

Structural Model of Nanocomposite with Anisotropic Matrix

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A structural model of the nanocomposite (a thin anisotropic substrate on which a double-periodical system of nanorods been grown) is proposed. To determine the effective elastic parameters of nanocomposite the method of regular structures was used. Numeric results were achieved by the method of mechanical quadrature.

Keywords: nanomposite, anisotropic matrix, structural model, effective elastic modules

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1. INTRODUCTION

The problem of determining the effective mechanical properties of nanocomposites is widely discussed in the literature [1-4]. The present work contains the analytical solution of the averaging problem of the elastic properties of an anisotropic 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 [5] 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

Let us assume that a regular (doubly periodic) system of nanorods (nanotubes) has been grown on the substrate (Fig. 1) which is a thin anisotropic plate or film. Nanorods are directed along the axis Ox_1 and continuously bonded with a substrate. Let us denote the main structure periods with ω_1 and ω_2 ($\text{Im } \omega_1 = 0$, $\text{Im}(\omega_2 / \omega_1) > 0$). The rods are placed along the parallel segments $L_k = (a_k, b_k)$, $\text{Im } a_k = \text{Im } b_k = h_k$, $k = \overline{1, N}$ their centres form doubly periodic point systems $0,5(a_k + b_k) + ih_k + m\omega_1 + n\omega_2$ ($m, n = 0, \pm 1, \pm \dots$). We denote by $\langle \sigma_{ij} \rangle$ ($i, j = 1, 2$) the average stresses acting in the domain occupied by this system.

Within the framework of the line contact model the load from the substrate to the rod L_k in a point t_0 is transferred via the tangent contact force $q_k(t)$, $t \in L_k$. Composing the equilibrium equation of the rod element L_k in Ox_1 axis dimension, we express the normal force in it through the linear contact force $q_k(t)$.

$$Q_k(t_0) = -\int_{t_0}^{b_k} q_k(t) dt \quad (k = \overline{1, N}) \quad (1)$$

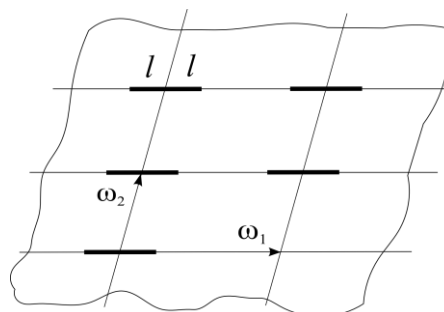


Fig. 1 – Scheme of the regular structure

In accordance with the line contact model, let us demand that the normal stress σ_{22} , displacements u_1 , u_2 and their derivatives be continuous and the stress σ_{12} be discontinuous along the segment L_k . We have

$$\begin{aligned} [\sigma_{22}]_k &= 0, [\partial_1 u_1]_k = [\partial_1 u_2]_k = 0, \\ [\sigma_{12}]_k &= \frac{-q_k(t)}{\delta}, \partial_i f = \frac{\partial f}{\partial x_i} \end{aligned} \quad (2)$$

where $[f]_k$ is a jump of function f on L_k , more precisely $[f]_k = f^-(t) - f^+(t)$ where the sign $(-)$ corresponds to the lower edge of rod L_k while we are moving from its beginning a_k to the end b_k , δ is the substrate thickness. The stresses and displacements in anisotropic medium are defined by the formulas [5,6]

$$\{\sigma_{11}, \sigma_{12}, \sigma_{22}\} = 2 \text{Re} \sum_{v=1}^2 \{\mu_v^2, -\mu_v, 1\} \Phi'_v(z_v), \quad (3)$$

$$\{u_1, u_2\} = 2 \text{Re} \sum_{v=1}^2 \{p_{1v}, p_{2v}\} \Phi_v(z_v), \quad z_v = x_1 + \mu_v x_2$$

$$p_{1v} = s_{11}\mu_v^2 + s_{12} - s_{16}\mu_v, \quad p_{2v} = s_{12}\mu_v + s_{22}\mu_v^{-1} - s_{26},$$

where μ_v – roots of characteristic equation

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$$(\mu_1 \neq \mu_2, \text{Im } \mu_\nu > 0, \nu = 1, 2)$$

$$s_{11}\mu^4 - 2s_{16}\mu^3 + (2s_{12} + s_{66})\mu^2 - 2s_{26}\mu + s_{22} = 0. \quad (4)$$

The material elastic flexibilities s_{ij} are represented in the Hook's law for anisotropic body [6]

$$\begin{aligned} e_{11} &= s_{11}\sigma_{11} + s_{12}\sigma_{22} + s_{16}\sigma_{12} \\ e_{22} &= s_{12}\sigma_{11} + s_{22}\sigma_{22} + s_{26}\sigma_{12} \\ 2e_{12} &= s_{16}\sigma_{11} + s_{26}\sigma_{22} + s_{66}\sigma_{12} \end{aligned} \quad (5)$$

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

$$\begin{aligned} X + iY &= \int_{AB} (X_n + iY_n) ds = -ig(z) \Big|_A^B \\ g(z) &= \sum_{\nu=1}^2 \left\{ (1 + i\mu_\nu) \varphi_\nu(z_\nu) + (1 + i\overline{\mu_\nu}) \overline{\varphi_\nu(z_\nu)} \right\} \end{aligned} \quad (6)$$

3. INTEGRAL REPRESENTATIONS OF THE SOLUTIONS

Let us assume that

$$\begin{aligned} \Phi_\nu(z_\nu) &= z_\nu A_\nu + \frac{\alpha_\nu^*}{2\pi i \delta} \int q(t) \ln \sigma(t_\nu - z_\nu) dt_\nu, \\ \Phi'_\nu(z_\nu) &= A_\nu - \frac{\alpha_\nu^*}{2\pi i \delta} \int q(t) \zeta(t_\nu - z_\nu) dt_\nu, \\ \text{Im } q(t) &= 0, \quad t_\nu = \text{Re } t + \mu_\nu \text{Im } t, \quad t \in L = UL_k \end{aligned} \quad (7)$$

Where $\zeta(z_\nu), \sigma(z_\nu)$ - determined on the periods $\omega_1^{(\nu)} = \omega_1, \omega_2^{(\nu)} = \text{Re } \omega_2 + \mu_\nu \text{Im } \omega_2$, Weierstrass dzeta and sigma functions [7,8] in affine plane of z_ν , $q(t) = \{q_k(t), t \in L_k\}$ is unknown density that should be determined, the constants A_ν are to provide presence of average stresses $\langle \sigma_{ij} \rangle$ in the structure, coefficients α_ν^* are defined based on conjugation conditions (2).

According to Sokhotskiy-Plemel formulas [5], let us write down limiting values of the function $\Phi'_\nu(z_\nu)$ at the edges of segments L_k . As a result we have

$$\begin{aligned} \left\{ \Phi'_\nu(z_\nu) \right\}_{z \rightarrow t_0 \in L_k}^\pm &= A_\nu - \frac{\alpha_\nu^*}{\delta} \left\{ \pm \frac{q_k(t_0)}{2} + \right. \\ &\left. + \frac{1}{2\pi i} \int_L q(t) \zeta(t_\nu - t_0^{(k)}) dt_\nu \right\} \\ t_{\nu 0}^{(k)} &= \text{Re } t_0^{(k)} + \mu_\nu \text{Im } t_0^{(k)}, \quad t_0 \in L_k \end{aligned} \quad (8)$$

Where the upper sign refers to the upper (lower) edge of the segment L_k while we are moving from its beginning a_k to the end b_k .

Substitution of the limiting values (8) into Eq. (2) and taking into account Eq. (3) yields the system of linear algebraic equations of the Vandermonde type, which is uniquely solvable due to $\mu_1 \neq \mu_2$ [5].

$$\text{Re } \sum_{\nu=1}^2 \mu_\nu^{n-1} \alpha_\nu^* = B_n \quad (n = 0, 1, 2, 3), \quad (9)$$

$$B_0 = -s_{12}/2s_{22}, \quad B_1 = 0, \quad B_2 = 1/2, \quad B_3 = s_{16}/2s_{11}$$

Thus functions (7) with coefficients α_ν^* , determined by the system (9), provide conditions of continuous conjugation of the nanorod with the substrate.

Let us determine the increments of the function $\Phi'_k(z_k)$ at the periods ω_1 and $\omega_2^{(\nu)}$. We deduce from Eqs. (7) with consideration of the quasi-periodicity of Weierstrass zeta-function the following expressions.

$$\Phi'_\nu(z_\nu + \omega_m^{(\nu)}) - \Phi'_\nu(z_\nu) = \alpha_\nu \delta_m^{(\nu)} c \quad (m, \nu = 1, 2) \quad (10)$$

where

$$c = \frac{1}{2\pi i} \int_L q(t) ds, \quad \alpha_\nu = \frac{\alpha_\nu^*}{\delta}, \quad \delta_m^{(\nu)} = 2\zeta\left(\frac{\omega_m^{(\nu)}}{2}\right), \quad t = s + ih_k$$

It follows from the Eqs. (3) and (10) that the fulfillment of the condition $c = 0$ produces the doubly periodicity of the stress field in the nanocomposite structure.

Now let us demonstrate that the displacement vector and the main stress vector on arc AB are quasi-periodic. For this purpose the increments of function $\Phi_\nu(z_\nu)$ at the periods are deduced with respect to group property of sigma-function [7].

$$\Phi_\nu(z_\nu + \omega_m^{(\nu)}) - \Phi_\nu(z_\nu) = \omega_m^{(\nu)} A_\nu - \frac{\alpha_\nu \delta_m^{(\nu)}}{2\pi i} \int t_\nu q(t) dt_\nu \quad (11)$$

The integral in (11) can be simplified, taking into account conditions $c = 0$ and $h_k = \text{const}$, as follows

$$\int_L t_\nu q(t) dt_\nu = \int_L (s + \mu_\nu h_k) q(t) ds = \int_L q(t) s ds. \quad (12)$$

Hence it yields

$$\begin{aligned} \Phi_\nu(z_\nu + \omega_m^{(\nu)}) - \Phi_\nu(z_\nu) &= A_\nu \omega_m^{(\nu)} - \alpha_\nu \delta_m^{(\nu)} l, \\ l &= \frac{1}{2\pi i} \int_L q(t) s ds \end{aligned}$$

Increments of the displacement and the resultant vector of forces in the arc are to be obtained from Eqs. (3), (6) with presence of the Eq. (12). We find out that

$$\begin{aligned} \{u_1, u_2\}_z^{z+\omega_m} &= 2 \text{Re} \sum_{\nu=1}^2 \{p_{1\nu}, p_{2\nu}\} \left(A_\nu \omega_m^{(\nu)} - \alpha_\nu \delta_m^{(\nu)} l \right) \\ \{X, Y\}_z^{z+\omega_m} &= 2 \text{Re} \sum_{\nu=1}^2 \{\mu_\nu, -1\} \left(A_\nu \omega_m^{(\nu)} - \alpha_\nu \delta_m^{(\nu)} l \right) \end{aligned} \quad (13)$$

Considering the two latter equations (13), as well as formulas (6), the constants A_ν ($\nu = 1, 2$) can be calculated based on the condition of the existing of the medium stresses $\langle \sigma_{ij} \rangle$ ($i, j = 1, 2$) in the structure. Thus we have:

$$\langle \sigma_{22} \rangle \omega_1 = 2 \text{Re} \sum_{\nu=1}^2 \left(A_\nu \omega_1 - \alpha_\nu \delta_1^{(\nu)} l \right)$$

$$\begin{aligned}
\langle \sigma_{12} \rangle \omega_1 &= -2 \operatorname{Re} \sum_{\nu=1}^2 \left(A_\nu \omega_1 - \alpha_\nu \delta_1^{(\nu)} l \right) \mu_\nu \\
\left\{ \langle \sigma_{11} \rangle \sin \alpha - \langle \sigma_{12} \rangle \cos \alpha \right\} \omega_2 &= \\
&= 2 \operatorname{Re} \sum_{\nu=1}^2 \mu_\nu \left(A_\nu \omega_2^{(\nu)} - \alpha_\nu \delta_2^{(\nu)} l \right) \\
\left\{ \langle \sigma_{22} \rangle \operatorname{ctg} \alpha - \langle \sigma_{12} \rangle \right\} \omega_2 &= 2 \operatorname{Re} \sum_{\nu=1}^2 \left(A_\nu \omega_2^{(\nu)} - \alpha_\nu \delta_2^{(\nu)} l \right)
\end{aligned} \quad (14)$$

After transforming of the first three equations in (14) we will find out that,

$$\begin{aligned}
2 \operatorname{Re} \sum_{\nu=1}^2 D_\nu \mu_\nu^k &= R_k \quad (k=0,1,2), \\
R_0 &= \langle \sigma_{22} \rangle, R_1 = -\langle \sigma_{12} \rangle, R_2 = \langle \sigma_{11} \rangle - \frac{2\pi i}{H \omega_1 \delta} \\
D_\nu &= A_\nu - \alpha_\nu l \frac{\delta_1^{(\nu)}}{\omega_1}, \quad H = \operatorname{Im} \omega_2
\end{aligned} \quad (15)$$

As the fourth equation in (14) is a linear combination of the first three equations mentioned above then the consistency condition of the system (14) should be written.

$$2 \operatorname{Re} \sum_{\nu=1}^2 \frac{\alpha_\nu}{\omega_1} 2\pi i l = 0, \quad (16)$$

It remains true due to the second equation in (9).

4. SYSTEM OF INTEGRAL EQUATIONS

Let us define the deformation compatibility conditions of the rods L_k with anisotropic substrate. According to Eq. (1) the rod deformation at the point $t_0 \in L_k$ is to be written down as follows:

$$e_{11}^c(t_0) = -\frac{1}{E_k F_k} \int_{t_0}^{b_k} q_k(t) dt, \quad (17)$$

where E_k, F_k is the Young's modulus and the nanorod's cross-sectional area.

The plate deformation along L_k is determined by formula (3)

$$e_{11}(t_0) = 2 \operatorname{Re} \sum_{\nu=1}^2 p_{1\nu} \left(A_\nu - \frac{\alpha_\nu}{2\pi i L} \int q(t) \zeta(t_v - t_{v0}^{(k)}) dt_v \right), \quad (18)$$

Considering the equations (15), (17) and (18) we transform the deformation compatibility condition of the substrate - nanorods to the following system:

$$\begin{aligned}
\sum_{m=1}^N \int_{-l_m}^{l_m} q_m(s_m) G(s_m, s_{0k}) ds_m - \\
-\frac{\pi}{E_k F_k} \int_{s_{0k}}^{l_k} q_k(s_k) ds_k &= f \quad (k=1, \overline{N}) \\
G(s_m, s_{0k}) &= \pi s_{11} s_m / \delta F_0 + \\
&+ \operatorname{Im} \sum_{\nu=1}^2 p_{1\nu} \frac{\alpha_\nu^*}{\delta} \left\{ \zeta(t_v^{(m)} - t_{v0}^{(k)}) - \frac{\delta_1^{(\nu)}}{\omega_1} s_m \right\}, \\
f &= \pi \left\{ s_{11} \langle \sigma_{11} \rangle + s_{12} \langle \sigma_{22} \rangle + s_{16} \langle \sigma_{12} \rangle \right\}, \quad F_0 = \omega_1 H \\
t_v^{(m)} &= s_m + \mu_\nu h_m, \quad t_{v0}^{(k)} = s_{0k} + \mu_\nu h_k, \quad -l_m \leq s_m, s_{0k} \leq l_m
\end{aligned} \quad (19)$$

If $m=n$ then the kernels $G(s_m, s_{0k})$ have singularities of Cauchy type, therefore the system (19) relates to a class of singular integro-differential equation systems.

The solution to such system is to be found in a class of unbounded functions at the ends of segments L_k [5]. Let us assume that

$$\begin{aligned}
q_k(s_k) ds_k &= \frac{Q_k(\beta)}{\sqrt{1-\beta^2}}, \\
s_k &= l_k \beta_k, \quad -1 < \beta_k < 1, \quad t \in L_k
\end{aligned} \quad (20)$$

In accordance with (20) a unique solution to the system (19) exists when the additional conditions take place:

$$\int_{-l_k}^{l_k} q_k(s_k) ds_k = 0 \quad (k=1, \overline{N}) \quad (21)$$

Equations (21) are conditions of equilibrium of nanorods. It should be noted that in case they are true, the system (14) will be automatically consistent.

5. AVERAGING OF NANOCOMPOSITE ELASTICITY PROPERTIES.

Independently of a cell microstructure, the regular (doubly periodic) structure is similar (in macro level) to homogeneous anisotropic medium. This means that during the transition from the arbitrary point z to the it congruent point $z+m\omega_1+n\omega_2$ the increments of displacements can be compared in the structure of nanocomposite and in the modeled homogeneous medium.

As result we have

$$\begin{aligned}
\omega_1 \langle e_{11} \rangle &= u_1(z+\omega_1) - u_1(z) = 2 \operatorname{Re} \sum_{\nu=1}^2 p_{1\nu} \Phi_\nu \Big|_{z_\nu}^{z_\nu+\omega_1} \\
\langle e_{11} \rangle h + (\langle e_{12} \rangle - \langle \varepsilon \rangle) H &= 2 \operatorname{Re} \sum_{\nu=1}^2 p_{1\nu} \Phi_\nu \Big|_{z_\nu}^{z_\nu+\omega_2^{(\nu)}}, \quad (22) \\
\omega_1 (\langle e_{12} \rangle + \langle \varepsilon \rangle) &= 2 \operatorname{Re} \sum_{\nu=1}^2 p_{2\nu} \Phi_\nu \Big|_{z_\nu}^{z_\nu+\omega_1}, \\
(\langle e_{12} \rangle + \langle \varepsilon \rangle) h + \langle e_{22} \rangle H &= 2 \operatorname{Re} \sum_{\nu=1}^2 p_{2\nu} \Phi_\nu \Big|_{z_\nu}^{z_\nu+\omega_2^{(\nu)}}, \\
h &= \operatorname{Re} \omega_2, \quad H = \operatorname{Im} \omega_2
\end{aligned}$$

where $\langle e_{ij} \rangle$ and $\langle \varepsilon \rangle$ are the averaged deformations and the averaged rotation of the fundamental cell, increments of $\Phi_\nu(z_\nu)$ function are determined in (12).

Considering the Eqs. (22), (12) and Legendre relation [7,8] in affine plane:

$$\delta_1^{(\nu)} \omega_2^{(\nu)} - \delta_2^{(\nu)} \omega_1 = 2\pi i \quad (\nu=1,2),$$

the average deformations can be found:

$$\begin{aligned}
\langle e_{11} \rangle &= s_{11} \langle \sigma_{11} \rangle + s_{12} \langle \sigma_{22} \rangle + s_{16} \langle \sigma_{12} \rangle - \frac{2\pi i l}{H \delta \omega_1} s_{11}, \quad (23) \\
\langle e_{22} \rangle &= s_{12} \langle \sigma_{11} \rangle + s_{22} \langle \sigma_{22} \rangle + s_{26} \langle \sigma_{12} \rangle - \frac{2\pi i l}{H \delta \omega_1} s_{12}, \\
2 \langle e_{12} \rangle &= s_{16} \langle \sigma_{11} \rangle + s_{26} \langle \sigma_{22} \rangle + s_{66} \langle \sigma_{12} \rangle - \frac{2\pi i l}{H \delta \omega_1} s_{16}.
\end{aligned}$$

Therefore, the average deformations depend upon the functional $2\pi il$ determined on solutions to the system (19), (21).

Let us suppose that $q_k^0(s_k)$ is the standard solution to the system corresponding to its right part $f = 1$. In this case the common solution will be determined through the standard one as follows:

$$q_k(s_k) = \pi \{s_{11} \langle \sigma_{11} \rangle + s_{12} \langle \sigma_{22} \rangle + s_{16} \langle \sigma_{12} \rangle\} q_k^0(s_k).$$

and the functional

$$2\pi il = \pi \{s_{11} \langle \sigma_{11} \rangle + s_{12} \langle \sigma_{22} \rangle + s_{16} \langle \sigma_{12} \rangle\} \gamma, \quad 24$$

$$\gamma = \sum_{k=1}^N \int_{-l_k}^{l_k} q_k^0(s_k) s_k ds_k$$

Then the Hook's law for nanocomposite macromodel can be obtained from (23), by entering the functional (24). It yields

$$\begin{aligned} \langle e_{11} \rangle &= \langle s_{11} \rangle \langle \sigma_{11} \rangle + \langle s_{12} \rangle \langle \sigma_{22} \rangle + \langle s_{16} \rangle \langle \sigma_{12} \rangle \\ \langle e_{22} \rangle &= \langle s_{12} \rangle \langle \sigma_{11} \rangle + \langle s_{22} \rangle \langle \sigma_{22} \rangle + \langle s_{26} \rangle \langle \sigma_{12} \rangle \\ 2 \langle e_{12} \rangle &= \langle s_{16} \rangle \langle \sigma_{11} \rangle + \langle s_{26} \rangle \langle \sigma_{22} \rangle + \langle s_{66} \rangle \langle \sigma_{12} \rangle, \end{aligned} \quad (25)$$

Here the effective (average, macroparameters) characteristics of a structure are determined by the following equations:

$$\begin{aligned} \langle s_{11} \rangle &= s_{11} \left(1 - \frac{\pi s_{11}}{\delta F_0} \gamma \right), \quad \langle s_{12} \rangle = s_{12} \left(1 - \frac{\pi s_{11}}{\delta F_0} \gamma \right), \\ \langle s_{16} \rangle &= s_{16} \left(1 - \frac{\pi s_{11}}{\delta F_0} \gamma \right), \quad \langle s_{22} \rangle = s_{22} \left(1 - \frac{\pi s_{12}^2}{s_{22} \delta F_0} \gamma \right), \\ \langle s_{26} \rangle &= s_{26} \left(1 - \frac{\pi s_{12} s_{16}}{s_{26} \delta F_0} \gamma \right), \quad \langle s_{66} \rangle = s_{66} \left(1 - \frac{\pi s_{16}^2}{s_{66} \delta F_0} \gamma \right), \\ \langle s_{12} \rangle &= \langle s_{21} \rangle, \langle s_{16} \rangle = \langle s_{61} \rangle, \langle s_{26} \rangle = \langle s_{62} \rangle, \quad F_0 = H \omega_1 \end{aligned} \quad (26)$$

6. NUMERICAL RESULTS

A composite substrate – nanorods is considered. A substrate material is a silicon (Si). The fundamental cell is of square shape. The characteristics of substrate material are $s_{11} = s_{22} = 7.7 \text{ GPa}^{-1}$, $s_{12} = -2.1 \text{ GPa}^{-1}$ [9].

The results of the calculations are represented in Figures 2.

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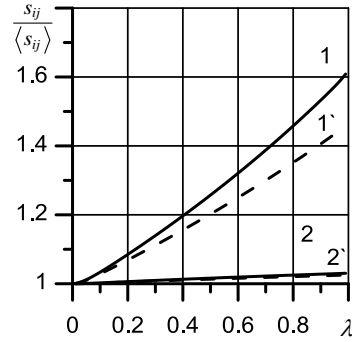


Fig. 2 – Dependence of the macroparameters as function of rods length. The substrate thickness equals $\delta = 150 \text{ nm}$ (solid line) and $\delta = 200 \text{ nm}$ (dash line).

The curves 1 (1') and 2 (2') are plotted for the ratio $a_{11}/\langle a_{11} \rangle$ and $a_{22}/\langle a_{22} \rangle$. The calculations are given for the following parameters of the composite: the cell size is $\omega_1 = 200 \text{ nm}$ and $|\omega_2| = 200 \text{ nm}$, the relative rod length is $\lambda = 2l/\omega_1$, Young's module of rods is $E = 1000 \text{ GPa}$ [3]. There are eight uniformly distributed nanorods with circle cross-section ($R = 5 \text{ nm}$) in a cell.

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 stated boundary problem about the compatible deformation of the rods and anisotropic substrate is reduced to the system of singular integro-differential equations with elliptical kernels. The effective moduli of elasticity of such medium obtained in the closed form via functionals built on the solution of system, containing the complete set of data about the geometric and physical properties of the nanostructure fundamental cell. As the result of numerical experiments, the dependences of macroparameters via relative length of rod are received. In case the substrate thickness equals to $\delta = 150$ (200) nm, the macroparameter $s_{11}/\langle s_{11} \rangle$ ranges from 1.0007 to 1.6086 (1.4599) and macroparameter $s_{22}/\langle s_{22} \rangle$ changes from 1.0001 to 1.0304 (1.0252).