

It is needed to note that the practice to write the formulas for effective physical constants in the form of brackets is useful and very common in the theory of effective constants. The well-known Hashin-Shtrikman bracket for shear modulus [Broutman and Krock (1974)]

$$\mu^{(-HS)} \leq \mu^{-eff} \leq \mu^{+eff} \leq \mu^{(+HS)} \quad (11)$$

corresponds to the understanding that for different schemes of evaluation of effective constants the composite material “soft matrix – stiff fillers”) has the moduli close to the lower bound and the composite material “stiff matrix – soft fillers” has the moduli close to the upper bound.

The characteristic bracket for one of shear moduli of fibrous composite has the form [Broutman and Krock (1974)]

$$\begin{aligned} \mu^{(m)} + \frac{c^{(f)}}{\frac{1}{\mu^{(f)} - \mu^{(m)}} + c^{(f)} \frac{K^{(m)} + 2\mu^{(m)}}{2\mu^{(m)}(K^{(m)} + \mu^{(m)})}} &\leq \mu_{23}^{eff} \\ &\leq \mu^{(f)} + \frac{c^{(m)}}{\frac{1}{\mu^{(m)} - \mu^{(f)}} + c^{(f)} \frac{K^{(f)} + 2\mu^{(f)}}{2\mu^{(f)}(K^{(f)} + \mu^{(f)})}}. \end{aligned} \quad (12)$$

The formulas for evaluating the effective moduli can have also the form of equalities.

Further the fibrous unidirectional composites will be considered and for calculation of their effective properties the equalities will be just used. It should be noted that for modeling such composites the transversally isotropic medium is convenient. It has one symmetry axis and the isotropy plane perpendicular to this axis; in the linear case it is characterized by the matrix with five independent constants C_{1111} , C_{3333} , C_{4444} , C_{1313} , C_{2211} . These constants are utilized mainly in wave analysis. In non-wave problems, the technical constants are used most often (Young and shear moduli, Poisson ratio) E , G , ν (for longitudinal direction) and E' , G' , ν' (for transversal direction). Then $E' = 2G'(1 + \nu')$.

Among the plenty of models of composite materials the mentioned above model of averaged (effective) elastic moduli is chosen (it can be referred to structural mechanics and takes into account the internal structure of materials by values of effective moduli). As it was commented above (see also [Broutman and Krock (1974); Guz A.N. (1993)]), calculation of effective moduli is based in most cases on assumption that components of the composite are described by the continuum and their properties are isotropic. This fact will be taken into account later, when the properties of composite materials under consideration being described. For calculating the constants,

further will be used the proposed in [Van Fo Fy (1971)] analytical formulas for effective constants of unidirectional fibrous composites which are in a good concordance with experimental observations of fibrous composites

$$E = c^m E^m + c^f E^f + \frac{4\mu^m c^m c^f (v^f - v^m)^2}{[1 - c^f (1 - 2v^m)] + c^m (1 - 2v^m) (\mu^m / \mu^f)}$$

$$G = \mu^m \frac{1 + c^f + c^m (\mu^m / \mu^f)}{c^m + (1 + c^f) (\mu^m / \mu^f)},$$

$$\nu = \nu^m - \frac{2(1 - v^m) c^f (v^m - v^f)}{[1 - c^f (1 - 2v^m)] + c^m (1 - 2v^f) (\mu^m / \mu^f)},$$

$$\frac{1}{E'} = \frac{\nu^2}{E} + \frac{1}{4\mu} + \frac{1 - 2v^m}{4\mu^m} \cdot \frac{c^m + (1 - 2v^f) (\mu^m / \mu^f)}{1 - c^f (1 - 2v^m) + c^m (1 - 2v^f) (\mu^m / \mu^f)}$$

$$G' = \mu^m \frac{(3 - 4v^m) + c^f + (1 - c^m) (\mu^m / \mu^f)}{(3 - 4v^m) c^m + [1 - (3 - 4v^m) c^f] (\mu^m / \mu^f)}, \quad (13)$$

where is assumed that the matrix and fibers are isotropic, and by E^m , E^f , μ^m , μ^f , ν^m , ν^f the Young and shear moduli, Poisson ratios of matrix and fiber are denoted. The values of effective density are evaluated by a conventional technique using the Voigt-Reuss bracket

$$\begin{aligned} \rho^V &= c^m \rho^m + c^f \rho^f; \quad \frac{1}{\rho^F} = \frac{c^m}{\rho^m} + \frac{c^f}{\rho^f}; \quad (14) \\ \rho^{eff} &= (1/2) (\rho^V + \rho^F). \end{aligned}$$

Further the effective density ρ^{eff} , six technical elastic constants E , E' , G , G' , ν , ν' (longitudinal tension, transversal tension, longitudinal shear, transversal shear, Poisson ratios for transversal tension and longitudinal shear) and two classical elastic constants

$$C_{1111}^{eff} = E' \frac{1 - \nu^2 (E'/E)}{(1 + \nu') [(1 - \nu') - 2\nu^2 (E'/E)]}, \quad (15)$$

$$C_{3333}^{eff} = E \frac{1 - \nu}{(1 - \nu') - 2\nu^2 (E'/E)} \quad (16)$$

will be evaluated.

There is a need to note that the common feature of all formulas is an absence in the formulas of the explicit geometrical parameters in the form of layer thickness, fiber or granule radius and an indirect presence of these parameters in the form of the volume fractions. Therefore the indicated inability of the model of effective constants to respond to changing the characteristic for composite materials scales (the characteristic size of internal structure, the filler sizes) excites

sometimes the criticism in the case of application of the model to nanocomposite materials. But it is the price, which we oblige to pay for using the notion of continuum.

Further the basic continuum model will be used in computer modeling in two variants: the linear model of effective elastic constants which is associated with the classical theory of elasticity and the physically and geometrically nonlinear model of effective elastic constants used the well studied in the nonlinear theory of elasticity Murnaghan potential. The choice of this potential is substantiated with the special property of the potential to describe properly the wave velocities in transversely isotropic media and by the author's intention to study the propagating in such a media harmonic waves and their evolution.

The last model reflects the possibility of nonlinear elastic deformation of the composites (in our case the composite inherits this nonlinearity from the isotropic nonlinearity of the epoxy matrix, which includes a small amount of the non-linearly deforming polystyrene).

In the model, a transversally isotropic continuum is assumed additionally to be quadratically nonlinear according to the Murnaghan elastic potential [Guz (2004); Rushchitsky et al (2005)]. It is necessary for elimination of contradiction to use the modified for the case of transversal isotropy Murnaghan potential, in concordance with which the third order constants in the direction along the fibers A_3 , B_3 , C_3 and across the fibers $A_1 = A_2$,

$B_1 = B_2$, $C_1 = C_2$ are different

$$W(\epsilon_{ik}) = -C_{ikik}(1 - \delta_{ik})(\epsilon_{ik})^2 + (1/2)C_{iimm}(\epsilon_{mm})^2 + (1/3)A_i\epsilon_{ik}\epsilon_{ik}\epsilon_{ik} + B_i(\epsilon_{ik})^2\epsilon_{ik} + (1/3)C_i(\epsilon_{ii})^3, \quad (17)$$

$$C_{1111} = C_{2222}, \quad C_{2233} = C_{1133},$$

$$C_{1313} = C_{2323}, \quad C_{1212} = (1/2)(C_{1111} - C_{1122}),$$

It is necessary to note that the Murnaghan potential is utilized for description of nonlinear deformation of the wide class of materials used in engineering sciences and the presented in (10) constants of the third order are determined for these materials quite exactly [Guz (2004)].

3 Mechanical properties of matrix and fillers

Four types of fibrous unidirectional composite materials will be further considered. We think all types of fibers as being made of carbon and the matrix material is made both epoxy rosin EPON-828 with properties: density $\rho = 1.21 \cdot 10^3 \text{ kg/m}^3$, Young modulus $E = 2.68 \text{ GPa}$; shear modulus $\mu = 0.96 \text{ GPa}$; Poisson ratio $\nu = 0.40$ – and consists of a mixture of the rosin EPON-828 and the polystyrene. The last one is the product of polymerization of styrene $[-CH_2 - CH(C_6H_5) -]_n$ with properties within the framework of nonlinear Murnaghan model: density $\rho = 1.05 \cdot 10^3 \text{ kg/m}^3$; elastic moduli of the second order: Young modulus $E = 2.56 \text{ GPa}$; shear modulus $\mu = 1.14 \text{ GPa}$; Poisson ratio $\nu = 0.30$; elastic moduli of the third order: $A = -10.8 \text{ GPa}$; $B = -7.85 \text{ GPa}$; $C = -9.81 \text{ GPa}$ (Murnaghan constants).

Since the organic epoxy rosin EPON-838 is assumed as the material of matrix and this rosin from technological reasons (for avoiding the crystallization) contains always the addition of high-molecular polymers [Lubin (1982)], then the presence in computer modeling of some hypothetical material consisting of chaotic mixture of epoxy rosin and high-molecular polystyrene seems to be not contradicting the nature of the rosin and quite possible.

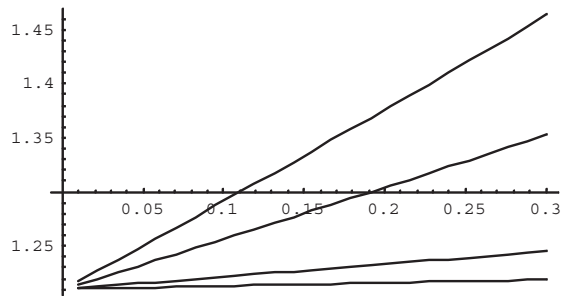


Figure 3: Dependence of density ρ^{eff} on c^f for 4 types of composites (from top – microW, microT, nanoZZ, nanoCH).

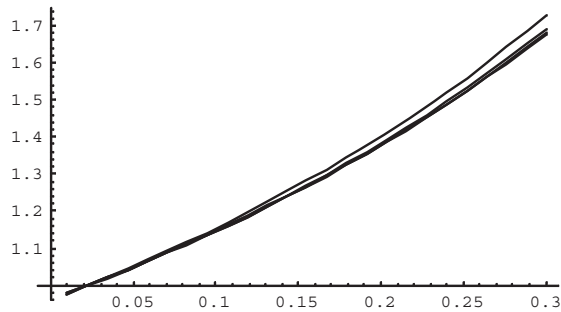


Figure 5: Dependence of transverse shear modulus G^{eff} on c^f for 4 types of composites (upper plot – microT).

It is necessary to note that the matrix made of the mixture of epoxy rosin with polystyrene is the material with the soft characteristics of non-linearity. The material with the heavy characteristics of nonlinearity is found rarely enough, it is studied here in the form of the matrix consisting of the mixture of the epoxy rosin with the Pyrex – glass. For this glass the following physical properties are assumed: $\rho = 9.95 \cdot 10^3 \text{ kg/m}^3$; $\lambda = 1.45 \text{ GPa}$; $\mu = 0.941 \text{ GPa}$; $A = 124 \text{ GPa}$; $B = -252 \text{ GPa}$; $C = 350 \text{ GPa}$. Additions to epoxy rosin are assumed to be the tenth portion of the mixture as a whole.

Fillers have the following characteristics:

Filler N1 – industrial carbon microfiber Thornel-300 with properties: mean diameter $8 \mu\text{m}$, density $\rho = 1.75 \cdot 10^3 \text{ kg/m}^3$ Young modulus $E = 228 \text{ GPa}$; shear modulus $\mu = 88 \text{ GPa}$; Poisson ratio $\nu = 0.30$.

Filler N2 – graphite whiskers with properties:

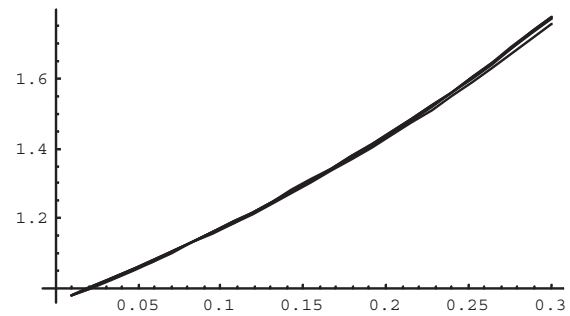


Figure 4: Dependence of longitudinal shear modulus G^{eff} on c^f for 4 types of composites.

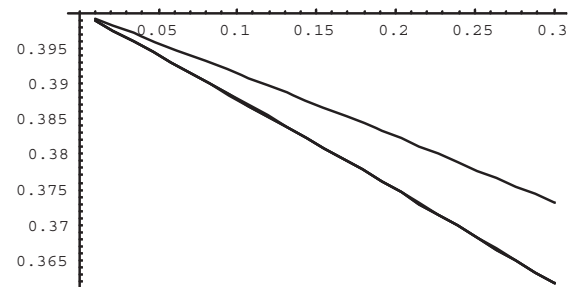


Figure 6: Dependence of Poisson ratio ν^{eff} on c^f for 4 types of composites (upper plot – nanoZZ).

mean diameter $1 \mu\text{m}$, density $\rho = 2.25 \cdot 10^3 \text{ kg/m}^3$, Young modulus $E = 1.0 \text{ GPa}$; shear modulus $\mu = 385 \text{ GPa}$; Poisson ratio $\nu = 0.30$.

Filler N3 – zig-zag carbon nanotubes with properties: mean diameter 10 nm , density $\rho = 1.33 \cdot 10^3 \text{ kg/m}^3$, Young modulus $E = 0.648 \text{ GPa}$; shear modulus $\mu = 221 \text{ GPa}$; Poisson ratio $\nu = 0.33$.

Filler N4 – chiral carbon nanotubes with properties: mean diameter 10 nm , density $\rho = 1.40 \cdot 10^3 \text{ kg/m}^3$, Young modulus $E = 1.24 \text{ GPa}$; shear modulus $\mu = 477 \text{ GPa}$; Poisson ratio $\nu = 0.30$.

Shown data about the matrix and fibers (further microT, microW, nanoZZ, nanoCH) are utilizing for computer modeling the physical constants in basic models. The modelling is described in next paragraph, where changing in value of basic constants in dependence with the degree of fiber

volume concentration as well as the distinction and similarities between micro- and nanocases are studied. Some of the results are predictable. For example, certain of the constants are very sensitive to the fiber properties (Young and shear moduli) big distinctions and some of constants are almost identical for all types of fibers.

4 Computer modeling of mechanical properties of fibrous composites

Within the framework of the linear model of effective constants the constants ρ^{eff} , E^{eff} , G^{eff} , ν^{eff} , E'^{eff} , G'^{eff} , ν'^{eff} , C_{1111}^{eff} , C_{3333}^{eff} are considered. The results of modeling are shown on next plots.

Everywhere the abscissa axis corresponds to the volume fraction of fibers c^f (it is assumed to be small – up to 0.3). The restriction to small filling of fibers is caused by that in this case the utilized formulas are exact sufficiently, on the one hand, and at present level of technology progress and nanoparticles or nanofibers cost the denser filling of matrix seems to be problematic, on the other hand.

It can be noted that Figs. 3-6 show the weak non-linearity in dependence of both shear moduli on the volume fraction of fibers. This type of non-linearity is characteristic for majority of parameters in the case of small filling by fibers what can be seen from next plots. Also Figs. 4-6 show that corresponding parameters are not sensitive to the difference between micro- and nanofiber properties.

The strong nonlinear dependence of Poisson ratio ν'^{eff} and a shift of its values to the range (0.5; 0.7) can be noted as one of interesting results. A commenting the shift can be found in [Guz and Rushchitsky (2004a)].

So, Fig. 9 seems to be very similar to Fig. 5 and testifies the almost full insensitiveness of transversal Young modulus E'^{eff} and transverse shear modulus G'^{eff} on fiber properties. At the same time both parameters are changed significantly with changing the filling degree.

Thus, if we assume that two groups of parameters differ essentially microcomposites from nano

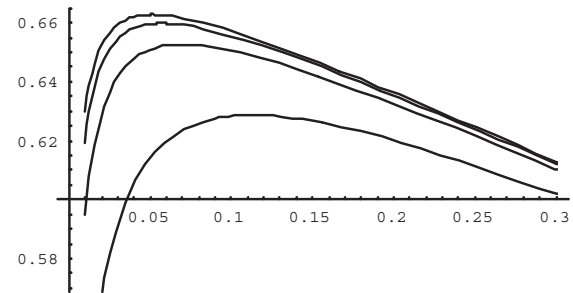


Figure 7: Dependence of Poisson ratio ν^{eff} on c^f for 4 types of composites (from top – microW, nanoZZ, nanoCH, microT).

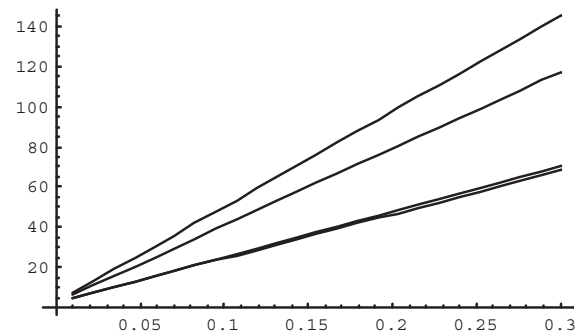


Figure 8: Dependence of longitudinal Young modulus E^{eff} on c^f for 4 types of composites (from top – nanoCH, microW, nanoZZ, microT).

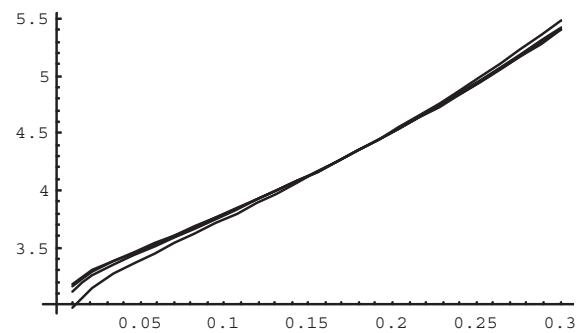


Figure 9: Dependence of transversal Young modulus E'^{eff} on c^f for 4 types of composites (microW, nanoCH, nanoZZ are practically identical).

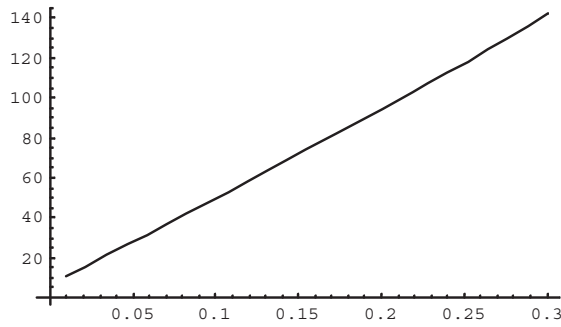


Figure 10: Dependence of elastic modulus C_{1111}^{eff} on c^f for 4 types of composites (from top – nanoCH, microW, nanoZZ, microT).

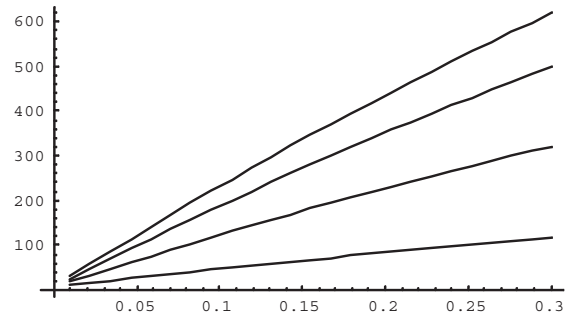


Figure 11: Dependence of elastic modulus C_{3333}^{eff} on c^f for 4 types of composites (from top – nanoCH, microW, nanoZZ, microT).

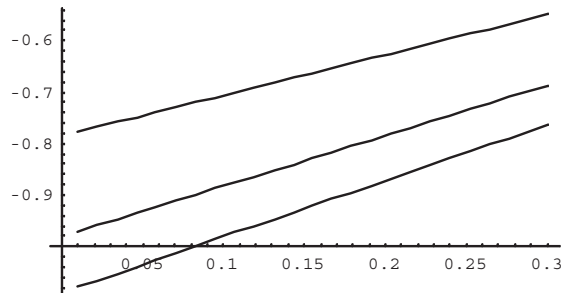


Figure 12: Dependence of constants A (lower plot), B (upper plot), C (middle plot) on c^f for the matrix rosin-styrene.

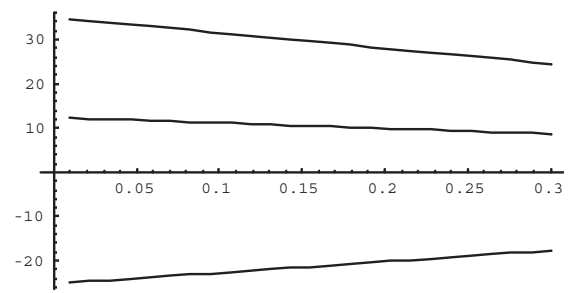


Figure 13: Dependence of constants A (middle plot), B (lower plot), C (upper plot) on c^f for the matrix rosin-Pyrex.

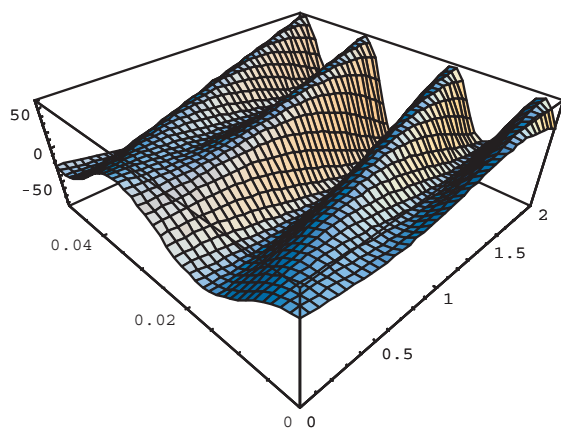


Figure 14: Evolution of the running harmonic longitudinal plane wave for microT.

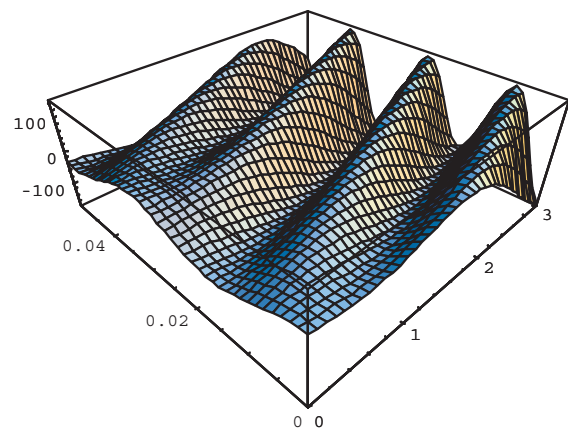


Figure 15: Evolution of the running harmonic longitudinal plane wave for nanoCH.

ones – Young and shear moduli as the mechanical group and fiber diameter as the geometrical group – then pictures above show a differing influence of the first group on mechanical constants of composites.

The most significant difference can be seen in the cases of longitudinal Young modulus E^{eff} and elastic modulus C_{3333}^{eff} .

Two plots on Figs. 12 and 13 show the variation of elastic constants of the third order (Murnaghan constants, in GPa) against volume fraction of fibers. As it can be seen they are changed not very much within the chosen range of filling with fibers.

5 Comparative analysis of waves in of carbon-polymer micro- and nanocomposites

The problems on propagation of harmonic waves are indicative not only in that they show the distinction between wave pictures in micro- and nanocomposites, but also they are very convenient for detection of the range of applicability of structural models of composite materials. The point is that the harmonic wave contains in its analytical representation the wave length as an independent parameter. Therefore the analysis of applicability of models can always forego the modeling of wave picture within framework of models adopted here. From the viewpoint of that by the use of comparison of the wave length with the characteristic length of internal structure of composite, the limit values of the wave length can be indicated. The limit ones in that the values less of the limit ones are to short for neglecting the peculiarities of internal structure of representative volume.

Thus, for micro- and nanocomposites the ranges of wave lengths or frequencies, in which the linear model of effective constants is applicable, can be compared. The case in point is the upper limit (short waves) because the long waves will have any restrictions from below. The assumption that exceeding the wave length of characteristic size of internal structure of materials l_{CSM} in 8-10 times is the limit one seems to be natural and substantiated by experimental observations.

Also is seems to be natural that the limit wave lengths are calculated for microcomposites in microns whereas for nanocomposites in nanometers and the difference is approximately three orders.

From point of view of frequencies, this means a transition from the ultrasound range to the hyper-sound range.

It will be displayed in the wave theory in differing on the same order times of evolution progress of initially harmonic wave.

Let us consider now three different waves propagating in a fibrous composite material which is described within the nonlinear model of effective constants by elastic Murnaghan potential and properties of which are described above. The first wave is the running longitudinal plane wave evolution of which is caused by the quadratic nonlinearity of the propagation medium [Guz and Rushchitsky 2004b]. The second wave is the running transverse plane wave and its evolution is caused by the cubic nonlinearity of the propagation medium [Rushchitsky et al 2003]. The third wave is already not the running plane but the cylindrical and it is propagated from the cylindrical cavity and is caused by the harmonic oscillations on the cavity boundary. The evolution of this wave is caused by the quadratic nonlinearity of the propagation medium [Rushchitsky 2005c].

For realization of computer modeling (the interactive system *Mathematica 5.1* was used) many necessary parameters are at first evaluated.

The characteristic size of internal structure l_{CSM} was determined in assumption that: fibres are placed within the quadratic structure; the fiber radius is r^f and the volume fraction of fibers is $c^f = 0, 1$: $l_{CSM} = \sqrt{10\pi r^f}$.

The wave length λ_3 was fixed as conditionally extremely possible for each material within the framework of continuum approach, namely as exceeding the CSM 4π times: $\lambda_3 = 4\pi l_{CSM}$.

The wave number k_3^* was recalculated through the known wave length: $k_3^* = (1/(2l_{CSM}))$.

The phase velocity in linear approximation v_3^{ph} was determined by the formula $v_3^{ph} = (\omega/k_3^*) = \sqrt{C_{3333}/\rho^{eff}}$.

The extremely possible frequency ω_3 was calculated through the wave number k_3^* and the phase velocity v_3^{ph} .

The initial amplitude u_3^0 was chosen from a reason of weak accumulation of changes of the profile on the distance of one wave period, namely such that it is significantly less of the wave length λ_3 (for all materials, the ratio of u_3^0 to λ_3 was chosen equal 0,1).

The extremely possible time t_L was recalculated through the known extremely possible distance d_L using the zero phase $\varphi = k_L^* d_L - \omega_L t_L = 0 \rightarrow t_L = (d_L / v_L^{ph})$.

Parameter d_L expresses quantitatively the fact of essential dependence of the distance which must run the wave for displaying the evolution of its initial profile on the wave length and the same dependence of the minimally admissible wave length on the characteristic size of internal structure. Comparison of parameter d_L for microT, microW, nanoZZ, nanoCH with identical fiber volume fraction $c^f = 0.1$ and for the quadratically nonlinear elastic harmonic longitudinal plane wave shows that within the condition of propagation of the wave with the minimally admissible wave length the distinction is estimated by orders – for the first material with carbon microfibers of diameter $8 \mu\text{m}$ the distance d_L is $1,127 \mu\text{m}$ (more than one millimeter); for the second material reinforced by microwhiskers of diameter $1 \mu\text{m}$ the distance d_L is about $141 \mu\text{m}$; for materials with fibers in the form of zig-zag and chiral nanotubes (Z-CNT and C-CNT with diameter 10 nm) the necessary distance is decreasing up to 1407 nm . So, in this case the basic nonlinear phenomenon – transformation of harmonic impulse into its second harmonics – occurs for micromaterials on distances of microlevel and for nanomaterials on distances of nanolevel. Respectively, durability of the evolution process for microcomposites is 224 and $14,58 \mu\text{s}$, whereas for nanocomposites it is evaluated in ns – 175 and 127 .

On Fig. 15 and 16 all stages of evolution development (from the initial profile in the form of the first harmonics to the form of the second harmon-

ics or, simpler, the process of transformation of the profile with one hump into the profile with two humps on the same semi-period) of running harmonic longitudinal plane wave propagating in composite materials for mentioned above initial parameters are shown.

In next list of four parameters the first position corresponds to microT and the second one to nanoCH:

The characteristic size of internal structure $l_{CSM} - 22.42 \mu\text{m}; 28\text{nm}$.

The critical wave length $\lambda_3 - 281.8 \mu\text{m}; 352 \text{ nm}$.

The critical wave number $k_3^* - 2.23 \cdot 10^{-4} \text{ 1/m}; 0.1785 \text{ 1/m}$.

The phase velocity $v_3^{ph} - 5.031 \text{ km/s}; 11.08 \text{ km/s}$.

At the last two pictures, the critical initial amplitude u_3^0 and the frequency ω were chosen from a reason of quick evolution – $u_3^0 - 28.18 \mu\text{m}; 35.2 \text{ nm}; \omega - 100\text{MHz}; 100\text{GHz}$.

The unit on abscissa axis corresponds to running distance $100 \mu\text{m}$, on ordinate axis corresponds to running time $100 \mu\text{s}$, on applicate axis corresponds to $1 \mu\text{m}$ for microT, and on abscissa axis – 100nm , on ordinate axis – 100 ns , on applicate axis – 1 nm for nanoCH.

So, process of harmonic wave evolution for micro- and nanocomposites is similar. The main distinction consists in transition from one scale of distance (microns) and time (microseconds) to another one (nanometers and nanoseconds).

In conclusion, we should note that performed computer and analytical modeling testifies first of all the high values of elastic moduli of nanocomposite materials. These materials show really high strength to deformations and in concordance with experimental observations the continuum model of effective moduli describes this high level of strength of deformations and can be applied at the problem of prediction of mechanical properties of nanocomposite materials. The theoretical and next computer modeling of physical properties must be necessary based on certain models. The elaborated by authors approach used the classical continuum model, which authors think as the quite appropriate. But, of course, some problems of nanocomposites are beyond the framework of

this approach. In our opinion, this fact doesn't minimize the fundamental and classical importance of the approach.

All considerations shown above permit to conclude that there is no hope of our getting quick solutions of the nanocomposite problem in the near future.

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