

## TENSILITY AND COMPRESSIBILITY OF AXIALLY SYMMETRIC NANOCLUSTERS II: CYLINDRICAL NANOCLUSTERS

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A method to model the tensile properties of cylindrical nanoclusters is proposed. The isothermal size effect, appearing in the static simple tension test and in the dynamic process of uniaxial stretching, is discussed. A numerical simulation of this effect is presented.

### 1. Introduction

Many novel phenomena exist that are intrinsic to mesoscopic systems [1]. Particularly, as we shrink the mesoscale to the nanoscale, physics becomes increasingly dominated by the surfaces. It is in contrast to macroscopic systems that physical properties are dominated by the physics of bulk [2] (see also [3] – Introduction). The paper concerns the bulk nanostructured isolated solid clusters of ultrasmall size ( $\leq 100$  nm) called *nanoclusters* [3, 4]. Unfortunately, there are only limited data on the mechanical behavior – especially tensile properties – of nanoclusters. However, the fundamental understanding of mechanical properties of nanoclusters depends not only on experimental work, but also requires theoretical models. In the present paper we propose a framework for the modelling of tensile properties (static as well as dynamic – Secs. 3–5) of cylindrical nanoclusters (Sec. 2). This proposal is based on the simplified method of modelling of tensile properties of axially symmetric nanoclusters that has been proposed in [4].

### 2. Uniaxial Tension

Let us consider a circular cylinder  $\mathcal{B}$  of height  $h$  and radius  $r$ . If  $V = V(\mathcal{B})$ ,  $F = F(\partial\mathcal{B})$  and  $M = M(\partial\mathcal{B})$  denote the volume of  $\mathcal{B}$ , the surface field of the boundary  $\partial\mathcal{B}$  of  $\mathcal{B}$  and the total mean curvature of  $\partial\mathcal{B}$ , respectively, then [5]:

$$(2.1) \quad V = \pi r^2 h, \quad F = 2\pi r(h + r), \quad M = \pi(h + \pi r).$$

Introducing the slenderness  $x$  of the cylinder  $\mathcal{B}$ :

$$(2.2) \quad x = \frac{h}{r},$$

we can write Eq. (2.1) in the form:

$$(2.3) \quad V = \pi r^3 x, \quad F = 2\pi r^2(x+1), \quad M = \pi r(x+\pi).$$

It has been observed that the structurally most stable small metallic clusters have almost spherical shape. The oblate or prolate shape of such a cluster means that its structure is less stable [6]. Therefore, it is physically reasonable to consider a degree of sphericity of nanoclusters. For a compact and convex nanocluster  $\mathcal{B}$ , the measure  $\kappa$  of its degree of sphericity can be defined as [3]:

$$(2.4) \quad 0 < \kappa = r_V/r_F \leq 1, \\ r_V = (3V/4\pi)^{1/3}, \quad r_F = \frac{1}{2}(F/\pi)^{1/2},$$

where  $V = V(\mathcal{B})$ ,  $F = F(\partial\mathcal{B})$  and  $\kappa = 1$  if and only if  $\mathcal{B}$  is a ball. For the circular cylinder

we have:

$$(2.5) \quad \kappa = \kappa(x) = \sqrt[3]{6x/\sqrt{2(x+1)}}$$

where Eq. (2.3) was taken into account. It easy to see that the function  $\kappa(x)$ ,  $x > 0$ , takes its maximum value for  $x = 2$ . Thus a circular cylinder  $\mathcal{B}_0$  such that  $h_0 = 2r_0$  can be considered as the structurally most stable metallic cylindrical nanocluster (with the degree of sphericity  $\kappa(2) \simeq 0.935$ ).

Let  $\mathcal{B}_0$  be a distinguished circular cylinder of height  $h_0$  and radius  $r_0$ . Introducing designations:

$$(2.6) \quad \lambda_h = \frac{h}{h_0}, \quad \lambda_r = \frac{r}{r_0}, \quad x_0 = \frac{h_0}{r_0},$$

we can write the slenderness of  $\mathcal{B}$  in the form:

$$(2.7) \quad x = x_0 \frac{\lambda_h}{\lambda_r}.$$

If the circular cylinders  $\mathcal{B}_0$  and  $\mathcal{B}$  have the same center of symmetry (that coincides with the center of mass for the considered homogeneous nanoclusters), then  $\mathcal{B}$  can be identified with the image of  $\mathcal{B}_0$  under a linear mapping  $l = l(\mathbf{F}) : E^3 \rightarrow E^3$  where  $\mathbf{F}$  denotes the gradient of  $l$  (called a deformation tensor), i.e.  $\mathcal{B} = l(\mathbf{F})(\mathcal{B}_0)$ ;  $E^3$  denotes a three-dimensional Euclidean vector space. The tensor  $\mathbf{F}$  admits then a polar decomposition:

$$(2.8) \quad \mathbf{F} = \mathbf{R}\mathbf{U},$$

where  $\mathbf{R}$  is a proper orthogonal tensor, the stretch tensor  $\mathbf{U}$  is a positive definite and symmetric tensor with its eigenvalues,  $\lambda_i > 0$ ,  $i = 1, 2, 3$ , usually called *principal stretches*, defined by

$$(2.9) \quad \mathbf{U}\mathbf{e}_i = \lambda_i\mathbf{e}_i, \\ \mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}, \quad i, j = 1, 2, 3,$$

and such that, according to Eq. (2.6), we can take:

$$(2.10) \quad \lambda_1 = \lambda_2 = \lambda_r, \quad \lambda_3 = \lambda_h.$$

Further on we will deal with *pure deformations* ( $\mathbf{R} = \mathbf{1}$ ) preserving the shape of  $\mathcal{B}_0$ , that is such that:

$$(2.11) \quad \begin{aligned} \mathbf{F} &= \mathbf{U} = \lambda_r \mathbf{E}_r + \lambda_h \mathbf{E}_h, \\ \mathbf{E}_r &= \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2, \quad \mathbf{E}_h = \mathbf{e}_3 \otimes \mathbf{e}_3. \end{aligned}$$

Let  $\mathcal{B}_0$  be a homogeneous cylindrical nanocluster with its axis of symmetry parallel to the versor  $\mathbf{n} = \mathbf{e}_3$  and endowed with the uniform absolute temperature  $\theta \in T$ . Let us denote by  $\mathbf{T}(\mathcal{B}_0; \mathbf{U}, \theta)$  the generalized Cauchy stress tensor [3, 4] corresponding to a pure deformation of the nanocluster  $\mathcal{B}_0$  defined by Eqs. (2.6) and (2.11). This generalized stress tensor has, in the framework of the simplified model of tensility of axially symmetric nanoclusters being in the quasi-solid state [4], the following representation:

$$(2.12) \quad \begin{aligned} \mathbf{T}(\mathcal{B}_0; \mathbf{U}, \theta) &= T_{r,\theta}(h_0, r_0; \lambda_h, \lambda_r) \mathbf{E}_r + T_{h,\theta}(h_0, r_0; \lambda_h, \lambda_r) \mathbf{E}_h, \\ T_{r,\theta} &= p_\theta + t_{r,\theta}, \quad T_{h,\theta} = p_\theta + t_{h,\theta}, \end{aligned}$$

where

$$(2.13) \quad \begin{aligned} p_\theta &= \frac{\partial \Phi_\theta}{\partial V}, \quad t_{r,\theta} = \frac{\lambda_r}{2V} \left( \frac{\partial \Phi_\theta}{\partial F} \partial_{\lambda_r} F + \frac{\partial \Phi_\theta}{\partial M} \partial_{\lambda_r} M \right), \\ t_{h,\theta} &= \frac{\lambda_h}{V} \left( \frac{\partial \Phi_\theta}{\partial F} \partial_{\lambda_h} F + \frac{\partial \Phi_\theta}{\partial M} \partial_{\lambda_h} M \right), \end{aligned}$$

and the scalars  $\Phi_\theta, \theta \in I$ , define the Helmholtz free energy function  $\Psi$  according to the rule:

$$(2.14) \quad \begin{aligned} \Psi(\mathcal{B}_0; \mathbf{U}, \theta) &= \Phi_\theta(V, F, M), \\ V &= \lambda_h \lambda_r^2 V_0, \quad F = 2\pi r_0^2 \lambda_r (x_0 \lambda_h + \lambda_r), \\ M &= \pi r_0 (x_0 \lambda_h + \pi \lambda_r), \quad V_0 = \pi r_0^3 x_0. \end{aligned}$$

It follows from Eqs. (2.1)–(2.3), (2.6), (2.7), (2.13) and (2.14) that, independently of the choice of  $\mathcal{B}_0$ , we have:

$$(2.15) \quad \begin{aligned} 2V t_{r,\theta} &= 2\pi r^2 (x+2) \partial_F \Phi_\theta + \pi^2 r \partial_M \Phi_\theta, \\ V t_{h,\theta} &= 2\pi r^2 x \partial_F \Phi_\theta + \pi r x \partial_M \Phi_\theta. \end{aligned}$$

In the case of isothermally incompressible elasticity defined at each temperature  $\theta \in I$  by:

$$(2.16) \quad \begin{aligned} V &= V_0 \vartheta(\theta), \\ \det \mathbf{U} &= \lambda_h \lambda_r^2 = \vartheta(\theta), \end{aligned}$$

should be:

$$(2.17) \quad \mathbf{T} = -\bar{p}\mathbf{1} + T_{r,\theta}\mathbf{E}_r + T_{h,\theta}\mathbf{E}_h = \bar{T}_{r,\theta}\mathbf{E}_r + \bar{T}_{h,\theta}\mathbf{E}_h,$$

where

$$(2.18) \quad \bar{T}_{r,\theta} = -\bar{p} + T_{r,\theta}, \quad \bar{T}_{h,\theta} = -\bar{p} + T_{h,\theta}.$$

The components  $T_{r,\theta}$  and  $T_{h,\theta}$  are defined by Eqs. (2.12)–(2.15) and  $\bar{p}$  is an undefined scalar.

### 3. Generalized Simple Tension

The generalized simple tension state can be defined as an uniaxial tension such that [4]:

$$(3.1) \quad \forall \theta \in I, \quad T_{r,\theta} = 0,$$

that is (at each  $\theta \in I$ ):

$$(3.2) \quad 2V\partial_V\Phi_\theta + 2\pi r^2(x+2)\partial_F\Phi_\theta + \pi^2 r\partial_M\Phi_\theta = 0,$$

where Eqs. (2.12)–(2.15) were taken into account. In this case:

$$(3.3) \quad T_{h,\theta} = t_{h,\theta} - t_{r,\theta}$$

and thus, according to Eq. (2.15), we have:

$$(3.4) \quad VT_{h,\theta} = \pi r^2(x-2)\partial_F\Phi_\theta + \pi r\left(x - \frac{\pi}{2}\right)\partial_M\Phi_\theta.$$

An unstressed (in the generalized sense – [4]) cylindrical nanocluster  $\mathcal{B}_\theta$  of height  $h(\theta)$  and radius  $r(\theta)$ ,  $\theta \in I$ , is defined by Eq. (3.1) (i.e. by the condition (3.2)) and by the equation:

$$(3.5) \quad \forall \theta \in I, \quad T_{h,\theta} = 0,$$

equivalent (at each  $\theta \in I$ ) to the following condition:

$$(3.6) \quad r(x-2)\partial_F\Phi_\theta = \left(\frac{\pi}{2} - x\right)\partial_M\Phi_\theta.$$

The experimental simple tension data for usual elastic materials [7] suggest that the following condition is physically reasonable:

$$(3.7) \quad \forall \theta \in I, \quad (h - h(\theta))(r - r(\theta)) < 0, \quad h \neq h(\theta), \quad r \neq r(\theta).$$

For example, if

$$(3.8) \quad \begin{aligned} h &= \mu_h h(\theta), & r &= \mu_r r(\theta), \\ \mu_r &= \chi_\theta(\mu_h), & \mu_h &> 0, \end{aligned}$$

where  $\chi_\theta$  is a differentiable monotone decreasing positive function dependent, in general, on  $h(\theta)$  and  $r(\theta)$  as the parameters (cf. [4]), then the condition (3.7) is fulfilled. The generalized postulate of isothermal tensility in the generalized simple tension state [4] is defined here by Eq. (3.7) and by the following condition:

$$(3.9) \quad \forall \theta \in I, \quad T_{h,\theta}(h - (h(\theta))) > 0, \quad h \neq h(\theta).$$

It follows from Eq. (3.6) that an "unstressed" metallic circular cylinder  $\mathcal{B}_\theta, \theta \in I$ , can be structurally most stable, that is (Sec. 2):

$$(3.10) \quad x(\theta) = h(\theta)/r(\theta) = 2,$$

if

$$(3.11) \quad \partial_M \Phi_\theta = 0.$$

In a similar manner:

$$(3.12) \quad x(\theta) = \frac{\pi}{2},$$

if

$$(3.13) \quad \partial_F \Phi_\theta = 0.$$

Note that the degree of sphericity  $\kappa(\pi/2) \simeq 0.932$  (see Eq. (2.5)), means that an "unstressed" metallic cylindrical nanocluster of the slenderness  $x = \pi/2$  is almost such structurally stable as that one of the slenderness  $x = 2$  is ( $\kappa(2) \simeq 0.935$ ). It follows from Eqs. (2.3), (3.2), (3.4), (3.11) and (3.13) that we can take:

$$(3.14) \quad \begin{aligned} T_{h,\theta} &= -\frac{x-2}{x+2} \partial_V \Phi_\theta & \text{for } x(\theta) &= 2, \\ T_{h,\theta} &= -\frac{2}{\pi} \left(x - \frac{\pi}{2}\right) \partial_V \Phi_\theta & \text{for } x(\theta) &= \frac{\pi}{2}. \end{aligned}$$

Then, according to the conditions (3.2), (3.7) and (3.9), would be:

$$(3.15) \quad \partial_V \Phi_\theta < 0,$$

and

$$(3.16) \quad \begin{aligned} \partial_F \Phi_\theta &> 0 & \text{for } x(\theta) &= 2, \\ \partial_M \Phi_\theta &> 0 & \text{for } x(\theta) &= \frac{\pi}{2}. \end{aligned}$$

It ought to be taken into account that the conditions (3.2) and (3.8) can be inconsistent. However, it is not the case of isothermally incompressible elasticity defined by Eqs. (2.12) and (2.16)–(2.18). Namely, the condition

$$(3.17) \quad \bar{T}_{r,\theta} = 0,$$



leads to Eq. (3.4) with  $\bar{T}_{h,\theta}$  in place of  $T_{h,\theta}$  and constrained by the condition (2.16) only. In this case:

$$(3.18) \quad \begin{aligned} h &= h_0\lambda, & \lambda &= \lambda_h, \\ r &= r_0\lambda_r = r_0 \left( \frac{\vartheta(\theta)}{\lambda} \right)^{1/2}, \\ x &= h/r = x_0\lambda \left( \frac{\lambda}{\vartheta(\theta)} \right)^{1/2}, \end{aligned}$$

and the condition (3.8) reduces to the following equation:

$$(3.19) \quad r = r_0 \sqrt{\frac{h_0 \vartheta(\theta)}{h}}.$$

The component  $\bar{T}_{h,\theta}$  of the generalized tensile stresses is then also defined by Eqs. (3.4), (3.15) and (3.16) and reduces to a function of the variable  $\lambda > 0$  only (dependent on the parameters  $h_0, r_0$  and  $\theta$ ). Consequently, the analysis of tensility of nanoclusters that has been presented in [4] can be applied here.

#### 4. Liquid-like Response

The so-called liquid-like response [3, 8, 9] of nanoclusters being in the quasi-solid state [3] is defined by a Helmholtz free energy function  $\Psi$  of the following form [3]:

$$(4.1) \quad \begin{aligned} \Psi(\mathcal{B}_0; \mathbf{F}, \theta) &= \Phi_\theta(V, F, M), & \theta &\in I, \\ \Phi_\theta(V, F, M) &= a(\theta)V + b(\theta)F + c(\theta)M + d(\theta), \end{aligned}$$

where  $\mathbf{F} \in GL^+(E^3)$  denotes a deformation tensor,  $V = V(\mathcal{B})$  is the volume of the actual configuration  $\mathcal{B} = l(\mathbf{F})(\mathcal{B}_0)$  of the nanocluster  $\mathcal{B}_0$ ,  $F = F(\partial\mathcal{B})$  is the area of the boundary  $\partial\mathcal{B}$  of  $\mathcal{B}$ , and  $M = M(\partial\mathcal{B})$  is the total mean curvature of  $\partial\mathcal{B}$ . Further on we will consider the liquid-like response of cylindrical nanoclusters defined by Eqs. (2.1)–(2.3), (2.6), (2.11) and (2.14). Moreover, we will assume, taking into account Eqs. (3.4), (3.15), (3.16) and (4.1) that:

$$(4.2) \quad a(\theta) < 0, \quad b(\theta) \geq 0, \quad c(\theta) \geq 0, \quad b(\theta)^2 + c(\theta)^2 > 0.$$

Let us denote:

$$(4.3) \quad \varepsilon(\theta) = |a(\theta)|, \quad \gamma(\theta) = b(\theta), \quad \omega(\theta) = 2\pi c(\theta), \quad \delta(\theta) = |d(\theta)|/4\pi.$$

The above defined scalars have the following physical interpretations ([9] – Part I). The quantity  $\varepsilon(\theta)$  is the free energy density needed to change the nanocluster volume unit and it is a quantity conditioned by the bulk interatomic interactions only. The quantity  $\gamma(\theta)$  can be identified with the so-called surface tension defined as the free energy density needed to change the boundary surface field unit. The density  $\gamma(\theta)$  is conditioned by the interactions of atoms located on the boundary solid surface and it is a positive quantity at the considered temperatures lower than the melting temperature.

The quantity  $\omega(\theta)$  can be interpreted as the free energy density needed to change the nanocluster mean width  $d = M/2\pi$  and this quantity can be considered as the one conditioned by interactions between the boundary surface atoms and the bulk atoms located in a boundary layer. The quantity  $\delta(\theta)$  is conditioned by the nanocluster connectedness. This quantity does not influence elastic properties of the nanocluster but influences its heat capacity. Note that although we consider solid clusters being in the quasi-solid state [3, 4], the concept of the liquid-like response can be also useful for modelling of the contribution of interface curvatures (mean and Gaussian) to the surface internal energy density in incompressible fluids without memory effects [10]. The quantity  $\delta(\theta)$  is then responsible for a discontinuous change of the total internal energy needed to change the topological connectedness of a fluid body [10].

Let us consider the generalized simple tension of an isothermally incompressible cylindrical nanocluster defined by Eqs. (2.12)–(2.18), (3.17)–(3.19) and (4.1)–(4.3). In this case:

$$(4.4) \quad \begin{aligned} \bar{T}_{h,\theta}(\mathcal{B}_0; \lambda_h, \lambda_r) &= T_\theta(\lambda), \\ T_\theta(\lambda) &= \frac{\gamma(\theta)}{r_0} \left[ \left( \frac{\lambda}{\vartheta(\theta)} \right)^{1/2} - \frac{2}{x_0 \lambda} \right] + \frac{\omega(\theta)}{2\pi\vartheta(\theta)r_0^2} \left[ \lambda - \frac{\pi}{2x_0} \left( \frac{\vartheta(\theta)}{\lambda} \right)^{1/2} \right]. \end{aligned}$$

The (isothermal) uniaxial tensility function  $E_\theta(\mathcal{B}_0; \lambda)$  of the nanocluster  $\mathcal{B}_0$  at the temperature  $\theta \in I$  defined as [4]:

$$(4.5) \quad E_\theta(\mathcal{B}_0; \lambda) = \lambda \frac{dT_\theta}{d\lambda}(\lambda),$$

is then given by:

$$(4.6) \quad \begin{aligned} E_\theta(\mathcal{B}_0; \lambda) &= \frac{\gamma(\theta)}{2r_0} \left[ \left( \frac{\lambda}{\vartheta(\theta)} \right)^{1/2} + \frac{4}{x_0} \left( \frac{1}{\lambda} \right) \right] \\ &\quad + \frac{\omega(\theta)}{2\pi\vartheta(\theta)r_0^2} \left[ \lambda + \frac{\pi}{4x_0} \left( \frac{\lambda}{\vartheta(\theta)} \right)^{-1/2} \right]. \end{aligned}$$

Since, at the temperature  $\theta \in I$ , we have:

$$(4.7) \quad \begin{aligned} \forall \lambda > 0, \quad E_\theta(\mathcal{B}_0; \lambda) &> 0, \\ \lim_{\lambda \rightarrow 0} T_\theta(\lambda) &= -\infty, \quad \lim_{\lambda \rightarrow \infty} T_\theta(\lambda) = \infty, \end{aligned}$$

the considered uniaxial tensility of the cylindrical nanocluster  $\mathcal{B}_0$  is mechanically stable [4] and the generalized stress component  $T_\theta$  is a monotone increasing unbounded function. Moreover, it follows from Eqs. (4.5) and (4.7) that the condition:

$$(4.8) \quad \forall \theta \in I, \quad T_\theta(\lambda(\theta)) = 0, \quad \lambda(\theta) > 0,$$

and Eq. (3.18) with  $\lambda = \lambda(\theta)$  uniquely define the “unstressed” cylinders  $\mathcal{B}_\theta$ ,  $\theta \in I$ , of height  $h(\theta)$ , radius  $r(\theta)$  and the slenderness  $x(\theta)$ . Thereby, the uniquely defined scalar

$$(4.9) \quad E(\mathcal{B}_0; \theta) = E_\theta(\mathcal{B}_0; \lambda(\theta)),$$

can be interpreted as the *generalized isothermal Young's modulus* of the nanocluster  $\mathcal{B}_0$  at the temperature  $\theta \in I$  [4]. For example, if  $x_0 = 2$ , then  $E(\mathcal{B}_0; \theta)$  can be considered as the generalized Young's modulus of a structurally most stable metallic cylindrical nanocluster (Sec. 2).

It follows from Eqs. (4.6) and (4.9) that, for a fixed slenderness  $x_0$ , a very thin cylindrical nanocluster  $\mathcal{B}_0$  admits to neglect the surface tension effect with respect to the boundary curvature effect (see remarks following Eq. (4.2)). So, let us consider the case:

$$(4.10) \quad \forall \theta \in I, \quad \gamma(\theta) = 0.$$

Then, according to Eqs. (3.4), (3.18), (4.1)–(4.4) and (4.8), we have:

$$(4.11) \quad \lambda(\theta) = \vartheta(\theta)^{1/3}, \quad x(\theta) = x_0 = \pi/2.$$

Let us denote by  $E_0$  a reference Young's modulus, say this one corresponding to macroscopic samples of the considered nanomaterial at a reference temperature  $\theta_0 \in I$  (see e.g. [11]). It follows from Eqs. (4.6) and (4.9)–(4.11) that:

$$(4.12) \quad \frac{E(\mathcal{B}_0; \theta)}{E_0} = \frac{3}{4\pi\vartheta(\theta)^{2/3}} \left( \frac{l(\theta)}{d_0} \right)^2,$$

where it was denoted:

$$(4.13) \quad l(\theta) = \sqrt{\frac{2\omega(\theta)}{E_0}}, \quad d_0 = 2r_0.$$

It is observed that if the nanostructure size becomes smaller than an “intrinsic” characteristic length associated with a certain physical property, then this property changes [12, 13]. For example, if  $l(\theta)$  is interpreted as the intrinsic characteristic length associated with the nanocluster tensility in the simple tension test, then the inequality

$$(4.14) \quad \forall \theta \in I, \quad d_0 < l(\theta),$$

can be considered as a condition consistent with the assumption that we are dealing with a very thin cylindrical nanocluster.

## 5. Uniaxial Stretching Process

Let us denote by  $\mathcal{B}_0$  a cylindrical nanocluster of immovable center of mass located e.g. in the point  $\mathbf{X} = \mathbf{0}$ . We will study the isothermal stretching dynamics [4] of  $\mathcal{B}_0$  due to the influence of uniaxial surface load (tensile or compressive). It is assumed that if the applied cross-sectional load is referred to actual cross-sections of the nanocluster, then it takes the form:

$$(5.1) \quad \begin{aligned} \boldsymbol{\sigma}(\mathbf{x}, \tau) &= \sigma(\mathbf{x}, \tau) \mathbf{n}(\mathbf{x}, \tau) \otimes \mathbf{n}(\mathbf{x}, \tau), \\ \mathbf{x} &= x^i \mathbf{e}_i \in \partial \mathcal{B}_\tau, \quad \mathbf{x} = \mathbf{U}(\tau) \mathbf{X}, \quad \mathbf{X} \in \partial \mathcal{B}_0, \\ \mathcal{B}_\tau &= l(\mathbf{U}(\tau))(\mathcal{B}_0), \quad \tau \geq 0, \quad \mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}, \end{aligned}$$



where

$$(5.2) \quad \sigma(\mathbf{x}, \tau) = \begin{cases} \sigma(\mathcal{B}_0; \mathbf{U}(\tau), \theta) & \text{for } x^3 = \pm \frac{h}{2}, \quad (x^1)^2 + (x^2)^2 \leq r, \\ 0 & \text{for } -\frac{h}{2} < x^3 < \frac{h}{2}, \quad (x^1)^2 + (x^2)^2 = r, \end{cases}$$

$\mathcal{B}_\tau$  is a circular cylinder of height  $h = h(\tau)$  and radius  $r = r(\tau)$  being an actual configuration of  $B_0$ ,  $\mathbf{U}(\tau)$  denotes a time-dependent stretch tensor defined by Eqs. (2.9)–(2.11) with the time-dependent principal stretches  $\lambda_i = \lambda_i(\tau)$  and the time-independent principal orthonormal vectors  $\mathbf{e}_i$ ,  $i = 1, 2, 3$ ;  $\mathbf{n}(\mathbf{x}, \tau)$  is the unit outward normal to the boundary  $\partial\mathcal{B}_\tau$  of  $\mathcal{B}_\tau$  at the point  $\mathbf{x}$ , and  $\theta \in I$  is a time-independent temperature of  $\mathcal{B}_0$ .

If the influence of mass forces is neglected, then an isothermal uniaxial stretching process corresponding to the above defined cross-sectional load is described, in the framework of the simplified model of dynamics [4], by the following equation:

$$(5.3) \quad \mathbf{U}(\tau)\mathbf{J}(\mathcal{B}_0)\ddot{\mathbf{U}}(\tau) = -\mathbf{M}_{\text{int}}(\mathcal{B}_0; \tau) + \mathbf{M}_{\text{ext}}(\mathcal{B}_0; \tau),$$

where  $\mathbf{M}_{\text{int}}$  and  $\mathbf{M}_{\text{ext}}$  are dipole moments of internal and external surface forces acting on the boundary  $\partial\mathcal{B}_\tau$  of the actual configuration  $\mathcal{B}_\tau$  of  $\mathcal{B}_0$ , respectively:

$$(5.4) \quad \mathbf{M}_{\text{int}}(\mathcal{B}_0; \tau) = -V(\tau)\mathbf{T}(\mathcal{B}_0; \mathbf{U}(\tau), \theta),$$

where  $V(\tau) = \text{vol}\mathcal{B}_\tau$ ,  $\mathbf{T}(\mathcal{B}_0; \mathbf{U}(\tau), \theta)$  is the generalized Cauchy stress tensor [3, 4] defined by Eqs. (2.12)–(2.15) in the case of compressible elasticity or by Eqs. (2.16)–(2.18) in the case of isothermally incompressible elasticity, and

$$(5.5) \quad \mathbf{M}_{\text{ext}}(\mathcal{B}_0; \tau) = \int_{\partial\mathcal{B}_\tau} \mathbf{x} \otimes \sigma(\mathbf{x}, \tau)\mathbf{n}(\mathbf{x}, \tau)dF(\mathbf{x}).$$

It follows from Eqs. (2.11), (5.1), (5.2) and (5.5) that:

$$(5.6) \quad \begin{aligned} \mathbf{M}_{\text{ext}}(\mathcal{B}_0; \tau) &= M(\mathcal{B}_0; \tau)\mathbf{E}_h, \\ M(\mathcal{B}_0; \tau) &= \sigma(\mathcal{B}_\tau; \mathbf{U}(\tau), \theta)V(\tau). \end{aligned}$$

$\mathbf{J}(\mathcal{B}_0)$  is the inertia tensor of the cylindrical nanocluster  $B_0$  of the mass  $m$  determined with respect to its mass center  $\mathbf{X} = \mathbf{0}$  and has the following form:

$$(5.7) \quad \begin{aligned} \mathbf{J}(\mathcal{B}_0) &= J_r(r_0)\mathbf{E}_r + J_h(h_0)\mathbf{E}_h, \\ J_r(r_0) &= \frac{1}{4}mr_0^2, \quad J_h(h_0) = \frac{1}{12}mh_0^2. \end{aligned}$$

Further on we will restrict ourselves to the case of isothermally incompressible elasticity. It follows from (2.1), (2.12)–(2.18), (5.4), (5.6) and (5.7) that the equation (5.3) is then equivalent to the following system of equations:

$$(5.8) \quad \begin{aligned} \lambda_h J_h(h_0) \ddot{\lambda}_h &= -V\bar{T}_{h,\theta} + M, \\ \lambda_r J_r(r_0) \ddot{\lambda}_r &= -V\bar{T}_{r,\theta}, \end{aligned}$$

constrained by the condition (2.16). Assuming that

$$(5.9) \quad \bar{p} = p_\theta(\mathcal{B}_0; V, F, M),$$

we obtain the following equation:

$$(5.10) \quad \lambda_h J_h(h_0) \ddot{\lambda}_h - 2\lambda_r J_r(\tau_0) \ddot{\lambda}_r = m_\theta + V\sigma,$$

where it was denoted:

$$(5.11) \quad m_\theta = 4\pi r^2 \partial_F \Phi_\theta - \pi r(x - \pi) \partial_M \Phi_\theta,$$

and Eq. (2.15) was taken into account. The scalar  $m_\theta$  can be viewed as a component of an *effective dynamic dipole moment* in  $\mathbf{e}_3$ -direction. Note that it differs from the component  $\bar{M}_{h,\theta} = V\bar{T}_{h,\theta}$  of the dipole moment defined by Eqs. (2.12)–(2.18), (3.17) and appearing in the static simple tension test (Sec. 3). Consequently, a new (dynamic) characteristic slenderness  $x = x(\theta)$  appears. Namely, in contrast to Eqs. (3.4), (3.5) and (3.12), the condition (3.13) leads to:

$$(5.12) \quad m_\theta = 0 \quad \text{iff} \quad x(\theta) = \pi.$$

Let us consider the case of a constant actual cross-sectional load:

$$(5.13) \quad \sigma(\mathcal{B}_0; \mathbf{U}(\tau), \theta) = \sigma_0,$$

where  $\sigma_0$  can be dependent on the parameters  $h_0, r_0$  and  $\theta$ . It follows from the condition (2.16) that introducing designations:

$$(5.14) \quad \lambda_h(\tau) = \lambda(\tau/\tau_0), \quad \tau_0 = \sqrt{\frac{m}{h_0|\sigma_0|}},$$

$$\lambda' = \frac{d}{ds}\lambda, \quad s = \tau/\tau_0 \geq 0, \quad h_0 = x_0 r_0,$$

and

$$(5.15) \quad \xi_\theta = \frac{1}{|\sigma_0|r_0} \partial_F \Phi_\theta, \quad \zeta_\theta = \frac{1}{|\sigma_0|r_0^2} \partial_M \Phi_\theta,$$

we can rewrite Eq. (5.10) in the following nondimensional form:

$$(5.16) \quad \left[ \frac{2x_0^2}{3\vartheta(\theta)} \lambda^2 + \frac{1}{\lambda} \right] \lambda'' - 3 \left( \frac{\lambda'}{\lambda} \right)^2 = M_\theta(\lambda),$$

where it was denoted

$$(5.17) \quad M_\theta(\lambda) = 8\pi \left[ \frac{4}{x_0} \xi_\theta - \frac{x_0}{\vartheta(\theta)} \zeta_\theta \left( \lambda^2 - \frac{\pi\sqrt{\vartheta(\theta)}}{x_0} \lambda^{1/2} \right) + (\text{sgn } \sigma_0) \lambda \right],$$

and Eqs. (2.2), (3.18), (5.7) were taken into account.

For circular cylindrical nanoclusters with the liquid-like response (Sec. 4) we can take:

$$(5.18) \quad \xi_\theta = \frac{\gamma(\theta)}{|\sigma_0|r_0} \geq 0, \quad \zeta_\theta = \frac{\omega(\theta)}{2\pi|\sigma_0|r_0^2} > 0,$$

where Eqs. (4.1)–(4.3) were taken into account. Let us consider the case (see Sec. 4):

$$(5.19) \quad \forall \theta \in I, \quad \gamma(\theta) = 0.$$

If additionally:

$$(5.20) \quad x_0 = \pi,$$

then, according to Eqs. (3.18), (5.11) and (5.12), we have:

$$(5.21) \quad m_\theta = 0 \quad \text{iff} \quad \lambda = \sqrt[3]{\vartheta(\theta)}.$$

Note, that in the static case we have an analogous relation. Namely, if

$$(5.22) \quad x_0 = \frac{\pi}{2},$$

then, according to Eqs. (3.18), (4.4) and (5.19), we have:

$$(5.23) \quad M_\theta = VT_\theta = 0 \quad \text{iff} \quad \lambda = \sqrt[3]{\vartheta(\theta)}.$$

We see that “unstressed” nanoclusters  $\mathcal{B}_\theta$ ,  $\theta \in I$ , defined by Eq. (3.18) with  $\lambda = \vartheta(\theta)^{1/3}$ , appear in the static simple tension test as well as in the time-dependent uniaxial stretching process. The conditions (5.19), (5.20) and

$$(5.24) \quad \forall \theta \in I, \quad \vartheta(\theta) = 1$$

describe the case when an incompressible nanocluster  $\mathcal{B}_0$  is “unstressed” at each temperature  $\theta \in I$ . In this case, introducing designations:

$$(5.25) \quad \begin{aligned} M(\lambda) &= -8\pi\lambda[t(\lambda) - e], \quad e = \text{sgn}\sigma_0, \\ t(\lambda) &= \frac{T(\lambda)}{|\sigma_0|} = \zeta(\lambda - \lambda^{1/2}), \quad \zeta = n^2, \\ n &= k(\sigma)\frac{l(\theta)}{d_0}, \quad k(\sigma) = \sqrt{E_0/\pi|\sigma_0|}, \quad d_0 = 2r_0, \end{aligned}$$

where  $l(\theta)$  is defined by Eq. (4.13) and  $T(\lambda)$  denotes the generalized longitudinal stress  $T_\theta(\lambda)$  of Eq. (4.4) defined by the conditions (5.18), (5.19) and (5.24), we obtain the following dynamic equation:

$$(5.26) \quad \left(\frac{2\pi^2}{3}\lambda^2 + \frac{1}{\lambda}\right)\lambda'' - 3\left(\frac{\lambda'}{\lambda}\right)^2 = M(\lambda).$$

The considered dynamics depends on the external surface load  $\sigma_0$  ( $e = 1$  – tension or  $e = -1$  – compression) as well as on the intrinsic characteristic length  $l(\theta)$  associated with the nanocluster tensility in the simple tension test (Sec. 4). Note that, according to Eqs. (5.14) and (5.20), the parameter  $\zeta$  of Eq. (5.25) can be represented in the following form:

$$(5.27) \quad \zeta = \frac{\omega(\theta)\tau_0^2}{mr_0}.$$

Thus, if the characteristic time  $\tau_0$  of the considered uniaxial stretching process is kept constant, then  $\zeta$  is a monotone decreasing function of the nanocluster radius  $r_0$ . The following plots, representing numerical solutions of Eq. (5.26) with the initial conditions

$$(5.28) \quad \lambda(0) = 1, \quad \lambda'(0) = 0,$$

show the way in which the parameter  $\zeta$  influences the dynamics of uniaxial stretching process:

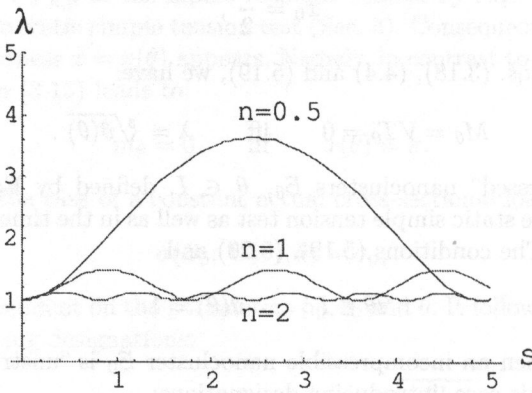


FIG. 1. Uniaxial stretching due to tensile surface load.

and

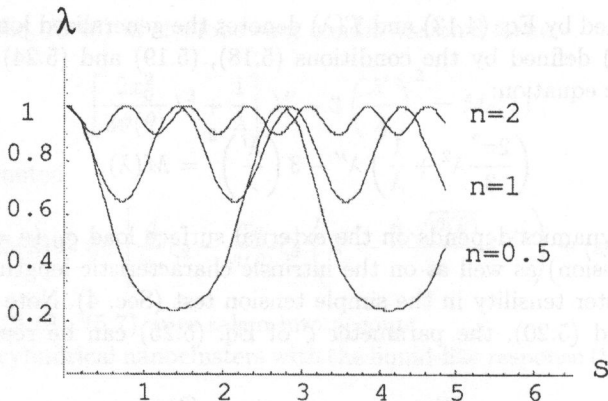


FIG. 2. Uniaxial stretching due to compressive surface load.

with the associated simple tension state:

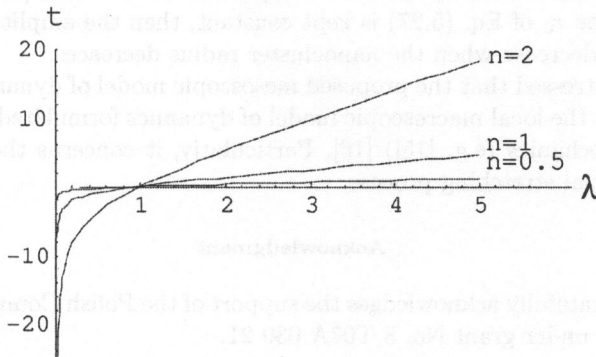


FIG. 3. Nondimensional generalized longitudinal stresses.

## 6. Final Remarks

Nanoclusters exhibit physical properties characteristic of neither the isolated atoms or molecules nor of the bulk materials (usual or nanostructured) [14] (see also [3] – Sec. 1). Consequently, on the nanoscale level, the notion of the state of matter takes a new meaning. The introduced notion of the quasi-solid state [3] is an example of the phenomenological mesoscopic representation of this phenomenon. Particularly, this notion is consistent with the observed dependence of isothermal mechanical properties of a nanocluster upon its size and shape [3, 4]. For example, it is predicted in the paper that the generalized Young's modulus of a cylindrical nanocluster (in the direction of its axis of symmetry) should increase when the nanocluster radius decreases (Sec. 4). Moreover, the static simple tension test as well as the nanocluster uniaxial stretching process depend explicitly on a characteristic intrinsic length (Secs. 4 and 5). The characteristic length is intrinsic in such a sense that it depends only on the boundary curvature effect (conditioned by interactions between the boundary surface atoms and the bulk atoms located in a boundary layer – Sec. 4) and on the Young's modulus of macroscopic nanostructured samples (conditioned by the bulk interatomic interactions; see also [11]).

The dynamics of deformation processes of nanoclusters is not recognized as yet. We propose [3, 4, 9] an approximate mesoscopic phenomenological model of this dynamics based on the assumption that, due to macroscopically small sizes of a nanocluster, we can restrict ourselves to its time-dependent spatially uniform deformations and temperatures. The equations governing the deformation processes of nanoclusters can be then derived basing oneself on the theory of such thermodynamic homogeneous processes [15] for which the associated thermodynamic functions (Helmholtz free energy, internal energy and entropy) and the generalized thermodynamic forces depend on the shapes and sizes of these clusters [9, 16]. Particularly, these equations can be applied to the description of the uniaxial stretching processes of cylindrical nanoclusters (Sec. 5, see also [4]). It leads, in the very thin cylindrical nanoclusters approximation (Sec. 4), to the one-dimensional nonlinear dynamic equation defined by Eqs. (5.25)–(5.27). This equation and the initial conditions of Eq. (5.28) define, according to Figs. 1 and 2,



the axial elongation or shortening processes of the nanocluster taking the form of its undamped vibrations forced by the time-independent actual cross-sectional load. If the characteristic time  $\tau_0$  of Eq. (5.27) is kept constant, then the amplitude and period of these vibrations decrease when the nanocluster radius decreases.

It should be stressed that the proposed mesoscopic model of dynamics is, in general, inconsistent with the local macroscopic model of dynamics formulated in the framework of continuum mechanics (e.g. [15]) [16]. Particularly, it concerns the above discussed vibrational uniaxial stretching process.

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#### References

1. Y. IMRY, *Introduction to mesoscopic physics*, Oxford University Press, New York 2002.
2. M. ROUKES, *Nanophysics*, Sci. Am., Special Issue (Nanotech), September, 42–49, 2001.
3. A. TRZĘSOWSKI, *On the quasi-solid state of solid nanoclusters*, Journal of Technical Physics, **44**, 4, 339–350, 2003.
4. A. TRZĘSOWSKI, *Tensility and compressibility of axially symmetric nanoclusters I: Simplified modelling*, Journal of Technical Physics, **45**, 2, 2004.
5. L.A. SANTALÓ, *Integral geometry and geometric probability*, Addison-Wesley, London 1976.
6. M. BRACK, *Metallic clusters and magic numbers*, Sci. Amer. (Polish edition), No. 2(78), 34–39, 1998.
7. J.G. MURPHY, G.A. ROGERSON, *A method to model simple tension experiments*, Int. J. Eng. Sci., **40**, 499–510, 2002.
8. A. TRZĘSOWSKI, *On liquid-like response of the size-effect body*, Bull. Ac. Polon. Sci., Sci. Tech., **28**, 7–8, 127–133, 1980.
9. A. TRZĘSOWSKI, *Nanomaterial clusters as macroscopically small size-effect bodies (Part I and II)*, Arch. Mech., **52**, 155–197, 2000.
10. A. BLINOWSKI, A. TRZĘSOWSKI, *Surface energy in liquids and the Hadwiger integral theorem*, Arch. Mech., **33**, 133–146, 1981.
11. C. KOCH, *Bulk behavior of nanostructured materials*, [in:] *Nanostructure science and technology*, R.W. SIEGEL, E. HU, M.C. ROCO [Eds.], Kluwer Academic Publishers, Dordrecht 1999.
12. L.I. TRUSOW, V.G. GRYNOW, *Highly dispersed systems and nanocrystals*, Nanostruc. Mat., **1**, 251–254, 1992.
13. R.W. SIEGEL, *Creating nanophase materials*, Sci. Amer., **275**, 42–47, 1996.
14. D.M. COX, *High surface area materials* [in:] *Nanostructure science and technology*, R.W. SIEGEL, E. HU, M.C. ROCO [Eds.], Kluwer Academic Publishers, Dordrecht 1999.
15. C. TRUESDELL, *Rational thermodynamics*, McGraw-Hill, New York 1969.
16. A. TRZĘSOWSKI, *On constrained size-effect bodies*, Arch. Mech., **36**, 185–193, 1984.

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