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MECHANICS

Dynamics of Nanotube Twisting in a Viscous Fluid

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The synthesis of nanotubular formations and the study of their structure and properties represent a new line of inquiry in materials science [1]. The development of this branch is stimulated by the unusual properties of nanotubes and composite materials produced on their basis [1].

Promising original materials for obtaining nanotubes are compounds with a layered structure [2], for example, hydrosilicates [3]. Irrespective of the structure of the original components, under hydrothermal conditions, nanotubes start to form only after intermediate compounds with a layered structure have been formed; it is precisely from these compounds that nanotubes are formed in the next stage of the synthesis [3, 4]. The investigation of the conditions and dynamics of layer twisting for compounds with a layered structure and their subsequent recrystallization with the formation of nanotubes with a certain morphology is of great importance for understanding the mechanism of nanotube formation.

The possibility of nanotube formation by spontaneous twisting of layers under the action of internal stresses was mentioned as early as 1930 [5]. There are some works devoted to the mechanics of nanotube formation by means of the twisting of stressed nanolayers and the effect of the size factor on the mechanical properties of materials (see, for example, [6–8]). At the same time, the dynamics of the process of nanotube twisting as they are formed in fluid media has not yet been analyzed. A salient feature of nanotube formation in hydrothermal or other fluid media is that the viscous medium affects the twisting process. A double layer is rolled due to internal stresses caused by the incomplete structural correspondence of the constituent layers. Examples of layered chemical compounds with such a structure are compounds with a serpentine structure [2–5]. Under certain conditions (with increase in the interlayer space thickness δ" due to the intercalation of water or other components of the surrounding medium between the layers), a double layer of thickness δ' can be twisted into a circular cylinder, or a nanotube with an initial radius R_0 (Fig. 1) of the order of a few nanometers. The angular velocity ω of the nanotube is determined by the balance of two moments, namely, the internal force moment $M_E = \frac{E\delta'^3}{R}$ and the viscous friction moment $M_V = 2\pi\alpha R^2\mu\omega$. The Reynolds number of the viscous flow around the twisted nanotube can be estimated as $\mathrm{Re} = \frac{\delta'^3 E\rho}{2\pi\alpha R\mu^2}$. Here, E is Young's modulus of the nanotube, μ and ρ are the dynamic viscosity

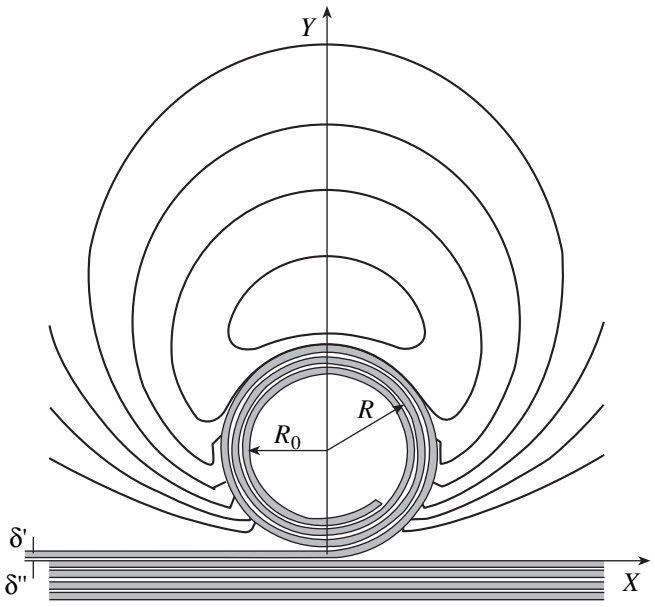

Fig. 1. Streamlines around a nanotube twisted from a double layer on the boundary of a viscous fluid.

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and density of the fluid, and α is a dimensionless parameter. For our estimates, we let $\alpha = 1$, $R \sim 5 \times 10^{-9}$ m, $\delta' \sim 2 \times 10^{-10}$ m, $E \sim 10^{11}$ Pa, $\mu \sim 10^{-2}$ kg/(m s), and $\rho \sim 300$ kg/m^3. The above values are typical of nanotube formation from layered compounds with a serpentine structure under hydrothermal conditions (near the critical point of water). In this case, we obtain Re ~ 10^{-4}. Although the values of the mechanical parameters, density, and viscosity can change in going over to nanodimensional objects [7, 9], these variations have little effect on the Reynolds number, which turns out to be low; this makes it possible to use the quasi-stationary Stokes approximation [10] for describing the flow. The solution to the biharmonic equation for the stream function Ψ with homogeneous conditions for Ψ and $\frac{\partial \Psi}{\partial n}$ imposed on the flat boundary of the layer and the condition $\nabla\Psi = -\omega r$ on the tube surface have the form

$$\Psi = 2R^2\omega\left[\frac{4Ry^3}{(x^2+y^2)^2} - \frac{3y^3}{x^2+y^2}\right] \quad (1)$$

The streamline pattern presented in Fig. 1 shows a vortex generated by the rotating nanotube. Using Eq. (1), we obtain $M_V = 2\pi\alpha R^2\mu\omega$, where $\alpha \approx \frac{12R_0}{\pi\delta'}$.

Let us write the total potential energy of the nanotube and that part of the double layer that has not yet been twisted in the form

$$U = \frac{E\delta'^3 L_0}{24R_0^2}L + \frac{E\delta'^3 L_0}{24}\int_0^{L_0-L}\left(\frac{1}{R(\zeta)} - \frac{1}{R_0}\right)^2 d\zeta, \quad (2)$$

where L and L_0 are the length of the nontwisted part of the nanolayer and its initial value, respectively; ζ is the coordinate measured along the nanotube coils; and R_0 is the equilibrium radius of the nanotube coil. Expression (2) makes it possible to calculate the elastic force moment M_E applied to the nanotube and the normal stress σ on its inner surface. Then the equality of the moments $M_E = M_V + M_A$, where M_A is the moment of the forces of nanotube adhesion to the nanolayer, yields the following equation of the dynamics of the outside radius R_2:

$$\frac{dr_2}{d\tau} = \frac{1}{r_2}\left[(1+\lambda r_1^4)\frac{r_2-0.5}{r_2^2} - \lambda r_1^2(r_1-0.5)\right] - \frac{m_A}{r_2^2}, \quad (3)$$

$$m_A = \frac{12R_0}{E\delta'^3}M_A.$$

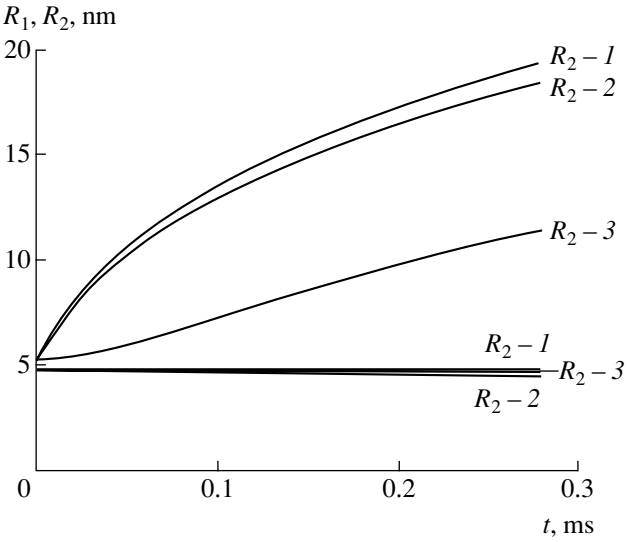

Fig. 2. Time dependence of the inner (R_1) and outer (R_2) radii of nanotube *1* without relative slipping of the coils in the case where the dimensionless adhesion force moment $m_A = 0$ and with regard for coil slipping in the case of (*2*) $m_A = 0$ and (*3*) $m_A = 0.5$.

Here,

$$r_1 = \frac{R_1}{R_0}, \quad r_2 = \frac{R_2}{R_0}, \quad \tau = \frac{E\delta'^3\delta}{48\pi^2\mu\alpha R_0^4}t,$$

$$\lambda = \frac{2\pi^2\alpha R_0^4}{L_0^2\delta^2}.$$

As the nanotube twists, its inner radius R_1 decreases, which leads to the displacement of the viscous fluid out of the hollow space of the tube. Equating the mechanical stress on the inside surface of the nanotube and the mean stress in the viscous fluid within the nanotube, we obtain the following equation for the dynamics of the inner radius:

$$\frac{dr_1}{d\tau} = -\lambda r_1^3\left(\frac{r_1-0.5}{r_1^2} - \frac{r_2-0.5}{r_2^2}\right). \quad (4)$$

Figure 2 presents the calculated dynamics of the outer and inner radii of a nanotube with the initial conditions $R_1(0) = R_0 - 0.5\delta$ and $R_2(0) = R_0 + 0.5\delta$ for different values of the adhesion force moment. It is assumed that the length and thickness of the original nanolayer are equal and have the order of 2 μm. As a limiting variant, we considered the nanotube twisting without relative slipping of its coils (in this case, Eqs. (3) and (4) can be considerably simplified). The characteristic time of twisting is proportional to the fluid viscosity.

Thus, the viscosity has a considerable effect on the layer twisting time. Within the considered range of viscosity ($\mu \sim 10^{-2}$–10^{-1} kg/(m s)), the characteristic time of twisting for a layer with a serpentine structure having a thickness of several micrometers amounts to several tenths of a second to several milliseconds (Fig. 2). The adhesion force moment can also have an appreciable effect on the nanotube twisting rate. Comparing the calculated time of twisting to the actual duration of the process of nanotube formation from layered compounds with the serpentine structure [2–4], as well as the calculated and measured nanotube lengths, we can conclude that the most prolonged stage of nanotube formation (at least, under hydrothermal conditions) is not layer twisting, but material recrystallization by means of mass transfer of the components through the hydrothermal medium. At the same time, in certain cases (in particular, at nanotube formation from exfoliated layered compounds in high-viscosity media), the twisting process can limit the nanotube formation rate. This situation can occur, for example, when nanocomposites are obtained by the method described in [11] in the cases where the nanolayers being formed are internally stressed double layers.

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