Nanocones rolling in hydro-thermal medium and flows in conical domains

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Abstract. In many applications of tubular nanostructures it is necessary to describe fluid flows through these systems, which have many specific features. Moreover, these flows play an important role in the processes of nanotubes formation. Our report is devoted to the description of these processes in conical nanostructures. Hydro-thermal method of nanotube formation is very effective. But it is often leads to formation of nanostructures of different morphology, particularly, nanocones. Process of nanocone formation due to rolling from plane structure in hydro-thermal medium is considered. The system comes to equilibrium if there is lattices correspondence between neighbor layers. Due to this reason the conical angle depends on the lattice parameters. This dependence is analyzed. Movement of the conical surface during the formation process leads to the appearance of flow in conical domain which has an influence on the formation process.

1. Introduction
Recently, the increasing interest was attracted to the problem of synthesis, studying of structural features, behaviour and properties of substance in nano-sized state. It is related, first of all, with unusual physical and chemical, optical, mechanical and other properties of such systems (see, e.g., [1]), and also with great prospects of practical use of nanocrystal constructional. The unusual behaviour of such objects in that case when at least one of characteristic sizes of particles does not exceed 10 nanometers is most expressed in nanotubes, owing to minimally admissible radius, capillary forces reach extremely possible value that opens unlimited possibilities for intercalation and synthesis of new composite nanomaterials and nanodevices with operated properties. It is worth noting, that so far there are no appropriate mathematical models of processes of nanotube formation. It limits the possibilities of forecasting of synthesis dynamics and its results.

The problem of nanotube formation is closely related with the problem of flows in nano-sized structures. Simple estimations [2] show that the Reynolds number for such flow is very small. Consequently, it is possible to use the Stokes approximation. Low Reynolds number flows in conical domains are intensively investigated [3], [4] starting from the well-known Moffatt work [5] It is possible to use two models for our structure: the domain between two cones with common vertex and the domain between two parallel cones. The first model allows one to obtain the solution in an analytical form (in this case one can make separation of the variables). For the second model one obtains the result by approximate calculations only.
### 2. Nanotube formation

The process of nanotube formation consists of several stages. The initial state is a sandwich structure of stressed double plane layers. Final result is the ensemble of nanotubes [7] in hydro-thermal medium (Fig. 1).

![Non-organic nanotubes Mg(Fe,Co,Ni)$_3$Si$_2$O$_5$(OH)$_4$](image)

Fig. 1. Non-organic nanotubes Mg(Fe,Co,Ni)$_3$Si$_2$O$_5$(OH)$_4$

The first stage is a separation of one double layer from the sample. The second stage is rolling of this layer and formation of tubular (cylindrical or conical) structure [2]. And the final stage is evolution of the ensemble of nanotubes in the hydro-thermal medium [6]. In the present paper we deal with the second stage. The case of cylinder was considered in [2]. To describe the dynamics of nanocone formation we use the model of stressed elastic layer. Taking into account the elastic forces, adhesion and liquid viscous friction, one obtains the corresponding dynamical equation. As a result, the average angular velocity of nanocone rolling is given by the following formula

$$\omega = \frac{E\delta^4}{144\mu \sin^2 \gamma} \left[ \frac{2 \cot \gamma (r_2 - r_1) - \cot^2 \gamma \ln \frac{r_2}{r_1}}{(r_2 + r_1)(r_2^2 + r_1^2)} \right].$$

Here $E$ is the Young’s modulus for nanocone, $\delta$ is the width of the double layer, $\gamma$ is the nanocone angle, $r_1$ and $r_2$ are radii of two cone boundaries, $\mu$ is the viscosity.

As for the length of the nanocone and the cone angle it depends not only on the parameters of the initial nanoplate, but also on the lattice constant for the layer. There is lattice correspondence of neighbor layers in equilibrium state. Absence of such correspondence leads to transformation of the structure into one closer to equilibrium. The majority of nanotubes in the set of experimentally obtained nanorolls have parameters close to the equilibrium one. Correlation between the lattice constants and the interlayer distance predetermines the angle and length of the nanocone. For given nanotube parameters it is obtained by simple calculations in MathCad. It is in correlation with the experiment results: it is shown that these parameters aren’t arbitrary. There are preferable angles and lengths (one can see it on Fig.1).
3. Flow in nanocone
It is necessary to describe the flow in more details to determine the parameters of the rolling process. We consider axisymmetric Stokes flow in the space between two cones with common vertex and semivertex angles \( \theta_1, \theta_2, \theta_1 < \theta_2 \). A Stokes streamfunction \( \psi(r, \theta) \) exists and is related to the velocity components \( (u, v) \) along the direction of the unit vector \( (e_r, e_\theta) \) according to

\[
\begin{align*}
  u &= \frac{1}{r^2 \sin \theta} \frac{\partial \psi}{\partial \theta}, \quad v = -\frac{1}{r \sin \theta} \frac{\partial \psi}{\partial r}
\end{align*}
\]

The fluid motion is governed by the fourth-order equation

\[
\left( \frac{\partial^2}{\partial r^2} + \frac{1-\xi^2}{r^2} \frac{\partial^2}{\partial \xi^2} \right)^2 \psi = 0,
\]

where \( \xi = \cos \theta \). Let us introduce new function by

\[
\psi(r, \theta) = \Re \left( r^{\mu+3/2}(1-\xi^2) f_\mu(\xi) \right),
\]

where \( \Re(\mu) > 1/2 \). Then \( f_\mu \) is easily determined by successively solving the equations

\[
\frac{d}{d\xi} ((1-\xi^2)g_\mu) + (\mu - 1/2)(\mu - 3/2)g_\mu = 0,
\]
\[
\frac{d}{d\xi} ((1-\xi^2)f_\mu) + (\mu - 1/2)(\mu - 3/2)f_\mu = g_\mu.
\]

To obtain the general solution, for \( \mu \neq 3/2 \),

\[
f_\mu = AP_{\mu+1/2}(\xi) + BP_{\mu-3/2}(\xi) + CQ_{\mu+1/2}(\xi) + DQ_{\mu-3/2}(\xi),
\]

where a prime denotes differentiation of a Legendre function. Impermeable and no-slip boundary conditions apply at each solid surface bounding the fluid. Hence, one obtains

\[
f_\mu(\xi_1) = f_\mu(\xi_2) = 0, \quad f'_\mu(\xi_1) = f'_\mu(\xi_2) = 0,
\]

where \( \xi_1 = \cos \theta_1, \xi_2 = \cos \theta_2 \). Correspondingly, \( \mu \) is determined by the following equation

\[
\begin{vmatrix}
P_{\mu+1/2}(\xi_1) & P_{\mu-3/2}(\xi_1) & Q_{\mu+1/2}(\xi_1) & Q_{\mu-3/2}(\xi_1) \\
P'_{\mu+1/2}(\xi_1) & P'_{\mu-3/2}(\xi_1) & Q'_{\mu+1/2}(\xi_1) & Q'_{\mu-3/2}(\xi_1) \\
P_{\mu+1/2}(\xi_2) & P_{\mu-3/2}(\xi_2) & Q_{\mu+1/2}(\xi_2) & Q_{\mu-3/2}(\xi_2) \\
P'_{\mu+1/2}(\xi_2) & P'_{\mu-3/2}(\xi_2) & Q'_{\mu+1/2}(\xi_2) & Q'_{\mu-3/2}(\xi_2)
\end{vmatrix} = 0.
\]

For each mode \( \mu = \mu_n \ (n = 1, 2, 3, \ldots) \), the radial and polar velocities are

\[
\begin{align*}
  u(r, \xi) &= \Re \left( -r^{\mu+1/2}(1-\xi^2)f_\mu \right), \\
v(r, \xi) &= (1-\xi^2)^{1/2} \Re \left( (1-\xi^2)r^{\mu+1/2}f_\mu \right),
\end{align*}
\]

4. Discussion
The stream function for the flow caused by a source, for example, posed at the cone vertex is obtained as a series in the obtained eigenfunctions. For the case of point source one gets the solution in an explicit form. It is possible also to consider line circle source at the cone boundary (it gives the axisymmetric flow too and reduces to point source in our two-dimensional problem). Rigorous theory of point-like sources for the Stokes flow [8] is based on the theory of self-adjoint extensions of symmetric operators (see, e.g., [9]). It is shown that the there are eddies in the flow. It has an influence on the nanotube formation process. In the case of moving boundary (rolling nanocone) one should replace two homogeneous boundary conditions by the corresponding inhomogeneous ones. If we assume that the nanotube wall is slightly penetrable, then it is necessary to replace the last pair of the boundary conditions by inhomogeneous ones.
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