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Stability Loss in Nanotube Reinforced Composites

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Abstract: The two models in the three-dimensional theory of stability of the nanotube reinforced composite materials are discussed. The model of “infinite fibers” and the model of “short fibers” are considered. The primary objective is attended to “short fibers” model. All results are obtained in the framework of the three-dimensional linearized theory of stability of deformable bodies.

Keywords: Stability problem, composite material, nanocomposite, short fibers, nanotube, three-dimensional linearized theory of stability, finite difference method.

1 Introduction

The main failure mechanism of fibrous composites under unidirectional compression, including composite materials reinforced by nanotubes, is a loss of stability in the structure of filler material. The approaches for building the theory of nanocomposites and a series of new results in the mechanics of nanocomposites are presented in [Guz A.N., Roger A.A., Guz I.A. (2005)], [Guz A.N. (2006)], [Guz A.N., Rushchitsky J.J. and Guz I.A. (2008)]. Overwhelming number of results in this direction is obtained in the model of infinite fibers, when only the periodic forms of stability loss (along the fibers) were analyzed. With such approach a number of problems of mechanics of deformable solids with respect to elastic and plastic models are investigated. These results are presented in numerous periodical publications and in some generalizing publications, for example, in [Guz AN (2004)], as well as [Guz A.N., Lapusta Yu.N. (1999)], [Babich I.Yu, Guz A.N. and Chekhov V.N. (2001)], [Guz A.N., Guz I.A. (2004)], [Guz A.N., Chekhov V.N. (2007)] and a series of other publications. Modern analyze of the approaches and results obtained with the three-dimensional linearized theory of stability of deformable bodies are presented in the generalizing publication [Guz A.N. (2001)].

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As a result of further researches, which are presented in [Guz A.N., Dekret V.A. (2008)], it was found that the values of critical strain for relatively short fiber which were obtained using the model of *infinite fibers*, significantly different from the values, which are obtained with the model of *short fibers*, when the matrix is considered as endless, and the filler is modeled as cylindrical fiber with finite size (Fig.1). Only recently the results with the model of *short fibers* were obtained for the one, two and periodical rows of short fibers which are presented in publications [Guz A.N., Dekret V.A. (2008), (2009)], [Dekret V.A. (2006), (2008a, b)].

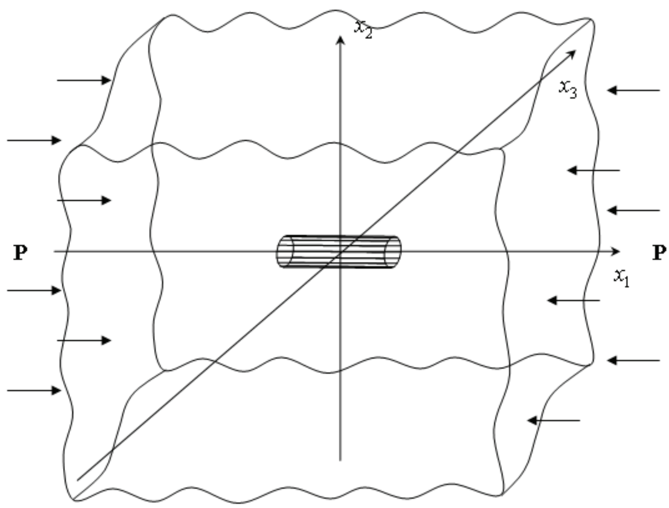

Figure 1: Model of composite reinforced by nanotube

2 On selection of geometric parameters of applicability of the models

It should be noted the results obtained with using the models of *infinite fibers* and the model of *short fibers* must be agreed. Obviously, for such conformity these results have to satisfy by the following conditions. The results obtained with using the model of *short fibers* have to approach asymptotically towards the results obtained with the model of *infinite fibers*, when the length of fibers tends to infinity.

In this connection, we need to define the values of geometric parameters that characterizes the "finiteness" of fibers. Such parameter can be the value of LD^{-1} that means the ratio of fiber length L to its diameter D. Some information about the limits of this parameter can be obtained from the classification of composite materials, which is offered in numerous monographic publications. The layered composite materials are defined as composite materials in which the geometric size of reinforcing elements to one direction is substantially less (by several orders of magnitude) than the geometric sizes to other two mutually perpendicular directions. The fibrous composite materials are defined as composite materials in which the geometric size of reinforcing elements to one direction is substantially more (by several orders of magnitude) than the geometric sizes to other two mutually perpendicular directions. The granular composite materials are defined as composite materials in which the geometric sizes of reinforcing elements in the three mutually perpendicular directions are the values of the same order.

From the above follows for the studying of loss of stability in the composite materials reinforced by nanotubes with using the model of *short fibers* the lower limit of parameter LD^{-1} we can choose as

$$LD^{-1} \geq 10 \tag{1}$$

It should be noted that follows publications on nanocomposites [Guz AN, Roger AA, Guz IA (2005)], [Guz A.N. (2006)], [Guz A.N., Rushchitsky J.J. and Guz I.A. (2008)] and other publications are contained the analysis of geometrical sizes of single-walled carbon nanotubes (SWCNT) and multi-walled carbon nanotubes (MWCNT), which can be considered as potential fillers in nanocomposites. In particular, in [Guz AN, Roger AA, Guz IA (2005)] are presented the publications where are studied the properties of single-walled, double-walled, three-walled and four-walled CNT with geometric parameter $LD^{-1} = 9,1$. Thus, in accordance with the accepted classification of composite materials (layered, fibrous, granular) and the existing examples of modern carbon nanotubes to determine the lower bounds of the geometric parameter LD^{-1} for the model of *short fibers* can be used expression (1).

Let us consider the information related to the choice of upper limits of the geometric parameter LD^{-1} for the model of *short fibers*. To define the upper limits of the geometric parameter LD^{-1} we can proceed from the following two considerations.

Firstly, we can proceed from condition that these two models of the composite materials must be agreed. In this case, the value of the upper limit of the geometrical parameter LD^{-1} must implement the asymptotical transition the results from the model of *short fibers* to the model of *infinite fibers*. Thus, it can be chosen as

$$LD^{-1} \leq k \cdot 1000, \tag{2}$$

where the value k should be chosen depending on the specific composite materials under consideration.

Secondly, we can proceed from the specific values of the geometric parameter LD^{-1} that correspond to various structures of composite materials, which are considered in researches of nanocomposites reinforced by carbon nanotubes. In the works [Guz A.N., Roger A.A., Guz I.A. (2005)], [Guz A.N. (2006)], [Guz A.N., Rushchitsky J.J. and Guz I.A. (2008)] is given the information about the geometric sizes of nanofibers which can be used as fillers in nanocomposites and is provided the analysis of publications in periodicals about it. It should be noted the following information about the geometric sizes:

Multi-walled carbon nanotube (MWCNT) obtained by chemical cooling of the vapors

$$D < 50nm; \quad L > 1000nm; \quad LD^{-1} > 200; \tag{3}$$

CNT ensembles

$$D = (30-50)\,nm; \quad L > 50000nm; \quad LD^{-1} \geq 1000; \tag{4}$$

nanoropes

$$D = (10-20)\,nm; \quad L > 100000nm; \quad LD^{-1} > 5000; \tag{5}$$

cup-stacked type carbon nano-fibers (CSNF),

$$D = (80-100)\,nm;\ \ L = (500-1000;\,2500-10000;\,200000)\,nm;\ \ LD^{-1} \leq 2500 \tag{6}$$

These data about the geometric parameters of various nanofibers allow to define the upper limits for the model of short fibers as expression (2) where the value k can be selected from the following range $0,5 < k \leq 5,0$.

Thus from the above analysis is followed the acceptability of the expression (2) to determine the upper limits of the geometric parameter LD^{-1} for comparative analysis of the results which is obtained for problems of stability of fibrous composites with the models of *infinite fibers* and *short fibers*.

3 Statement and technique of the solution of problem

In this paper we are restrict the study of stability of composite materials weakly reinforced by nanotubes in a plane strain. The composite material is modeled as a piecewise-homogeneous medium when the material in a component of composite is considered as uniform and the condition of continuity is satisfied at the contact of components. The components of composite are considered as linearly elastic and isotropic. Thus, using model of *short fibers*, we have got the plane model of composite under unidirectional compression, with conditions of plane deformation, it is presented at Fig.2.

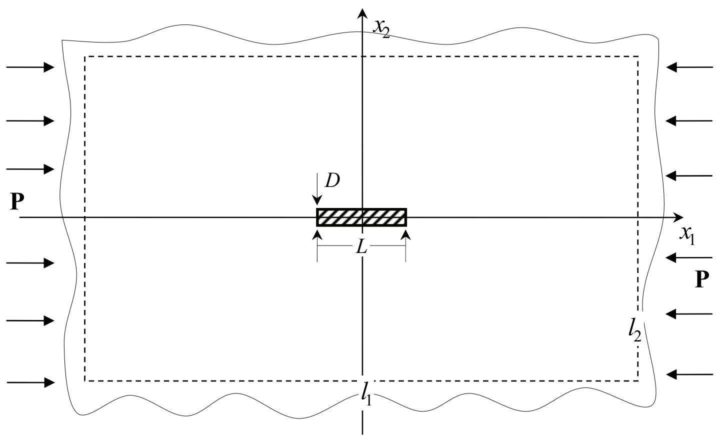

Figure 2: Plane model of nanocomposite

The stability analysis is performed using the static method of the three-dimensional linearized theory of stability when the initial state is determined from the equations of linear elasticity [Guz A.N. (1969)]. The statements of linear elasticity problem and stability problem are presented in detail in [Guz A.N., Dekret V.A (2008)]. Obviously, the solution of the problems by analytical methods is impossible; in this connection for the solution of problem of determination of the subcritical state and stability problem the numeral methods are used. In this paper we will consider in detail the technique of the numeral solution of problems.

The approximate solutions of the problems are performed using the finite difference method with the concept of the basic schemes as described in [Kokhanenko Yu.V. (2001)]. Difference mesh is placed in calculation area using lines $x_i = const$

$$\bar{\omega} = \left\{ \mathbf{x} = (x_1^m, x_2^n), \ m = \overline{0,M}, n = \overline{0,N} \right\}. \tag{7}$$

Herewith a material in each cell of mesh is homogeneous, i.e. every cell of mesh contains the material only of one kind of composite components (Fig.3). This mesh must be non-uniform at each direction as near the contact of components and near the boundary of the calculation area the grid lines should be placed more densely. The density of the mesh is selected as a result of computational experiment.

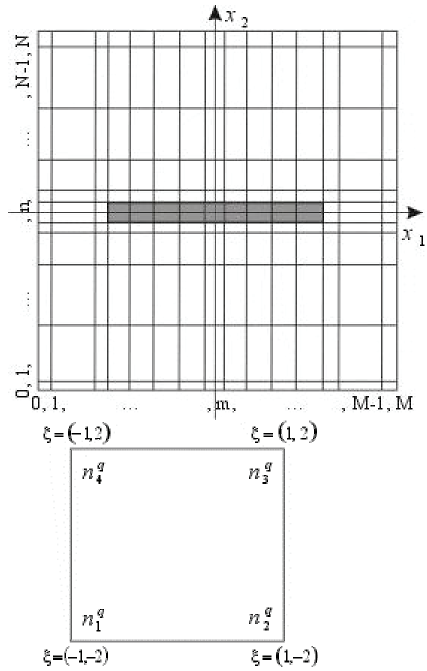

Figure 3: Calculation scheme of nanocomposite

The mesh of $\bar{\omega} = \omega \cup \gamma$, where ω- interior nodes, γ - boundary nodes, is a set of rectangular cells. Thus each cell of the mesh has got the mechanical and geometrical characteristics of material of the composite component. Each node grid is associated with vector parameter $\boldsymbol{\xi} = (\xi_1, \xi_2) = (\pm 1, \pm 2)$ (Fig.3).

Each node of mesh adjoin a number of cells (from 1 to 4) so each node $\mathbf{x} \in \bar{\omega}$ corresponds to the same number of vector parameters $\boldsymbol{\xi} \in \mathbf{x}$. The variable $x_i^{\xi_j}$ is coordinate of node adjacent to x_i at the direction x_j (if $\xi_j > 0$, then $x_i^{\xi_j} > x_i$); the difference derivatives of mesh functions u_i to x_j are written as

$$u_{i,\xi_j} = \frac{u_i^{\xi j} - u_i}{\eta_{\xi_j}}, \tag{8}$$

where $u_i^{\xi_j} = u(x_i^{\xi_j})$; $\eta_{\xi_j} = x_j^{\xi_j} - x_j$ - a step at the direction of x_j. The sign of parameter ξ_j determines the type of derivative with accordance of (18): if $\xi_j > 0$, then $\eta_{\xi_j} > 0$ and in u_{i,ξ_j} - the right derivative, and if $\xi_j < 0$, then $\eta_{\xi_j} < 0$ and - u_{i,ξ_j} the left derivative.

The discrete problems are constructed using variational-difference method with the concept of the basic schemes. The discrete problems are obtained through the appropriate summation of basic schemes for each node of the mesh $\bar{\omega}$. The components of the basic scheme are determined by approximation and minimizing the corresponding functional on the mesh.

The expression of the energy functional, which corresponds to the problem of determining the subcritical stress-strain state, is written as

$$J = \int\limits_{\Omega} \sigma_{ij}\varepsilon_{ij} d\Omega - 2\int\limits_{\Gamma} P_i u_i d\Gamma. \tag{9}$$

The components of the stress-strain state within the component of composite satisfy the equations of elasticity.

For approximation of the energy functional (9) at the mesh (7) need to replace the continued values by the mesh variables and the mesh functions which are defined in the nodes of $\bar{\omega}$. The integrals should be approximated by the trapezium rule. The partial derivatives of displacements vector are approximated with the expression (8). Thus, the following expressions of the basic operators are obtained from the condition of stationarity of energy functional (9) for each node of cell

$$a_i(\boldsymbol{\xi})\mathbf{u} = -H\frac{\sigma_{ji} + \sigma_{ji}^{\xi_j}}{\eta_{\xi_j}}, \ \mathbf{x} \in \varpi; \quad \varphi_i(\boldsymbol{\xi}) = -\frac{2H}{\eta_{\xi_j}} P_1, \ \mathbf{x} \in \gamma. \tag{10}$$

The difference problem of determining the stress-strain state, which corresponds to the problem of linear elasticity theory, can be written as

$$\mathbf{A}\,\mathbf{u} = \boldsymbol{\Phi}, \ \ \mathbf{x} \in \overline{\varpi} \text{ or } A_i\,\mathbf{u} = \Phi_i, \ \ \mathbf{x} \in \overline{\varpi} \tag{11}$$

where

$$A_i\,\mathbf{u} = \sum_{\boldsymbol{\xi}\in\mathbf{x}} a_i\,(\boldsymbol{\xi})\ \mathbf{u}, \ \ \Phi_i = \sum_{\boldsymbol{\xi}\in\mathbf{x}} \varphi_i\,(\boldsymbol{\xi})\,, \ \ \mathbf{x} \in \overline{\varpi}\,. \tag{12}$$

Hereafter the sign of sum means that the basic operators must be summed up for the parameters $\boldsymbol{\xi}$ that correspond to the node $\mathbf{x} \in \bar{\omega}$ of all surrounding cells.

It should be noted, in accordance with [Kokhanenko Yu.V. (2001)], the difference operators of problem (10) retain the properties of self-conjugacy and positive definiteness of the relevant differential operator. Thus, the problem of determining the subcritical stress-strain state is reduced to solving mesh equations (10), which can be represented as a system of linear equations with symmetric matrix.

The expression of the energy functional, which corresponds to the problem of stability, is written as

$$J=\int\limits_{\Omega}\sigma_{ij}\varepsilon_{ij}\,d\Omega-p\int\limits_{\Omega}\sigma_{ij}^{0}\frac{\partial u_m}{\partial x_i}\frac{\partial u_m}{\partial x_j}\,d\Omega. \tag{13}$$

For approximation of the energy functional (13) at the mesh (7) need to replace the continued values by the mesh variables and the mesh functions which are defined in the nodes of $\bar{\omega}$. The integrals should be approximated by the trapezium rule.

Then, from the condition of stationarity of functional (13) for each node of cell the following expressions of the basic operators are obtained

$$a_i(\boldsymbol{\xi})\mathbf{u}=-H\frac{\sigma_{ji}+\sigma_{ji}^{\xi_j}}{\eta_{\xi_j}},\ b_i(\boldsymbol{\xi})\mathbf{u}=-H\frac{\sigma_{jk}^{0}u_{i,\xi_k}+(\sigma_{jk}^{0}u_{i,\xi_k})^{\xi_j}}{\eta_{\xi_j}},\ \ \mathbf{x}\in\boldsymbol{\varpi}. \tag{14}$$

The difference problem of stability can be written as

$$\mathbf{A}\,\mathbf{u}=p\mathbf{B}\,\mathbf{u},\ \ \mathbf{x}\in\overline{\varpi}\text{ or }A_i\mathbf{u}=pB_i\mathbf{u},\ \ \mathbf{x}\in\overline{\varpi} \tag{15}$$

$$A_i\,\mathbf{u}=\sum_{\boldsymbol{\xi}\in\mathbf{x}}a_i\,(\boldsymbol{\xi})\,\mathbf{u},\ B_i\,\mathbf{u}=\sum_{\boldsymbol{\xi}\in\mathbf{x}}b_i\,(\boldsymbol{\xi})\,\mathbf{u},\quad \mathbf{x}\in\overline{\varpi} \tag{16}$$

As for the problem of determining of the subcritical state, difference operators of the problem (15) retain properties of self-conjugacy and positive definiteness of the differential operators. Thus, the problem of stability reduces to the solution of the mesh equations (15), which can be represented as an algebraic generalized eigenvalue problem.

The described method for constructing difference problems greatly simplifies the procedure of numerical solving of the problems. Thus, we can use the general expressions for the basic operators for all the problems of these classes, which are not depend on the method of their production, and can be obtained by other means, for example, using the finite element method [Kokhanenko Yu.V. (1998)].

To solve discrete problems were used well-known in the theory of difference schemes direct and iterative methods: the Kholetskii method, conjugate gradient method, subspace iteration method, the method of gradient descent.

4 The results of calculations

Let us consider the results of study of stability for the nanocomposites with polymer matrix which has Young's modulus $E_m=2,68$GPa and Poisson's ratio $\nu_m=0,4$.

To select the parameter values $E_a E_m^{-1}$ that are characteristic for the nanocomposites with polymer matrix was used the information about properties of nanofibers from the works [Guz A.N., Roger A.A., Guz I.A. (2005)], [Chen W.H., Cheng H.C. and Hsu Y.C. (2007)], [Wu C.J., Chou C.Y., Han C.N. and Chiang K.N. (2009)] and other publications.

So in the work [Guz A.N., Roger A.A., Guz I.A. (2005)] is proposed to use the value $E_m \approx (1,0-1,2)$TPa as Young's modulus of "averaged" CNT for calculations of properties of multi-walled and single-walled carbon nanotubes. In consideration of the properties of the polymer matrix the ratios of Young's modulus of components of the composite material reinforced by "averaged" CNT are used in range of $373 \leq E_a E_m^{-1} \leq 448$. The following results are obtained for the nanocomposites with a polymer matrix for wider set of parameter values as

$$E_a E_m^{-1} = 285; 373; 448; 500; 1000 \qquad (17)$$

The last two values $E_a E_m^{-1}$ (17) correspond to situation that may arise during the technological processes of creation of nanocomposites, which are connected to substantial dependence of properties of polymer matrix on temperature.

According to the above considerations, for comparative analysis the geometric parameters were changed in the interval which determined by the lower boundary of (1) and the upper boundary of (2)

$$10 \leq LD^{-1} \leq 2310 \qquad (18)$$

The results of calculations of the critical value of strain $|\varepsilon_{11}^{cra}|$ along the ax Ox_1 in the middle point of reinforcing elements (nanotube) on the geometric parameter LD^{-1} in the interval (18) are presented in Fig.4. The dashed lines depicts the results related to model of *infinite fibers*, solid line depicts the results related to model of *short fibers*.

It should be noted that Fig.4 presents the results only for the parameters $E_a E_m^{-1} = 373; 448; 1000$, because the results for $E_a E_m^{-1} = 285; 500$ are similar.

From the results shown in Fig.4 for the nanocomposites with a polymer matrix is follow the critical values of strain $|\varepsilon_{11}^{cra}|$ which are calculated within the model of *short fibers* with increasing geometric parameter LD^{-1} in the interval (18) asymptotically tend to the critical values of strain which are calculated within the model of *infinite fibers*.

When the geometric parameter LD^{-1} approaches to the value of $LD^{-1} = 2310$ that corresponds to the upper boundary of interval (18), the critical values are practically coincide for the models of *short fibers* and *infinite fibers*.

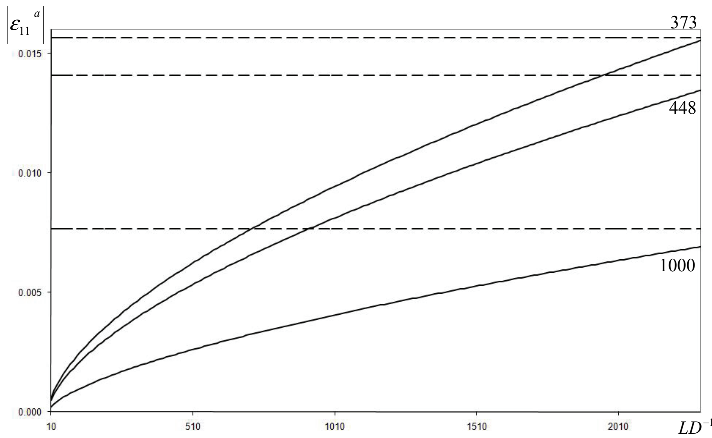

Figure 4: Dependence of the value of critical strain for a fiber on the geometrical parameters of fibers

5 Conclusion

The research of stability of the composite materials reinforced by nanotube is presented. The stability problem is formulated with application of the three-dimensional linearized theory of stability of deformable bodies and the model of piecewise-homogeneous medium, such approach is most strict and physically correct.

The results of research allow us to conclude that under compression directed along the nanotube may result the failure of the composite due to stability loss of its structure.

The results of study with the model of *short fibers* and with the model of *infinite fibers* are consistent, because results for the model of *short fibers* asymptotically tend to the results of the model of *infinite fibers* with increase of the length of fiber. However, the values of critical strain obtained in the framework of the model of *short fibers* with the values of geometrical parameters $LD^{-1} < 2000$ are differed significantly.

Therefore, the use of model of *short fibers* is preferable to study the stability of composite materials reinforced by nanotubes, which are the geometrical parameters in this range.

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