JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 5 No 3, 03020(5pp) (2013)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 5 № 3, 03020(5cc) (2013)

Model of the Elastic Plate Stiffened with the Regular System of Nanorods

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(Received 09 April 2013; published online 12 July 2013)

The structural model of the nanocomposite (a thin substrate), with a doubly periodic system of nanorods grown on it, is proposed. It is supposed that nanorod (nanotube) elastic moduli have been obtained by a molecular dynamic method or experimentally, and they are known. The problem is reduced to the integral equation from which the functionals determining the nanocomposite effective moduli are constructed. The results of computations are given.

Keywords: Nanocomposite, Structural model, Effective elastic modules

PACS numbers: 62.23.Pq, 62.25. – g, 02.70.Pt. 46.15. – x

1. INTRODUCTION

The problem of determining the effective mechanical properties of nanocomposites is widely discussed in the literature [1-5]. The present work contains the analytical solution of the averaging problem of the elastic properties of the plate (substrate) stiffened by the regular system of nanorods. A nanorod is defined as the discrete formation of atoms which interatomic bonds are realized through the forces of their interaction. While the interaction between the nanorods takes place through the material medium (substrate). Therefore, the nanocomposite mechanic problems can be set and solved using the structural theory of composite materials in the framework of continuum mechanics [6] taking into account certain mechanical characteristics of nanorods, which can be obtained, for example, by experiment or with the molecular dynamics methods considering the different interactions.

2. PROBLEM FORMULATION

The regular (doubly periodic) system of nanorods (nanotubes) is grown on a substrate, which is a thin plate or sufficiently rigid film. They are directed along the axis Ox and continuously bonded with the substrate (Fig. 1). Let us use ω_1 and ω_2 ($\mathrm{Im}\,\omega_1 = 0$, $\mathrm{Im}\,(\omega_2/\omega_1) > 0$) to denote main periods of the structure. The rod is a segment L with length $2l$ where end-points are $a = -l$, $b = l$. Rods centres form a doubly periodic system of points $P = m\omega_1 + n\omega_2$ ($m, n = 0, \pm 1, \pm 2,\ldots$). We denote by $\langle\sigma_{ik}\rangle$ ($i, j = 1, 2$) the average stress acting in the domain occupied by this system.

Within the framework of the given model the load is transferred from the substrate to the rod with the help of tangential stresses $q_0(t)$. While composing the equilibrium equation of the rod element in the direction of the axis Ox, we express the normal force in the rod via the linear tangential load of intensity $q_0(t)$

$$P(t_0) = -\int_{t_0}^{b} q_0(t)dt,\ P(b) = 0,$$
$$P(t) = -\int_{a}^{b} q_0(t)dt = 0,\ \mathrm{Im}\,t = 0. \tag{1}$$

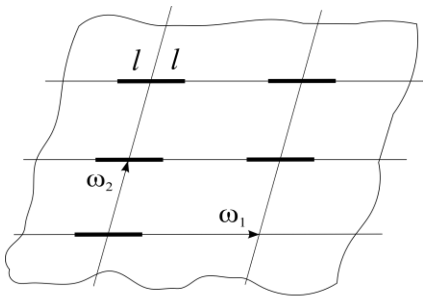

Fig. 1 – Scheme of the regular structure

Based on the model of the plane stress state [7] the displacements and stresses in the substrate can be expressed in terms of two analytic functions in the domain under consideration by the formulas

$$h(z) = 2\mu(u_1 + iu_2) = \kappa\varphi(z) - z\overline{\Phi}(z) - \overline{\psi}(z), \tag{2}$$
$$(\sigma_{11} + \sigma_{22}) = 4\,\mathrm{Re}\,\Phi(z),$$
$$(\sigma_{22} - \sigma_{11} + 2i\sigma_{12}) = 2\ \bar{z}\Phi'(z) + \Psi(z)\ ,$$
$$\Phi(z) = \varphi'(z),\ \Psi(z) = \psi'(z).$$

The resultant vectors of the forces acting in the structure along any arc is defined by formula (per unit thickness of the substrate)

$$(X + iY) = \int_{AB} (X_n + iY_n)ds = -ig(z)_A^B. \tag{3}$$

where

$$g(z) = \varphi(z) + z\overline{\Phi}(z) + \overline{\psi}(z).$$

Integral representations of analytic functions, which ensure doubly periodic distribution of the stress tensor in the plate, we take of the form [6]

$$\delta\Phi(z) = \frac{1}{2\pi(\kappa+1)}\int_L q_0(t)\zeta(t-z)dt + A_1, \tag{4}$$
$$\delta\Psi(z) = \frac{\kappa}{2\pi(\kappa+1)}\int_L q_0(t)\zeta(z-t)dt -$$
$$-\frac{1}{2\pi(\kappa+1)}\int_L q_0(t)\ \wp_1(z-t) + \bar{t}\wp(z-t)\ dt + A_2,$$

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where $\kappa = (3 - \nu)/(1 + \nu)$; ν – Poisson's ratio of the substrate material; A_1, A_2 – constants determined from the conditions of existence in the structure of the specified average stress $\langle\sigma_{ik}\rangle$; $\wp(z)$ and $\zeta(z)$ – the doubly periodic and the quasi-periodic Weierstrass functions [8]; $\wp_1(z)$ – the special meromorphic function [9], δ – substrate thickness.

3. QUASIPERIODICITY OF THE DISPLACEMENT VECTOR AND THE RESULTANT VECTOR OF FORCES ON THE ARC

Integrating the functions (4), we have

$$\delta\varphi(z) = -\frac{1}{2\pi(\kappa+1)}\int_L q_0(t)\nu_*(t-z)dt + A_1 z\,, \qquad (5)$$

$$\delta\psi(z) = \frac{\kappa}{2\pi(\kappa+1)}\int_L q_0(t)\nu_*(z-t)dt -$$

$$-\frac{1}{2\pi(\kappa+1)}\int_L q_0(t)\left\{\wp_1^{(-1)}(z-t) + \bar{t}\,\wp^{(-1)}(z-t)\right\}dt + A_2 z$$

where [6]

$$\nu_*'(z) = \zeta(z)\,,\ \ \wp^{(-1)} = -\zeta(z)\,,\ \ \wp_1^{(-1)}(z) = \int\wp_1(z)dz\,,$$

$$\nu_*(z+\omega_m) - \nu_*(z) = \pi i + \delta_m(z+\omega_m/2),$$

$$\delta_m = 2\zeta(\omega_m/2),\ \ (m=1,2)$$

$$\wp_1^{(-1)}(z+\omega_m) - \wp_1^{(-1)}(z) = -\bar{\omega}_m\zeta(z) + \gamma_m z + \gamma_m^*,$$

$$\gamma_2\omega_1 - \gamma_1\omega_2 = \delta_1\bar{\omega}_2 - \delta_2\bar{\omega}_1\,,\ \ \delta_1\omega_2 - \delta_2\omega_1 = 2\pi i.$$

According to (5), we get

$$\delta(z)_z^{z+\omega_n} = A_1\omega_n + B\delta_n\ \ (n=1,2)\,, \qquad (6)$$

$$\delta\,h(z)\Big|_z^{z+\omega_n} = \omega_n(\kappa A_1 - \bar{A}_1) - \bar{A}_2\bar{\omega}_n$$

$$-\,B\left[\bar{\delta}_n(1-\kappa) + \bar{\gamma}_n\right] + B\kappa\delta_n,$$

$$\delta g(z)\Big|_z^{z+\omega_n} = 2\omega_n\operatorname{Re}A_1 + \bar{A}_2\bar{\omega}_n + B\left[\delta_n + (1-\kappa)\bar{\delta}_n + \bar{\gamma}_n\right],$$

$$B = \frac{1}{2\pi(\kappa+1)}\int_L t q_0(t)dt\,.$$

Let us write the conditions of existence in the structure of the averaged stresses $\langle\sigma_{ik}\rangle$. Assuming, that lattice is a rectangular ($\omega_2 = iH$), and by using formula (3) for the resultant vector of forces on the arc, we have

$$\left[\langle\sigma_{11}\rangle + i\langle\sigma_{12}\rangle\right]H = -ig(z)\Big|_z^{z+\omega_2}\,,$$

$$\left[\langle\sigma_{21}\rangle + i\langle\sigma_{22}\rangle\right]\omega_1 = -ig(z)\Big|_{z+\omega_1}^{z}\,. \qquad (7)$$

Conditions (6) and (7) result in the system of equations for the constant A_1 and A_2

$$\begin{cases} H\left\{\langle\sigma_{11}\rangle + i\langle\sigma_{12}\rangle\right\}\delta = -i\left\{2(\operatorname{Re}A_1)\omega_2 + \bar{A}_2\bar{\omega}_1 + \right. \\ \qquad\qquad \left. +\left[\delta_2 + \bar{\delta}_2(1-\kappa) + \bar{\gamma}_2\right]B\right\} \\ \omega_1\left\{\langle\sigma_{12}\rangle + i\langle\sigma_{22}\rangle\right\}\delta = i\left\{2\operatorname{Re}A_1\omega_1 + \bar{A}_2\bar{\omega}_2 + \right. \\ \qquad\qquad \left. +\left[\delta_1 + \bar{\delta}_1(1-\kappa) + \bar{\gamma}_1\right]B\right\} \end{cases}$$

The solution to this system is

$$\operatorname{Re}A_1 = \delta\frac{\langle\sigma_{11}\rangle + \langle\sigma_{22}\rangle}{4} + \frac{B}{F}\left[\pi(1+\kappa)/2 - H\operatorname{Re}\delta_1\right], \qquad (8)$$

$$A_2 = \delta\frac{\langle\sigma_{22}\rangle - \langle\sigma_{11}\rangle + 2i\langle\sigma_{12}\rangle}{2} -$$

$$-\frac{B}{F}\left[\pi(1+\kappa) + H(\gamma_1 - \kappa\delta_1)\right],$$

$$F = \omega_1 H.$$

In virtue of the structure symmetry it was taken into account that both lattice constants δ_1, γ_1, and the functional B are real quantities.

Thus, the integral representations (4) in the presence of Eqs. (8) are correct in the sense that they provide: double-periodicity of the stress field in the structure; quasi-periodicity of the displacement vector and the resultant vector of forces on the arc connecting the congruent points, the existence of the specified average stresses $\langle\sigma_{11}\rangle$, $\langle\sigma_{12}\rangle$, $\langle\sigma_{22}\rangle$, at any density satisfying condition

$$\int_L q_0(t)dt = 0\,. \qquad (9)$$

4. INTEGRAL EQUATIONS OF THE STRUCTURE SUBSTRATE-NANORODS

According to (2), the deformation e_{11} of the substrate along the nanorod axis is defined by the following formula at $z = t_0 \in L$

$$2\mu e_{11} = \partial_1\operatorname{Re}\left\{\kappa\varphi(z) - z\bar{\Phi}(z) - \bar{\psi}(z)\right\} =$$

$$= \operatorname{Re}\left\{(\kappa-1)\Phi(z) - \bar{z}\Phi'(z) - \Psi(z)\right\}.$$

The deformation of the rod at the point $t_0 \in L$ in view of (1) is

$$e_0 = -\frac{1}{E_0F_0}\int_{t_0}^{l} q_0(t)dt\,,$$

where E_0, F_0 – the Young's modulus and the nanorod cross-section area, respectively

By setting deformation of the substrate equal to deformation of the rod on L, we get the singular integrodifferential equation

$$\int_L q_0(t)K(t-t_0)dt + \beta_*(t_0)\int_{t_0}^{b} q_0(t)dt + M_*\left\{q_0(t)\right\} = N_*\,, \qquad (10)$$

$$K(t) = \operatorname{Re}\left\{\zeta(t) + \frac{t\bar{\wp}(t) - \bar{\wp}_1(t)}{2\kappa - 1}\right\},$$

$$M_*\left\{q_0(t)\right\} = \left[\frac{\pi(1+\kappa)^2}{2(2\kappa-1)F} - \frac{(2\kappa-1)\operatorname{Re}\delta_1 - \operatorname{Re}\gamma_1}{(2\kappa-1)\omega_1}\right]\int_L t q_0(t)dt,$$

$$\beta_*\left\{t_0\right\} = \frac{4\pi E\delta}{(1+\nu)(5-3\nu)E_0F_0(t_0)},$$

$$N^* = \frac{\pi(\kappa+1)\delta}{2(2\kappa-1)}\left[(3-\kappa)\langle\sigma_{22}\rangle - (1+\kappa)\langle\sigma_{11}\rangle\right].$$

Where E – the elastic modulus of the substrate material; δ and ν – the thickness and the Poisson's ratio of the substrate. The equation (10) combined with the additional condition (9) clearly determines the solution $q_0(t)$ on L.

However, we can not make computations using the system (9), (10). First, we have to reduce it to the dimensionless form and equalize the orders of its terms.

Let us introduce the dimensionless variables

$$\xi = \frac{t}{l},\ \xi_0 = \frac{t_0}{l},\ \lambda = \frac{2l}{\omega_1},\ q_0(t) = \langle\sigma\rangle q(\xi),$$
$$w = \frac{t}{\omega_1} = \frac{\lambda\xi}{2},\ \langle\sigma\rangle = \langle\sigma_{11}\rangle + \langle\sigma_{22}\rangle,\ \frac{H}{\omega_1} = \varepsilon.$$

Then, taking into account the decompositions [6],

$$\omega\zeta(t) = \frac{1}{w} - \sum_{j=1}^{\infty}\rho_{2j+2}w^{2j+1},$$
$$\omega_1^2\rho(t) = \frac{1}{w^2} + \sum_{j=1}^{\infty}(2j+1)\rho_{2j+2}w^{2j},$$
$$\omega_1\rho_1(t) = \sum_{j=1}^{\infty}(2j+2)\rho_{2j+3}^{(1)}w^{2j+1},$$
$$\rho_{2j+2} = \sum_{m,n}{}' \left(\frac{1}{m+n\alpha}\right)^{2j+2},$$
$$\rho_{2j+3}^{(1)} = \sum_{m,n}{}' \frac{m+n\bar{\alpha}}{(m+n\alpha)^{2j+3}} \quad (m,n = 0,\pm1,\pm2,\pm,...)$$

we represent the system (9), (10) as

$$\int_{-1}^{1} q(\xi)G(\xi-\xi_0)d\xi + +\beta(\xi_0)\int_{\xi_0}^{1} q(\xi)d\xi + M\{q(\xi)\} = N \qquad (11)$$

Where

$$G(\xi) = \frac{1}{\xi} + \frac{\lambda}{2\kappa}\sum_{j=1}^{\infty}\left(\frac{\lambda\xi}{2}\right)^{2j+1}\left[(j-\kappa+1)\rho_{2j+2} - (j+1)\rho_{2j+3}^{(1)}\right]$$
$$M\{q(\xi)\} = \frac{\lambda^2}{8\kappa\varepsilon}\Big[0{,}5\pi(\kappa+1)^2 + +4\varepsilon\left[r_2 - (2\kappa-1)r_1\right]\Big]\int_{-1}^{1}\xi q(\xi)d\xi\Big],$$
$$\beta(\xi_0) = \frac{4\pi E\delta l}{(1+\nu)(3-\nu)E_0F_0(\xi_0)},$$
$$N = \frac{\pi(\kappa+1)\delta}{4\kappa}\left[(3-\kappa)\frac{\langle\sigma_{22}\rangle}{\langle\sigma\rangle} - (1+\kappa)\frac{\langle\sigma_{11}\rangle}{\langle\sigma\rangle}\right],$$
$$r_1 = 1 - \sum_{j=1}^{\infty}\frac{\rho_{2j+2}}{2^{2j+2}},\ r_2 = -1 + \sum_{j=1}^{\infty}\left[-\frac{2j+1}{2^{2j+2}}\rho_{2j+2} + \frac{j+1}{2^{2j+1}}\rho_{2j+3}^{(1)}\right]$$

The additional condition is

$$\int_{-1}^{1} q(\xi)d\zeta = 0 \qquad (12)$$

5. NANOCOMPOSITE MODEL

Let us suppose that $q^c(\xi)$ is the standard solution to the system of equations (11), (12) determined by formula (where $\langle\sigma_{11}\rangle \neq 0$, $\langle\sigma_{22}\rangle \neq 0$, $\langle\sigma_{12}\rangle = 0$)

$$q(\xi) = [(k+1)\langle\sigma_{11}\rangle + (k-3)\langle\sigma_{22}\rangle]\delta q^c(\xi). \qquad (13)$$

According to (13) functional B can be written as follows

$$B = \frac{l^2 b_{11}^c\delta}{2\pi(k+1)}\left[(k+1)\langle\sigma_{11}\rangle + (k-3)\langle\sigma_{22}\rangle\right].$$

Where

$$b_{11}^c = \int_{-1}^{1}\xi q^c(\xi)d\xi .$$

The average deformations in the structure can be found by formulas from [6]

$$\langle e_{11}\rangle = \frac{1}{\omega_1}u_1(z)\Big|_z^{z+\omega_1},$$
$$\langle e_{22}\rangle = \frac{1}{\operatorname{Im}\omega_2}u_2(z)\Big|_z^{z+\omega_2} - \frac{\operatorname{ctg}\alpha}{\omega_1}u_2(z)\Big|_z^{z+\omega_1},$$
$$2\langle e_{12}\rangle = \frac{1}{\omega_1}\left[u_2(z) - u_1(z)\operatorname{ctg}\alpha\right]\Big|_z^{z+\omega_1} + \frac{1}{\operatorname{Im}\omega_2}u_1(z)\Big|_z^{z+\omega_2}.$$

By performing the prescribed in Eqs. (6) operations of the calculation of displacement increments in congruent points and taking into account, that $\operatorname{Re}\omega_2 = 0$ in case considered here, we obtain the equations of the structure macromodel.

$$\langle e_{11}\rangle = \langle a_{11}\rangle\langle\sigma_{11}\rangle + \langle a_{12}\rangle\langle\sigma_{22}\rangle$$
$$\langle e_{22}\rangle = \langle a_{21}\rangle\langle\sigma_{11}\rangle + \langle a_{22}\rangle\langle\sigma_{22}\rangle \qquad (14)$$

where

$$\langle a_{11}\rangle = \frac{1}{\langle E_1\rangle} = \frac{1}{E}(1+\Delta),\ \langle a_{12}\rangle = -\frac{\nu}{E}(1+\Delta),$$
$$\langle a_{22}\rangle = \frac{1}{\langle E_2\rangle} = \frac{1}{E}(1+\nu^2\Delta),\ \Delta = \frac{(k+1)l^2 b_{11}^c}{F}.$$

As it follows from (14), the macromodulus $\langle a_{11}\rangle$ has the most sufficient changes, the absolute value of $\langle a_{12}\rangle$ is equal to $\nu\langle a_{11}\rangle$, the value of $\langle a_{22}\rangle E$ changes as $1 + O(\nu^2)$. It can be explained by the fact that the rods are oriented along the axis Ox and their presence has insignificant effect on the shift deformations of the structure.

6. ANALYSIS OF NUMERICAL RESULTS

Let us consider a nanocomposite of tetragonal structure $\omega_1 = 100$ nm, $\omega_2 = \omega_1 i$, which is a silicon substrate with carbon nanotubes (CNTs) grown on it. According to [10], we choose the following mechanical properties of the substrate material: Young's modulus of 165 GPa, Poisson's ratio = 0.22. Based on [11], the Young's modulus of CNTs may vary in range 900-1800 GPa and the diameter of the tubes is 10-30 nm. The curves for the nanocomposite relative macromoduli $\langle E_i^r\rangle = \langle E_i\rangle/E$ $i = 1, 2$ and $\langle\nu^r\rangle = \langle\nu\rangle/\nu$ are constructed in the following figures.

Fig. 2, 3 show the relative effective mechanical properties of the tetragonal structure nanocomposite as functions of the parameter $\lambda = 2l/\omega_1$. Here the CNT Young's modulus is $E_0 = 1800$ GPa, thickness of the substrate is $\delta = 150$ nm. Plotted in Fig. 2, curves 1-3 correspond to the moduli $\langle E_1^r\rangle, \langle E_2^r\rangle$ and $\langle \nu^r\rangle$, and the diameter of the nanotube is 30 nm, while Fig. 3 shows the changes in values of the averaged Young's modulus $\langle E_1^r\rangle$ with the nanotube length increasing. The curves 1-3 are constructed for nanotube diameters: 10, 20, 30 nm, respectively.

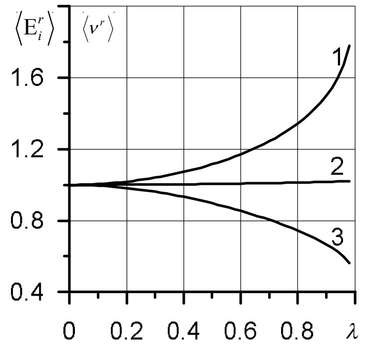

Fig. 2 – Dependences of the relative macromoduli of the tetragonal structure nanocomposite ($\omega_1 = 100$ nm) versus parameter λ. Substrate thickness is $\delta = 150$ nm, nanotube diameter is 30 nm

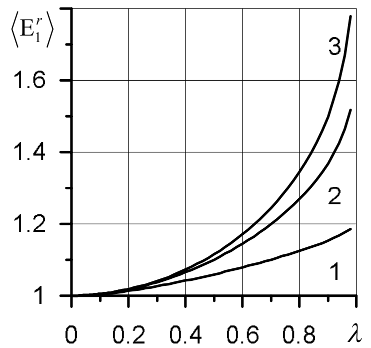

Fig. 3 – Dependences of the relative macromodulus of the tetragonal structure nanocomposite (100 nm) as a function of the parameter λ, substrate thickness is $\delta = 150$ nm, the curves 1-3 are plotted for nanorods with diameters 10, 20 and 30 nm, respectively

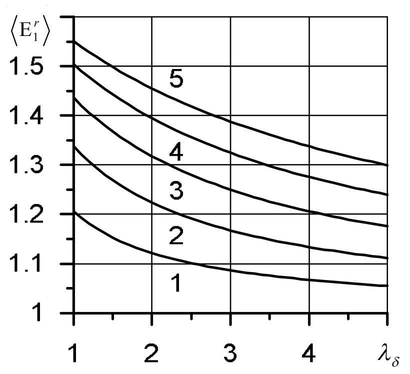

Fig. 4 – Dependences of the relative macromodulus of the tetragonal structure nanocomposite (100 nm)as a function of the parameter $\lambda_\delta = 2\delta/\omega_1$. The curves 1-5 are constructed for nanorods with diameter 10, 15, 20, 25 and 30 nm, respectively. The relative nanorod length is $\lambda = 0.9$

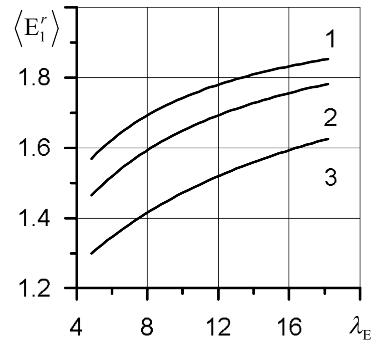

Fig. 5 – Dependences of the relative macromodulus of the tetragonal structure nanocomposite (100 nm) as a function of the parameter $\lambda_E = E_0/E$. The curves 1-3 are plotted for different substrate thickness 100, 150, 300 nm, respectively. The relative nanorod length is $\lambda = 0.96$

The dependence of the nanocomposite mechanical characteristics as functions of the substrate thickness is shown in Fig. 4. The curves 1-5 represent changes of the macromodulus $\langle E_1^r\rangle$ versus $\lambda_\delta = 2\delta/\omega_1$ when the nanotube diameter is 10, 15, 20, 25 and 30 nm, respectively. Here the Young's modulus of CNTs is $E_0 = 1800$ GPa, the relative length of the tube is $\lambda = 0.9$.

Let us consider the influence of nanotube Young's modulus values on the values of nanocomposite macromodulus. Fig. 5 shows the dependence of the macromodulus $\langle E_1^r\rangle$ versus $\lambda = E_0/E$. The curves 1-3 are plotted for various substrate thickness: 100, 150, 300 nm, in the case of the fixed relative nanorod length $\lambda = 0.96$.

7. CONCLUSION

The paper presents the model of the nanocomposite (the doubly periodic system of nanorods (nanotubes) grown on a thin substrate) constructed by the regular structures method. The effective moduli of elasticity of such medium obtained in the closed form via functionals built on the solution of singular integral equations of the first kind, containing the complete set of data about the geometric and physical properties of the nanostructure fundamental cell.

As follows from the results, macromoduli strongly depend on the diameter and length of the nanotubes, the thickness of the substrate, as well as the mechanical characteristics of the pair substrate-nanorod. Thus, the relative macromodulus $\langle E_1^r\rangle$ has the most significant changes, the absolute value of relative average Poisson's ratio $\langle \nu^r\rangle$ is equal to $1/\langle E_1^r\rangle$, the value of $\langle E_2^r\rangle$ is changed as $1 + O(\nu^2)$. It can be explained by the fact that the rods are arranged along the axis Ox, and their presence has insignificant effect on the shear strain of the system.

It is possible to solve the inverse problem, i.e. to determine mechanical properties of nanorods, if the effective modules of substrate – nanorods system are obtained as a result of the experiment. It should be noted that a stable solution of such problem may be derived at rather close packing of nanorods in a lattice: the cell area F must be of the order l^2.

Модель упругой пластины подкрепленной регулярной системой наностержней

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Предложена структурная модель нанокомпозита, представляющего собой тонкую подложку, на которой выращена двоякопериодическая система наностержней. Предполагается, что модули упругости наностержня (нанотрубки) получены методом молекулярной динамики или экспериментально и известны. Задача сведена к интегральному уравнению, из которого получены функционалы, определяющие эффективные модули нанокомпозита. Приведены результаты расчетов.

Ключевые слова: Нанокомпозит, Структурная модель, Эффективные модули упругости.

Модель пружної пластини підкріплена регулярною системою нанострижнів

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Запропонована структурна модель нанокомпозиту, яка представлена у вигляді підкладки, на якій вирощена двоякоперіодична система нанострижнів. Передбачається, що модулі пружності нанострижня (нанотрубки) отримані методом молекулярної динаміки або експериментально і відомі. Задача зведена до інтегрального рівняння, з якого отримані функціонали, що визначають ефективні модулі нанокомпозиту. Приведені результати розрахунків.

Ключові слова: Нанокомпозит, Структурна модель, Ефективні модулі пружності.

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