On the Influence of Residual Surface Stresses on the Properties of Structures at the Nanoscale

Holm Altenbach, Victor A. Eremeyev and Nikita F. Morozov

Abstract We discuss the influence of residual surface stresses on the effective (apparent) properties of materials at the nanoscale such as the stiffness of rods. The interest to the investigation of the surface effects is recently grown with respect to progress in nanotechnologies. The surface and interface effects play an important role for nanofilms, nanocomposites, nanoporous materials, etc. Here we consider the Gurtin–Murdoch model of surface elasticity. With the help of the simple problem of uniaxial tension of a rod with residual surface stresses we analyze the behavior of the rod under tension and present the effective stiffness.

1 Introduction

Recently, the interest to the model of surface elasticity by Gurtin and Murdoch [6] grows fast with respect to development of nanotechnologies, see [3, 16]. The model [6] predicts the size effect observed in the case of nanosized materials [15]. Unlike to macro- and microsized specimen where the size effect can be explained by various mechanisms, see the review [2], the size effect in nanomechanics can be related to surface phenomena only. An elastic body with surface stresses can be considered as a classical elastic body with glued elastic membrane. The stress resultant tensor acting

H. Altenbach · V. A. Eremeyev (✉)
Institut für Mechanik, Fakultät für Maschinenbau, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany
e-mail: holm.altenbach@ovgu.de

V. A. Eremeyev
South Scientific Center of RASci & South Federal University, Rostov on Don, Russia
e-mail: victor.eremeyev@ovgu.de; eremeyev.victor@gmail.com

N. F. Morozov
St. Petersburg State University, Bibliotechnaya sq. 2, 198904 St. Petersburg, Russia
e-mail: morozov@NM1016.spb.edu

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in the membrane can be interpreted as surface stresses in the Gurtin–Murdoch model. The additional surface elasticity influences on the effective properties of materials [3, 16]. It was shown that within the linear theory of surface elasticity the presence of surface stresses lead to the stiffening of the material, see, for example, [1, 4, 17, 18]. The residual or initial surface stresses can play an important role with respect to the material behavior at the nanoscale. In particular, the residual surface stress change the free vibrations of materials [5, 10, 14]. The finite deformations of elastic solids within the framework of the model [6] including analysis of residual surface stresses are considered in [7–9]. Let us note that the using of nonlinear elasticity methods is necessary for the correct describing of the prestressed state of solids.

The paper is organized as follows. In Sect. 2 we recall the basic equations of elasticity with surface stresses. In Sect. 3 we discuss the constitutive equations in more details. Here we introduce the natural configurations for the elastic body and residual (initial) stresses as a result of mismatch of natural configurations for the bulk and surface materials, respectively. We formulate the constitutive equations for surface stresses with non-natural reference configuration. Finally, we illustrate influence of residual surface stresses on the effective tangent stiffness considering the uniaxial tension of a rod with surface stresses.

Throughout the paper we use the direct tensor and vector notations as in [11].

2 Boundary-Value Problem for Nonlinear Solids with Surface Stresses

Following [6] we recall the basic equations of elastic materials taking into account surface stresses. The deformation of an elastic body is described by the mapping

$$\mathbf{x} = \mathbf{x}(\mathbf{X}), \tag{1}$$

where $\mathbf{x}$ and $\mathbf{X}$ are the position vectors in the actual configuration χ and in the reference one κ, respectively, see Fig. 1.

The Lagrangian equilibrium equations and the boundary conditions take the following form:

$$\begin{aligned} &\nabla \cdot \mathbf{P} + \rho \mathbf{f} = \mathbf{0}\,, \quad (\mathbf{n} \cdot \mathbf{P} - \nabla_s \cdot \mathbf{S})|_{\Omega_s} = \mathbf{t}\,, \\ &\mathbf{u}|_{\Omega_u} = \mathbf{u}_0\,, \quad \mathbf{n} \cdot \mathbf{P}|_{\Omega_f} = \mathbf{t}\,. \end{aligned} \tag{2}$$

Here $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor, ∇ the Lagrangian three-dimensional (3D) nabla operator, ∇_s the surface (2D) nabla operator, $\mathbf{S}$ the surface stress tensor of the first Piola-Kirchhoff type acting on the surfaces Ω_s, $\mathbf{u} = \mathbf{x} - \mathbf{X}$ the displacement vector, $\mathbf{f}$ and $\mathbf{t}$ the body force and surface loads vectors, respectively, and ρ the density. We assume that on the part of the body surface Ω_u the displacements are given, while on Ω_f the surface stresses $\mathbf{S}$ are absent, see Fig. 1. Equation $(2)_2$ is

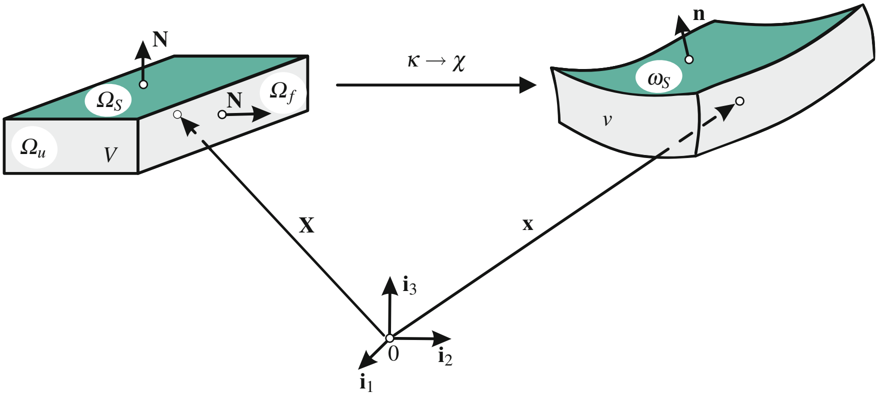


Fig. 1 Deformation of a body with surface stresses

the so-called generalized Young-Laplace equation describing the surface tension in solids. For solution of (2) we have to specify the constitutive equations for the stress tensors $\mathbf{T}$ and $\mathbf{S}$.

3 Constitutive Relations of Surface Elasticity

For the bulk material we use the standard constitutive relations of the nonlinear elasticity, see [12, 13],

$$\mathbf{P} = \frac{\partial \mathscr{W}}{\partial \mathbf{F}}, \quad \mathscr{W} = \mathscr{W}(\mathbf{F}), \tag{3}$$

where $\mathscr{W}$ is the strain energy density and $\mathbf{F} = \nabla \mathbf{x}$ the deformation gradient. In the theory of Gurtin and Murdoch [6] the stress tensor $\mathbf{S}$ is similar to the membrane stress resultants tensor and expressed with the use of the surface strain energy density $\mathscr{U}$

$$\mathbf{S} = \frac{\partial \mathscr{U}}{\partial \mathbf{F}_s}, \quad \mathscr{U} = \mathscr{U}(\mathbf{F}_s), \tag{4}$$

where $\mathbf{F}_s = \nabla_s \mathbf{x}\big|_{\Omega_s}$ is the surface deformation gradient.

Hence, to specify a hyperelastic solid with surface stresses one needs two constitutive equations for both the bulk and the surface behavior, that is for $\mathscr{W}$ and $\mathscr{U}$. Formally, in addition to (1) one needs the mapping $\Omega_s \to \omega_s$. Since we usually consider joint deformation of the volume V and the surface Ω_s in κ to the corresponding volume v and the surface ω_s in χ, it is enough to use the same mapping (1) for the deformation of the surface and the volume.

In the nonlinear elasticity one usually chooses a natural reference configuration. This means that $\mathscr{W}$ and $\mathbf{P}$ vanish without deformation or, in other words, $\mathscr{W}$ and $\mathbf{P}$

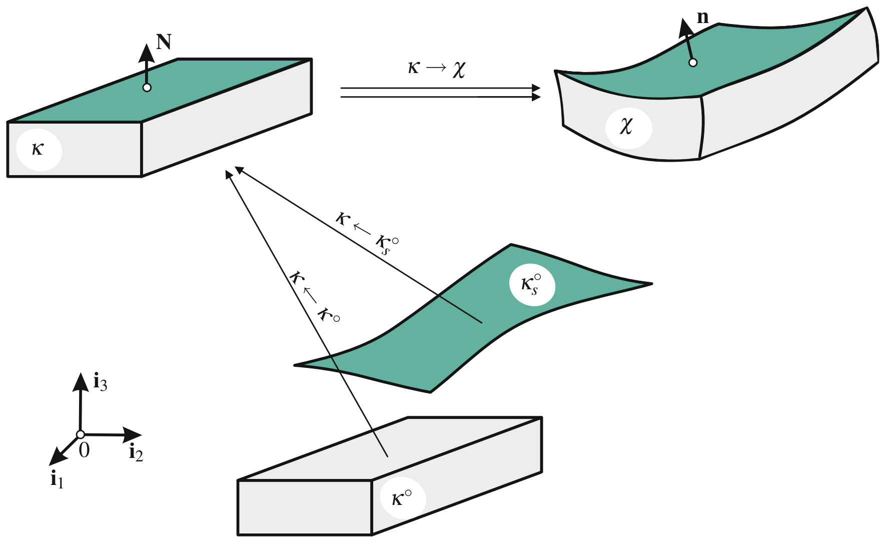


Fig. 2 Deformation of body with surface stresses: reference, actual, and two different natural configurations for surface and bulk material

possess the properties $\mathscr{W}(\mathbf{I}) = 0$, $\mathbf{P}(\mathbf{I}) = \mathbf{0}$, where $\mathbf{I}$ is the 3D unit tensor. In the case of surface elasticity one has to choose two natural reference configurations for $\mathscr{W}$ and $\mathscr{U}$ which do not coincide with each other, in general. This case is schematically shown in Fig. 2. Here κ_s° and κ° are the natural configurations taken different for the surface and the bulk material behavior. For example, if $\kappa_s^\circ = \kappa$ and $\kappa^\circ \neq \kappa_s^\circ$ there exist residual (initial) surface energy and surface stresses that is

$$\mathscr{U}(\mathbf{A}) = \mathscr{U}_0 \neq 0, \quad \mathbf{S}(\mathbf{A}) = \mathbf{S}_0 \neq \mathbf{0},$$

where $\mathbf{A} \equiv \mathbf{I} - \mathbf{N} \otimes \mathbf{N}$ is the surface unit tensor. In other words, here we assume that the reference configuration κ for the bulk material is natural one while for the attached on Ω_s membranes we assume the non-natural reference configuration κ with natural one κ_s°.

Let $\mathbf{F}_s^\circ$ and $\mathbf{F}_s^*$ be the surface deformation gradients related to mappings $\kappa_s^\circ \to \kappa$ and $\kappa_s^\circ \to \chi$, respectively. Then there is the multiplicative decomposition

$$\mathbf{F}_s^* = \mathbf{F}_s^\circ \cdot \mathbf{F}_s.$$

Since $\mathbf{F}_s^*$ corresponds to the mapping from the stress-free configuration to the actual one it can be used in the constitutive equations for $\mathscr{U}$ and $\mathbf{S}$. Keeping the same notation we re-write the constitutive equation for $\mathscr{U}$ as follows

$$\mathscr{U} = \mathscr{U}(\mathbf{F}_s^\circ \cdot \mathbf{F}_s),$$

where $\mathscr{U}$ satisfies the condition $\mathscr{U}(\mathbf{A}) = \mathbf{0}$. Tensor $\mathbf{F}_s^\circ$ can be considered as the given parametric tensor in the constitutive equations. The surface stress tensor $\mathbf{S}$ is given now by the relation

$$\mathbf{S} = \mathbf{F}_s^{\circ T} \cdot \frac{\partial \mathscr{U}}{\partial \mathbf{F}_s^*}. \tag{5}$$

The initial surface energy and surface stresses are given by

$$\mathscr{U}_0 = \mathscr{U}(\mathbf{F}_s^\circ), \quad \mathbf{S}_0 = \mathbf{F}_s^{\circ T} \cdot \left.\frac{\partial \mathscr{U}}{\partial \mathbf{F}_s^*}\right|_{\mathbf{F}_s^\circ}.$$

Using the material frame-indifference principle we write the strain energies as a functions of the right Cauchy–Green strain tensor and its surface analogues

$$\mathscr{W} = \mathscr{W}(\mathbf{C}), \quad \mathscr{U} = \mathscr{U}(\mathbf{F}_s^\circ \cdot \mathbf{C}_s \cdot \mathbf{F}_s^{\circ T}), \tag{6}$$

where $\mathbf{C} = \mathbf{F} \cdot \mathbf{F}^T$ and $\mathbf{C}_s = \mathbf{F}_s \cdot \mathbf{F}_s^T$. In the case the isotropic material behavior $\mathscr{W}$ and $\mathscr{U}$ are expressed via the principal invariants

$$\mathscr{W} = \mathscr{W}(I_1, I_2, I_3), \quad \mathscr{U} = \mathscr{U}(J_1, J_2), \tag{7}$$

where

$$I_1 = \mathrm{tr}\,\mathbf{C}, \quad I_2 = \frac{1}{2}\left[\mathrm{tr}^2\mathbf{C} - \mathrm{tr}\,\mathbf{C}^2\right], \quad I_3 = \det\mathbf{C},$$
$$J_1 = \mathrm{tr}\left(\mathbf{F}_s^\circ \cdot \mathbf{C}_s \cdot \mathbf{F}_s^{\circ T}\right), \quad J_2 = \mathrm{tr}\left(\mathbf{F}_s^\circ \cdot \mathbf{C}_s \cdot \mathbf{F}_s^{\circ T}\right)^2.$$

The corresponding surface stress tensor $\mathbf{S}$ takes the form

$$\mathbf{S} = 2\frac{\partial \mathscr{U}}{\partial \mathbf{C}_s} \cdot \mathbf{F}_s = 2\left[\frac{\partial \mathscr{U}}{\partial J_1}\mathbf{F}_s^{\circ T} \cdot \mathbf{F}_s^\circ + 2\frac{\partial \mathscr{U}}{\partial J_2}\mathbf{F}_s^{\circ T} \cdot \mathbf{F}_s^\circ \cdot \mathbf{C}_s \cdot \mathbf{F}_s^{\circ T} \cdot \mathbf{F}_s^\circ\right] \cdot \mathbf{F}_s. \tag{8}$$

As an example of the surface strain energy we consider the quadratic function

$$\mathscr{U} = \frac{1}{8}\lambda_\mathrm{s}(J_1 - 2)^2 + \frac{1}{4}\mu_\mathrm{s}(J_2 - 2J_1 + 2), \tag{9}$$

where λ_s and μ_s are the surface elastic moduli, which are also named the surface Lamé moduli. For (9) the tensor $\mathbf{S}$ has the form

$$\mathbf{S} = \left[\left(\frac{1}{2}\lambda_s(J_1 - 2) - \mu_s\right)\mathbf{F}_s^{\circ T} \cdot \mathbf{F}_s^\circ + \mu_s \mathbf{F}_s^{\circ T} \cdot \mathbf{F}_s^\circ \cdot \mathbf{C}_s \cdot \mathbf{F}_s^{\circ T} \cdot \mathbf{F}_s^\circ\right] \cdot \mathbf{F}_s. \tag{10}$$

In the case of infinitesimal deformations without initial deformations we have

$$\mathbf{C}_s \approx \mathbf{A} + 2\boldsymbol{\varepsilon}, \quad \mathbf{F}_s^\circ = \mathbf{A},$$

and Eqs. (9) and (10) reduce to the relations of the linear surface elasticity, see [1],

$$\mathscr{U} = \frac{1}{2}\lambda_s \mathrm{tr}^2\boldsymbol{\varepsilon} + \mu_s \mathrm{tr}\,\boldsymbol{\varepsilon}^2, \quad \mathbf{S} = \lambda_s \mathbf{A}\,\mathrm{tr}\,\boldsymbol{\varepsilon} + 2\mu_s\boldsymbol{\varepsilon},$$

where $\boldsymbol{\varepsilon}$ is the linear surface strain tensor.

Let us consider the uniform surface tension $\mathbf{F}_s^\circ = \lambda_\circ\mathbf{A}$ as an example of the initial surface deformation gradient. Here we have $J_1 = 2\lambda_\circ^2$, $J_2 = 2\lambda_\circ^4$, and

$$\mathscr{U}_0 = \frac{1}{2}(\lambda_s + \mu_s)(\lambda_\circ^2 - 1)^2, \quad \mathbf{S}_0 = (\lambda_s + \mu_s)\lambda_\circ^2(\lambda_\circ^2 - 1)\mathbf{A}.$$

Further we consider the influence of residual (initial) stresses on effective (apparent) stiffness of solids.

4 Uniaxial Tension

To illustrate the influence of surface stresses including residual ones let us consider the uniaxial tension of a circular cylinder made of incompressible material, see Fig. 3. The mapping (1) is now given by

$$x_1 = \lambda^{-1/2}X_1, \quad x_2 = \lambda^{-1/2}X_2, \quad x_3 = \lambda X_3, \tag{11}$$

where x_k, X_k, $k = 1, 2, 3$, are the Cartesian coordinates in the actual and reference configurations, respectively, and λ is the stretch parameter.

The corresponding deformation gradient $\mathbf{F}$ and the right Cauchy–Green strain tensor $\mathbf{C}$ are given by formulas

$$\mathbf{F} = \lambda^{-1/2}(\mathbf{i}_1 \otimes \mathbf{i}_1 + \mathbf{i}_2 \otimes \mathbf{i}_2) + \lambda\mathbf{i}_3 \otimes \mathbf{i}_3, \quad \mathbf{C} = \lambda^{-1}(\mathbf{i}_1 \otimes \mathbf{i}_1 + \mathbf{i}_2 \otimes \mathbf{i}_2) + \lambda^2\mathbf{i}_3 \otimes \mathbf{i}_3,$$

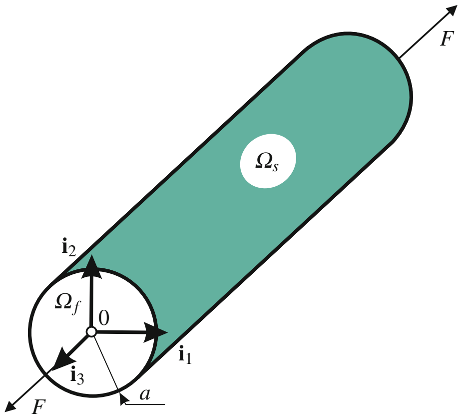
or with base vectors of cylindrical coordinates as follows

$$\mathbf{F} = \lambda^{-1/2}(\mathbf{e}_R \otimes \mathbf{e}_R + \mathbf{e}_\Phi \otimes \mathbf{e}_\Phi) + \lambda\mathbf{e}_Z \otimes \mathbf{e}_Z,$$
$$\mathbf{C} = \lambda^{-1}(\mathbf{e}_R \otimes \mathbf{e}_R + \mathbf{e}_\Phi \otimes \mathbf{e}_\Phi) + \lambda^2\mathbf{e}_Z \otimes \mathbf{e}_Z.$$

The principal invariants of $\mathbf{C}$ are

$$I_1 \equiv \mathrm{tr}\,\mathbf{C} = 2\lambda^{-1} + \lambda^2, \quad I_2 \equiv \frac{1}{2}\left[\mathrm{tr}^2\mathbf{C} - \mathrm{tr}\,\mathbf{C}^2\right] = 2\lambda + \lambda^{-2}, \quad I_3 \equiv \det\mathbf{C} = 1.$$

Fig. 3 Uniaxial tension of a circular rod of radius a subjected by the force F



In a similar way we calculate the surface deformation gradient $\mathbf{F}_s$ and the surface left Cauchy–Green strain tensor $\mathbf{C}_s$

$$\mathbf{F}_s = \lambda^{-1/2}\mathbf{e}_\Phi \otimes \mathbf{e}_\Phi + \lambda \mathbf{e}_Z \otimes \mathbf{e}_Z, \quad \mathbf{C}_s = \lambda^{-1}\mathbf{e}_\Phi \otimes \mathbf{e}_\Phi + \lambda^2 \mathbf{e}_Z \otimes \mathbf{e}_Z.$$

We assume $\mathbf{F}_s^\circ$ in the form

$$\mathbf{F}_s^\circ = \lambda_1 \mathbf{e}_\Phi \otimes \mathbf{e}_\Phi + \lambda_2 \mathbf{e}_Z \otimes \mathbf{e}_Z,$$

where λ_1 and λ_2 are positive numbers describing initial axisymmetric stretching of the surface Ω_s. Thus $\mathbf{F}_s^\circ \cdot \mathbf{C}_s \cdot \mathbf{F}_s^{\circ T}$ is given by

$$\mathbf{F}_s^\circ \cdot \mathbf{C}_s \cdot \mathbf{F}_s^{\circ T} = \lambda_1^2 \lambda^{-1} \mathbf{e}_\Phi \otimes \mathbf{e}_\Phi + \lambda_2^2 \lambda^2 \mathbf{e}_Z \otimes \mathbf{e}_Z,$$

and its invariants are

$$J_1 = \lambda_1^2 \lambda^{-1} + \lambda_2^2 \lambda^2, \quad J_2 = \lambda_1^4 \lambda^{-2} + \lambda_2^4 \lambda^4.$$

For the bulk material we use the neo-Hookean model

$$\mathscr{W} = \mu(I_1 - 3), \quad \mathbf{P} = 2\mu \mathbf{F} - p\mathbf{F}^{-T}, \tag{12}$$

where μ is the elastic modulus playing a role of the shear modulus in the case of infinitesimal deformations, p is the pressure in incompressible materials.

Obviously, in the case of uniaxial tension $(2)_1$ is fulfilled, the boundary condition $(2)_2$ reduces to

$$P_{RR}\Big|_a + \frac{1}{a} S_{\Phi\Phi} = 0. \tag{13}$$

Using (12) from (13) we obtain p

$$p = 2\mu\lambda^{-1} + \frac{1}{a}\lambda^{-1/2} S_{\Phi\Phi}.$$

This gives us the axial nominal stress

$$P_{ZZ} = 2\mu(\lambda - \lambda^{-2}) - \frac{1}{a}\lambda^{-3/2} S_{\Phi\Phi}. \tag{14}$$

From (10) it follows

$$\mathbf{S} = S_{\Phi\Phi}\mathbf{e}_\Phi \otimes \mathbf{e}_\Phi + S_{ZZ}\mathbf{e}_Z \otimes \mathbf{e}_Z,$$

where

$$S_{\Phi\Phi} = \left[\frac{1}{2}\lambda_\mathrm{s}(J_1 - 2) - \mu_\mathrm{s}\right]\lambda_1^2\lambda^{-1/2} + \mu_\mathrm{s}\lambda_1^4\lambda^{-3/2}, \tag{15}$$

$$S_{ZZ} = \left[\frac{1}{2}\lambda_\mathrm{s}(J_1 - 2) - \mu_\mathrm{s}\right]\lambda_2^2\lambda + \mu_\mathrm{s}\lambda_2^4\lambda^3. \tag{16}$$

Considering the integral equilibrium condition

$$F\mathbf{e}_\mathrm{z} = \iint\limits_{\Omega_f} \mathbf{e}_\mathrm{z} \cdot \mathbf{P}\,\mathrm{d}S + \int\limits_{\partial\Omega_f} \mathbf{e}_\mathrm{z} \cdot \mathbf{S}\,\mathrm{d}s$$

we obtain the formula

$$F = \pi a^2 P_{ZZ} + 2\pi a S_{ZZ}. \tag{17}$$

Substituting into (17) Eqs. (14) and (16) we obtain the dependence of the axial force F on the stretch parameter λ taking into account initial stretching λ_1 and λ_2

$$\frac{1}{\pi a^2}F = 2\mu(\lambda - \lambda^{-2}) + \frac{1}{a}\left(-\lambda^{-3/2}S_{\Phi\Phi} + 2S_{ZZ}\right). \tag{18}$$

Let us first consider the influence of surface stresses without residual ones. In Fig. 4 we present dependence F on λ.

Here

$$\overline{F} = \frac{F}{2\pi\mu a^2}$$

is the nominal axial stress. The dotted curve corresponds to the function

$$\overline{F}_0(\lambda) = \lambda - \lambda^{-2},$$

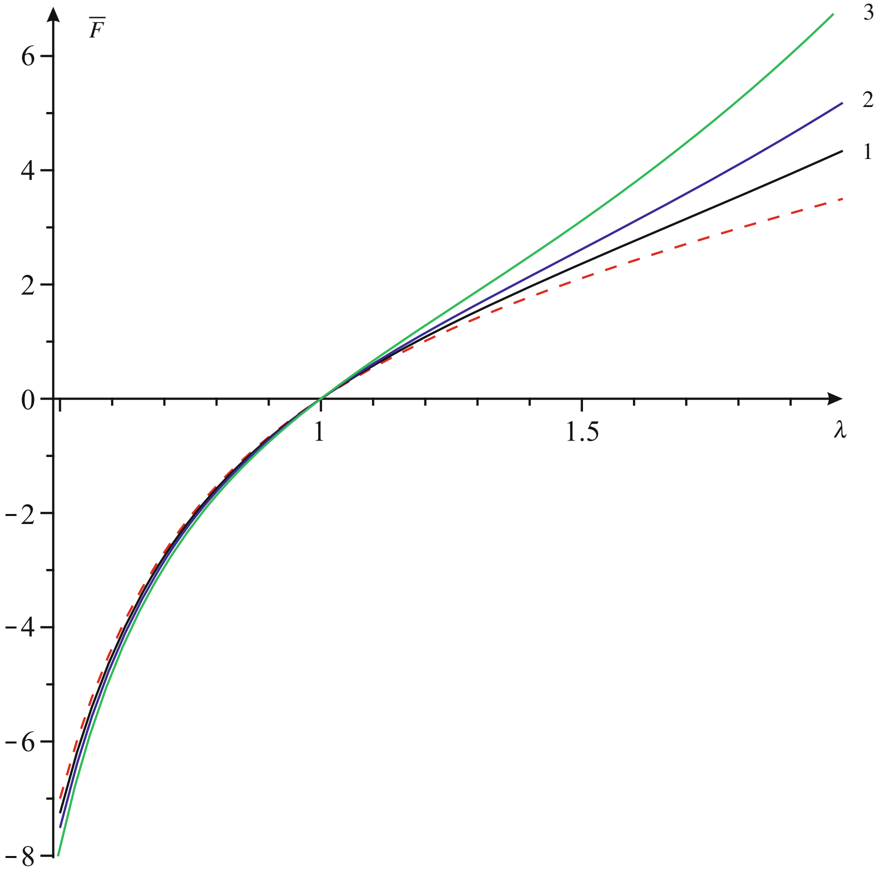


Fig. 4 $\overline{F}$ versus λ without residual surface stresses

which describe the uniaxial tension of a rod within the framework of neo-Hookean model. For simplicity let us assume that $\lambda_s = \mu_s$. We introduce the dimensionless parameter

$$\alpha = \frac{\mu_s}{2\mu a},$$

so $\overline{F} = \overline{F}(\lambda, \alpha)$ and $\overline{F}(\lambda, 0) = \overline{F}_0$. Curves 1, 2, 3 present the dependence $\overline{F}(\lambda)$ for the values $\alpha = 0.05; 0.1; 0.2$, respectively. It is seen that

$$\overline{F}(\lambda, \alpha_1) > \overline{F}(\lambda, \alpha_2) \quad \text{for} \quad \alpha_1 > \alpha_2 \geq 0, \quad \lambda > 1,$$

and

$$\overline{F}(\lambda, \alpha_1) < \overline{F}(\lambda, \alpha_2) \quad \text{for} \quad \alpha_1 > \alpha_2 \geq 0, \quad \lambda < 1.$$

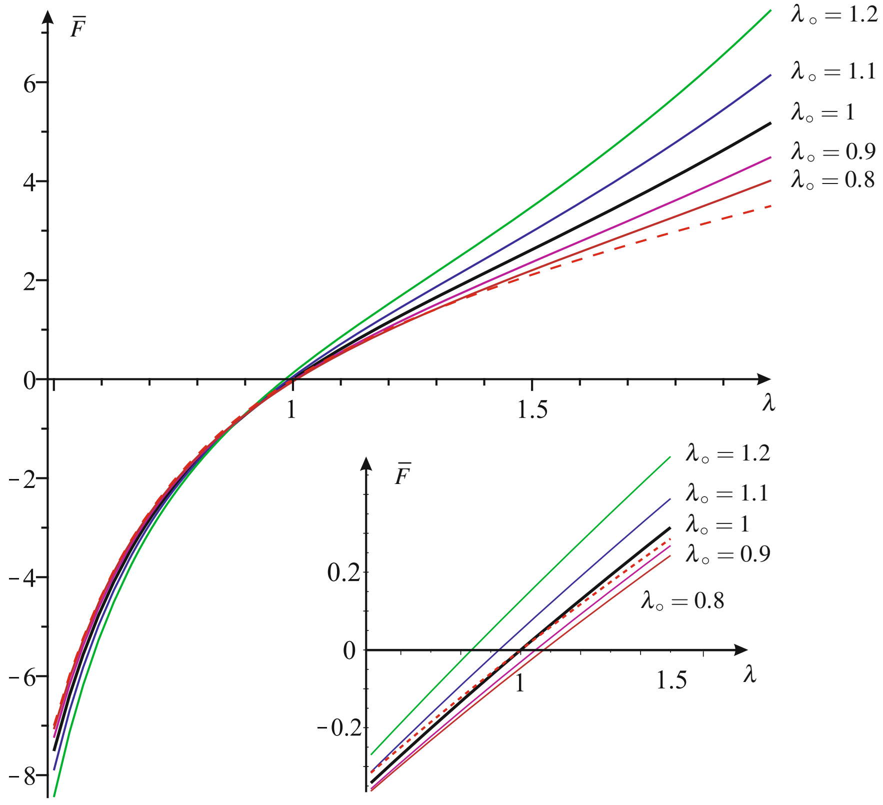


Fig. 5 $\overline{F}$ versus λ with uniform residual surface stresses

Calculating the tangent stiffness by the formula

$$E(\lambda, \alpha) = \frac{\partial \overline{F}}{\partial \lambda}$$

we conclude that

$$E(\lambda, \alpha_1) > E(\lambda, \alpha_2) \quad \text{for} \quad \alpha_1 > \alpha_2 \geq 0, \quad \lambda \neq 1.$$

This means that the rod with surface stresses becomes stiffer then the rod without the latter.

Let us consider the influence of uniform residual stresses $\lambda_1 = \lambda_2 = \lambda_\circ$. Here we have more complicated behavior, see Fig. 5. As in Fig. 4 the dotted curve corresponds function $\overline{F}_0(\lambda)$, others curves correspond to various values of $\lambda_\circ$. Here $\alpha = 0.1$ is assumed. One can see that initial stretching $\lambda_\circ > 1$ leads to the increase of $\overline{F}$ while initial compression $\lambda_\circ < 1$ leads to the decrease of $\overline{F}$. The detailed analysis near the

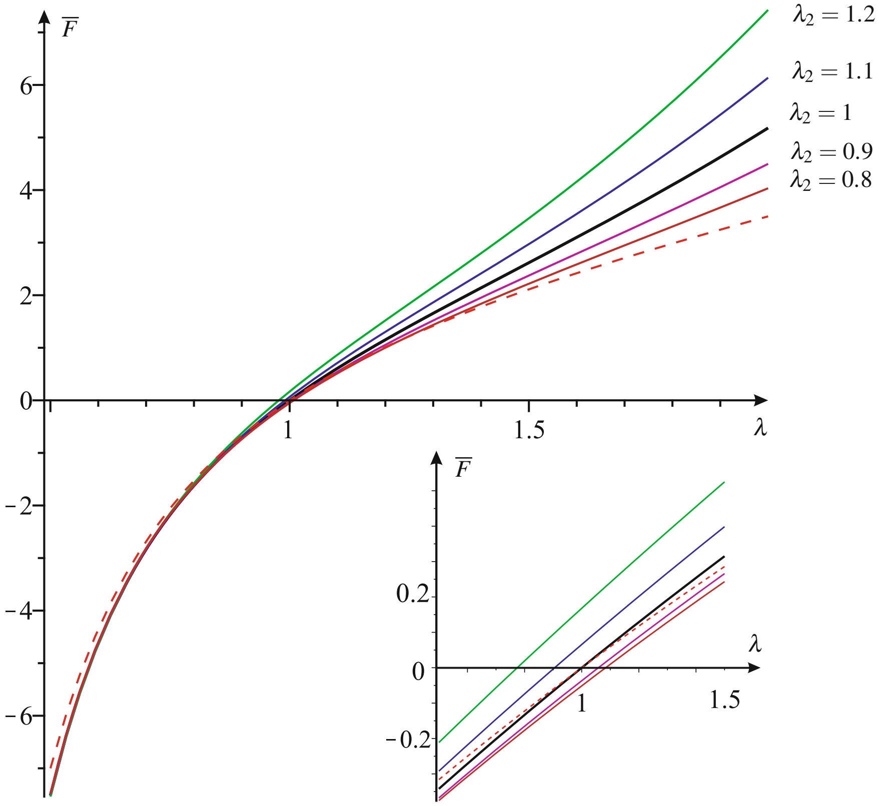


Fig. 6 $\overline{F}$ versus λ with uniaxial residual surface stresses

point $\lambda = 1$ shows that the values of λ, when $\overline{F} = 0$, are also shifted with respect to $\lambda_\circ$.

Finally, we consider the uniaxial initial stretching with $\lambda_1 = 1, \lambda_2 \neq 1$. Such state corresponds to the uniaxial stress tensor $\mathbf{S}_0 = S^0_{ZZ}\mathbf{e}_z \otimes \mathbf{e}_z$. Unlike to the uniform initial stretching this case relates to self-equilibrate initial stresses in the case of a cylindrical body. This means that $\mathbf{S}_0$ and $\mathbf{P} = \mathbf{0}$ satisfy the equilibrium conditions $(2)_{1,2}$. The corresponding dependencies are shown in Fig. 6. Here $\alpha = 0.1$ again is assumed.

Both uniform and uniaxial residual (initial) stretching change the effective tangent stiffness of the rod. In particular, initial compression leads to the decrease of the tangent stiffness in comparison with the tangent stiffness of the rod with surface stresses but without residual ones.

5 Conclusion

Here we discussed the influence of residual surface stresses on the effective (apparent) stiffness of nanodimensional specimen. It was shown that the presence of surface stresses leads to the increase of stiffness of nanosized specimen in comparison with bulk material while influence of residual stresses may result in the decrease or the increase of the effective stiffness of material.

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