

EFFECT OF NANOSIZED ASPERITIES AT THE SURFACE OF A NANO HOLE

Mikhail A. Grekov¹, Aleksandra B. Vakaeva¹

¹St. Petersburg State University
7/9, Universitetskaya nab., 199034, St. Petersburg, Russia
e-mail: m.grekov@spbu.ru, a.vakaeva@spbu.ru

Keywords: Nanosized Asperities, Nanohole, Surface Stress, Perturbation Method, Integral Equation, Stress Concentration.

Abstract. *The two-dimensional problem on a curvilinear nanohole in an infinite elastic body under arbitrary remote loading is solved. The shape of the hole is assumed to be weakly deviated from the circular one and the complementary surface stresses are acting at the boundary. The boundary conditions are formulated according to the generalized Laplace – Young law. The study is based on Gurtin – Murdoch surface elasticity model. Using Goursat – Kolosov complex potentials and the boundary perturbation technique, the solution of the problem is reduced to a singular integro-differential equation for any-order approximation. The algorithm of solving this integral equation is constructed in the form of a power series. Solutions of the integral equation and corresponding complex potentials are obtained for zero-order and first-order approximations. The size effect in the form of the dependence of the stress distribution at the surface on the size of the hole is demonstrated.*

1 INTRODUCTION

Material properties are determined by its chemical composition and structure. The study of surface phenomena is of great interest as it gives an opportunity to obtain an information about the physical and mechanical behavior of a whole material as, for example, in the case of mechanochemical corrosion [1, 2]. In particular, it concerns nanosized materials and structures widely used for developing functional devices in the semiconductor industry, nanoelectromechanical systems, gas and chemical sensors or even biomedical equipment [3].

During the past half-century, much effort to study the mechanical behavior of nanomaterials (beams, plates, wires, films, etc.) and composites containing nanosized inhomogeneities (inclusions, voids and holes) has been made in materials science, solid state science and nanomechanics (see reviews [3, 4, 5]). Investigation of material properties and elastic fields of nanostructures and nanocomposites is important for further development of nanotechnology involving analysis, design and fabrication of devices and structures at the nanoscale. At least one of the overall dimensions of nanomaterials and nano-inhomogeneities is in the nanometer range. This implies that the ratio of the volume occupied by the atoms at and near the corresponding surface/interface to the volume of the bulk or nano-inhomogeneity becomes significant. As a consequence, the energy of the atoms adjoining the surface/interface, called the surface free energy [6], and the surface stress relating the variation of the surface free energy to the variation of the surface strain [7] highly influence on material properties and elastic fields of nanomaterials and nanocomposites. The size dependency of an elastic state at the nanoscale is one of the corroborations of this influence [8, 9, 10].

The basic concepts of surface/interface free energy and surface/interface stress in solids were first formulated by Gibbs [6] and developed later by a lot of researchers. Gurtin and Murdoch [11, 12] and Gurtin et al. [13] elaborated the mathematical framework incorporating surface stress into continuum mechanics. Miller and Shenoy [8] performed atomistic simulations with the embedded atom method of nanosized plates and beams subjected to uniaxial loading and bending and found that their results were in excellent agreements with those obtained by means of the Gurtin – Murdoch continuum model.

Within the Gurtin – Murdoch model of the surface/interface elasticity, a number of classical problems related to elastic phenomena at the nanoscale have been studied and some size effects have been found for relevant nanoscale materials. For example, thin film, inclusion, inhomogeneity and surface defect formation problems were resolved in the works [14]–[26].

The influence of surface stress on the elastic field was reported in [21] for the case when the external forces applied to a flat surface have changed within a nanosized region (size effect). Incorporating surface stresses, size effect is appeared as the dependence of an elastic field near an elliptical nanohole [22] and nanoinclusion [16, 17] on their sizes, and the local instability of a plate with a circular nanohole on the hole size under uniaxial tension [23, 24]. Recently, analysis of elastic fields at the nanosized surface defects arising on a film coating due to diffusion has been carried out in [25, 26] using the surface elasticity theory [11, 12] coupled with the universal boundary perturbation technique.

In the previous paper [27], using the universal boundary perturbation method, we have solved the 2-D elasticity problem on a nearly circular hole in an infinite plane at the macrolevel. The results allowed us to evaluate the effect of deviation of the hole boundary from the circular one on the stress concentration and the stress-strain state near the curvilinear macrohole. In connection with the intensive development of nanotechnology and the use of nanomaterials and nanostructures in a variety of optical, electronic and other devices, it is important to study the

problem of changing the stress state near nanohole due to incorporating surface stress. So, the purpose of the present work is to study the effect of the surface stresses on an elastic field of a body containing a nearly circular nanohole. In order to solve the corresponding problem, we use Gurtin – Murdoch surface elasticity theory [11, 12] and the boundary perturbation technique developed in [25]–[29]. As a result, we come to the singular integro-differential equation in any order approximation of the perturbation method. The analytical solution of this equation and numerical results are given for the first-order approximation.

2 PROBLEM FORMULATION

We consider an infinite elastic plane of complex variable $z = x_1 + ix_2$ (i is the imaginary unit) with a nanohole the shape of which is weakly deviated from the circle of radius a with the center in the origin of Cartesian coordinates x_1, x_2 . The plane is under arbitrary remote loading and extra surface stresses at the boundary. The plane strain conditions are supposed to be satisfied. The boundary of the hole Γ is determined by the equation:

$$z \equiv \zeta = \rho e^{i\theta} = a(1 + \varepsilon f(s))s, \quad (1)$$

where $s = e^{i\theta}$, $f(s)$ is the continuous function and $|f| \leq 1$, ε is the small parameter which is equal to the maximum deviation of the hole boundary from the circular one of radius a , $\varepsilon > 0$, $\varepsilon \ll 1$.

The boundaries of the hole determined by the equation (1) are shown in Fig. 1 for $f(s) = \cos 2\theta$ and $a = 1$, and different values of the parameter ε . These different forms of the hole are used in our work to get numerical results.

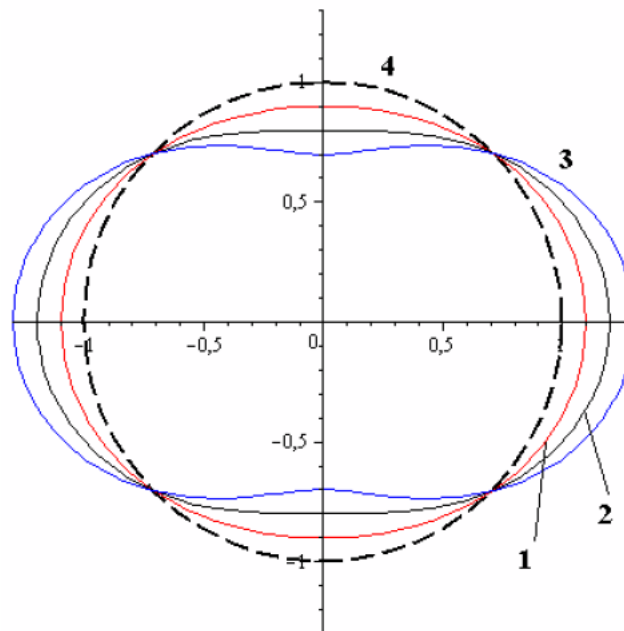


Figure 1: Boundaries of the hole described by the function $f(s) = \cos 2\theta$ in equation (1) for $a = 1$, $\varepsilon = 0, 1; 0, 2; 0, 3$ (curves 1, 2, 3) and $\varepsilon = 0$ (curve 4).

In the case of the 2-D problem, the condition at the boundary is described by the generalized

Laplace – Young law [14, 18] and has the form [22, 25]:

$$\sigma_n(\zeta) = \sigma_{nn} + i\sigma_{nt} = \frac{\sigma_{tt}^s}{R} - i\frac{1}{h}\frac{d\sigma_{tt}^s}{d\theta} + p(\zeta) \equiv t^s(\zeta) + p(\zeta), \quad \zeta \in \Gamma, \quad (2)$$

where σ_{nn}, σ_{nt} are normal and tangential stresses (in equation (2), the unit vectors \mathbf{n} and \mathbf{t} are the basis vectors of the local Cartesian coordinates n, t); $\sigma_{tt}^s = \tau$ is the surface stress, p is the external force. Metric coefficient h [30] and the curvature radius of the boundary R are evaluated in terms of the radius a by the formulas:

$$L = \frac{1}{h} = \frac{1}{\sqrt{x_1'^2 + x_2'^2}}, \quad K = \frac{1}{R} = \frac{x_1'x_2'' - x_2'x_1''}{h^3}$$

and can be written as

$$L = \frac{1}{\sqrt{(\delta')^2 + (1 + \delta)^2}}, \quad K = \frac{2(\delta')^2 - (1 + \delta)\delta'' + (1 + \delta)^2}{h^3}, \quad (3)$$

where $\delta = \varepsilon f(s)$.

At infinity, the stresses σ_{ij} ($i, j = 1, 2$) and rotation angle ω are specified as

$$\lim_{z \rightarrow \infty} \sigma_{ij} = \sigma_{ij}^\infty = s_{ij}, \quad \lim_{z \rightarrow \infty} \omega = 0. \quad (4)$$

In the case of the plane strain, the constitutive equations of the surface [11, 12] and volume [31] linear elasticities are respectively reduced to the following [21, 22]

$$\sigma_{tt}^s = \gamma_0 + (\lambda_s + 2\mu_s)\varepsilon_{tt}^s, \quad \sigma_{33}^s = \gamma_0 + \lambda_s\varepsilon_{tt}^s \quad (5)$$

and

$$\begin{aligned} \sigma_{nn} &= (\lambda + 2\mu)\varepsilon_{nn} + \lambda\varepsilon_{tt}, & \sigma_{tt} &= (\lambda + 2\mu)\varepsilon_{tt} + \lambda\varepsilon_{nn}, \\ \sigma_{nt} &= 2\mu\varepsilon_{nt}, & \sigma_{33} &= \lambda(\varepsilon_{tt} + \varepsilon_{nn}). \end{aligned} \quad (6)$$

In equations (5), (6), γ_0 is the residual surface stress; $\varepsilon_{nn}, \varepsilon_{nt}, \varepsilon_{tt}$ are the components of the volume strain tensor; ε_{tt}^s is the surface strain; λ_s, μ_s are the surface elastic constants similar to Lamé constants λ, μ .

To find the surface stress τ and solve the boundary value problem, we use the relations (2)–(6) and the inseparability condition of the surface and bulk, expressed in terms of hoop strains:

$$\varepsilon_{tt}^s(\zeta) = \varepsilon_{tt}(\zeta), \quad \zeta \in \Gamma. \quad (7)$$

3 BOUNDARY EQUATION FOR COMPLEX POTENTIALS

Goursat – Kolosov complex potentials and Muskhelishvili's method [31] are used in order to solve the problem. According to [27, 31], the vector of stresses $\sigma_n = \sigma_{nn} + i\sigma_{nt}$ at the area with the normal \mathbf{n} can be expressed via two functions Φ and Ψ holomorphic outside of their boundaries as

$$\sigma_n(z) = \Phi(z) + \overline{\Phi(z)} + \left[z\Phi'(z) + \overline{\Psi(z)} \right] \frac{d\bar{z}}{dz}, \quad z \in \Omega,$$

where $dz = |dz|e^{i\alpha}$, $d\bar{z} = \overline{dz}$, α is the angle between the axes \mathbf{t} and x_1 .

Following [31], we introduce the new function $\Upsilon(z)$ holomorphic in the finite region $D = \{z : \bar{z}^{-1} \in \Omega\}$ with the boundary $\tilde{\Gamma}$ which is symmetrical to the boundary Γ with respect to the unit circle:

$$\Upsilon(z) = -\overline{\Phi(\bar{z}^{-1})} + z^{-1}\overline{\Phi'(\bar{z}^{-1})} + z^{-2}\overline{\Psi(\bar{z}^{-1})}, \quad \bar{z}^{-1} \in \Omega.$$

Passing to the limit for $z \rightarrow \zeta \in \Gamma$, $z \in \Omega$ [27] and taking into account (2), we get the following boundary equation for complex potentials Φ and Υ :

$$\sigma_n(\zeta) = \Phi(\zeta) + \overline{\Phi(\zeta)} + \frac{\rho' - i\rho}{\rho' + i\rho} \left[\frac{1}{\bar{\zeta}^2} \left(\overline{\Phi(\zeta)} + \Upsilon\left(\frac{1}{\bar{\zeta}}\right) \right) + \left(\zeta - \frac{1}{\bar{\zeta}} \right) \overline{\Phi'(\zeta)} \right] \bar{s}^2, \quad (8)$$

where $\Phi(\zeta) = \lim_{z \rightarrow \zeta} \Phi(z)$ when $z \in \Omega$ and $\Upsilon(\zeta) = \lim_{z \rightarrow \zeta} \Upsilon(z)$ when $z \in D$.

4 BOUNDARY PERTURBATION PROCEDURE

Following perturbation method [25]–[29], we represent unknown functions Φ , Υ and the surface stress τ as power series in the small parameter ε :

$$\Phi(z) = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \Phi_n(z), \quad \Upsilon(z) = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \Upsilon_n(z), \quad \tau(\zeta) = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \tau_n(\zeta). \quad (9)$$

We also derive the expressions for all functions in (8). Taking into account expansions

$$K = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} K_n(s), \quad L = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} L_n(s), \quad (10)$$

we obtain for the zero-order and first-order approximations:

$$K_0 = 1, \quad L_0 = 1, \quad K_1 = -f''(s) - f(s), \quad L_1 = -f(s). \quad (11)$$

Substituting series (9), (10) into equation (8), we equate the sum of coefficients of the same power ε^n ($n = 0, 1, \dots$) to zero. Then we arrive at the Rimann–Gilbert boundary value problem on the jump of the holomorphic function $\Xi_n(z)$ for each-order approximation:

$$\Xi_n^+(s) - \Xi_n^-(s) = -\left(\tau_n(s) + s\tau'_n(s)\right) + F_n(s). \quad (12)$$

Here,

$$\Xi_n^\pm = \lim_{|z| \rightarrow 1 \mp 0} \Xi_n(z), \quad \Xi_n(z) = \begin{cases} \Phi_n(z), & |z| > 1, \\ \Upsilon_n(z), & |z| < 1. \end{cases}$$

According to Muskhelishvili [31], solution of the problem (12) can be written in terms of Cauchy type integrals

$$\Xi_n(z) = -I_n(z) + J_n(z) + S_n(z), \quad (13)$$

where

$$I_n(z) = \frac{1}{2\pi i} \int_{|\zeta|=1} \frac{\tau_n(\zeta) + \zeta\tau'_n(\zeta)}{\zeta - z} d\zeta, \quad J_n(z) = \frac{1}{2\pi i} \int_{|\zeta|=1} \frac{F_n(\zeta)}{\zeta - z} d\zeta, \quad (14)$$

and $S_0 = C + C_2 z^{-2}$, $S_n = 0$ ($n = 1, 2, \dots$), $4C = s_{11} + s_{22}$, $2C_2 = s_{22} - s_{11} - 2is_{12}$.

The functions F_n ($n = 1, 2, \dots$) in (13) are the known functions depending only on all previous approximations. So, in the zero-order and first-order approximations, we obtain:

$$F_0(s) = -p(s),$$

$$F_1(s) = -p'(s) - \bar{s}f(\bar{s})\frac{d\Upsilon_0(\bar{s}^{-1})}{d\bar{s}} + sf(s)\Phi_0'(s) + 2(f(s) - if_\theta'(s))\left(\overline{\Phi_0(s)} + \Upsilon_0(\bar{s}^{-1})\right) -$$

$$-2\bar{s}f(s)\overline{\Phi_0'(s)} - sf(s)\frac{d\tau_0(s)}{d\theta} + (f_\theta''(s) + f(s))\tau_0(s) + i\left(sf(s)\frac{d^2\tau_0(s)}{d\theta^2} - f(s)\frac{d\tau_0(s)}{d\theta}\right).$$

It is easy to see that the integral J_n in the equation (14) is a known function.

5 INTEGRAL EQUATION OF N-ORDER APPROXIMATION. FIRST-ORDER APPROXIMATION

As a result, we use the constitutive equations (5), (6) by Gurtin–Murdoch surface elasticity theory and inseparability condition (7) and obtain the following singular integro-differential equation in the unknown functions τ_n :

$$\tau_n(s) + \frac{M(\varkappa + 1)}{2a - M(\varkappa - 1)} \operatorname{Re} \left(\frac{1}{2\pi i} \int_{|\eta|=1} \frac{\tau_n(\eta) + \eta\tau_n'(\eta)}{\eta - s} d\eta \right) = G_n(s), \quad (15)$$

where $M = (\lambda_s + 2\mu_s)/2\mu$; $\varkappa = (\lambda + 3\mu)/(\lambda + \mu)$.

The function G_0 depends from the load $p(s)$ ($G_0 = 0$ when $p(s) = 0$), and functions G_n ($n > 0$) are expressed through all the previous approximations.

For any-order approximation, the solution of the integral equation (15) can be found in the form of a power series $\tau_n(\zeta) = \sum_{k=-\infty}^{\infty} a_{nk}\zeta^k$ for any external forces $p(s)$ and function $f(s)$. In the case of a hole free from external forces ($p(s) = 0$), the complex potentials in the zero-order approximation, which correspond to the solution of the appropriate boundary value problem for the circular hole, are determined as

$$\Phi_0(z) = C + C_2 z^{-2} - \overline{a_{02}} z^{-2}, \quad \Upsilon_0(z) = C + C_2 z^{-2} - a_{00} - 3a_{02} z^2, \quad (16)$$

where $a_{00} = 4H_1 C - \sigma_0$, $a_{02} = H_2 \overline{C_2}$ and

$$\sigma_0 = -\frac{\gamma_0}{a + M}, \quad H_1 = \frac{M(\varkappa + 1)}{4(a + M)}, \quad H_2 = \frac{M(\varkappa + 1)}{2a + M(\varkappa + 3)}. \quad (17)$$

So, surface stress is written in the form:

$$\tau_0 = a_{00} + a_{02}\zeta^2 + \overline{a_{02}}\zeta^{-2} \quad (18)$$

and hoop stress for the circular hole ($|z| = a$) is defined by the equality:

$$\sigma_{tt} = \sigma_0 + (1 - H_1)(s_{11} + s_{22}) + (2 - 3H_2)(s_{22} - s_{11}) \cos 2\theta - 2(2 - 3H_2)s_{12} \sin 2\theta. \quad (19)$$

This solution is identical to the solution obtained in [22] by the another way.

Consider a curvilinear hole the boundary of which is described by the relation (1) for the function $f(s) = \cos 2\theta$. The integral equation in the first-order approximation is

$$\tau_1(s) + \frac{M(\kappa + 1)}{2a - M(\kappa - 1)} \operatorname{Re} I_1(s) = G_1(s), \quad (20)$$

where

$$G_1(s) = -\frac{M(\kappa + 1)}{2a - M(\kappa - 1)} \operatorname{Re} J_1(s).$$

To find the surface stress τ_1 and therefore complex potentials Φ_1 and Υ_1 , represent τ_1 in the form of the power series. Following the algorithm as shown for any-order approximation, one can solve the boundary value problem in the first-order approximation.

To find the function G_1 , it is necessary to substitute equations (1), (11) and (16)-(18) in the equation (14). After that, one can obtain the solution of the equation (20) in the form:

$$\tau_1(\zeta) = \sum_{k=-5}^5 a_{1k} \zeta^k, \quad a_{1-k} = \overline{a_{1k}}, \quad k = \overline{0, 5} \quad (21)$$

for the boundary of the hole given by the function $f(s) = \cos 2\theta$.

Coefficients a_{1k} in the equation (21) depend on coefficients a_{00} and a_{02} of the first-order approximation and aren't given here because of bulky expressions. We substitute (21) into (12), (13) and obtain the complex potentials as

$$\Phi_1(z) = -I_1^-(z) + J_1^-(z), \quad \Upsilon_1(z) = -I_1^+(z) + J_1^+(z), \quad (22)$$

where $I_1^\pm(z) = I_1(z)$ and $J_1^\pm(z) = J_1(z)$ when $\pm|z| < \pm 1$.

Using expressions (9), (10) and complex potentials (16), (22), we obtain σ_{tt} for the hole determined by the function $f(s) = (s^2 + s^{-2})/2 = \cos 2\theta$:

$$\begin{aligned} \sigma_{tt} = \varepsilon \left(\Phi_1(s) + 2\overline{\Phi_1(s)} + \Upsilon_1(\bar{s}^{-1}) + s f(s) \Phi_0'(s) + \bar{s} f(\bar{s}) \left(2\overline{\Phi_0'(s)} + \frac{d\Upsilon_0(\bar{s}^{-1})}{d\bar{s}} \right) \right) + \\ + 2\varepsilon \left((i f_\theta'(s) - f(s)) \left(\overline{\Phi_0(s)} + \Upsilon_0(\bar{s}^{-1}) \right) + \bar{s} f(s) \overline{\Phi_0'(s)} \right) + \\ + \sigma_0 + (1 - H_1)(s_{11} + s_{22}) + (2 - 3H_2)(s_{22} - s_{11}) \cos 2\theta - 2(2 - 3H_2)s_{12} \sin 2\theta. \end{aligned} \quad (23)$$

6 NUMERICAL RESULTS

According to the equation (23), the hoop stress σ_{tt} depends on the radius a of the basic circular hole (size effect). The dependence of maximum values of σ_{tt} (when $\theta = 0$) in the case of the uniaxial tension s_{22} along the axis x_2 , and $p = \gamma_0 = 0$, is shown in Fig. 2. The plots are constructed for aluminium [22]. Surface elastic modulus [8, 15] lead to $M = 0, 1$ nm (continuous red lines in Fig. 2) or $M = -0, 152$ nm (dashed green lines in Fig. 2). Dotted lines correspond to the classical solution ($M = 0$).

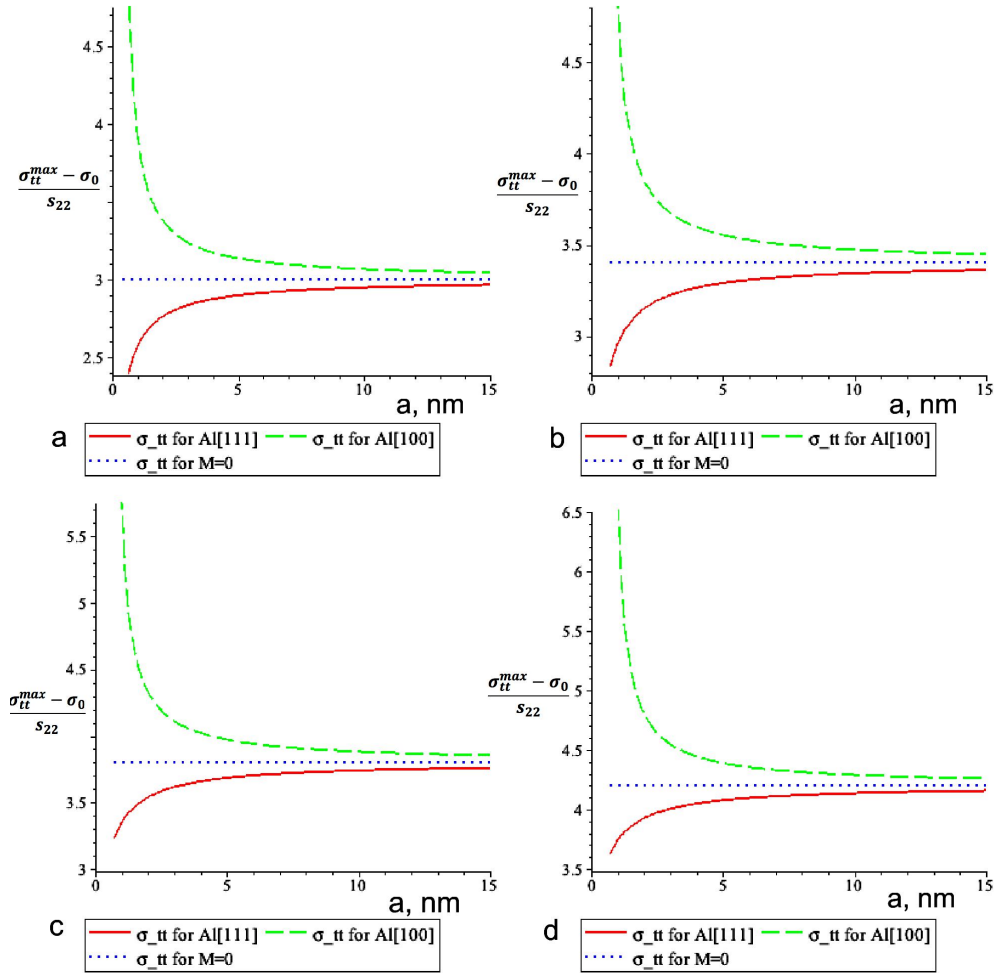


Figure 2: Dependence of maximum hoop stresses upon the radius a of the basic circular hole when $\varepsilon = 0; 0, 1; 0, 2; 0, 3$ (a, b, c, d).

7 CONCLUSIONS

In the paper, we have presented the solution of the two-dimensional boundary value problem on a nanohole slightly deviated from the circular one in an infinite elastic solid. In particular:

- The analytical approximate solution of the problem on a stress-strain state of an elastic solid containing nanosized asperities at the surface is constructed by means of the perturbation method developed in [27].
- Different forms of surface asperities have been considered.
- The rigorous mathematical algorithm of solving the problem to any-order approximation of the perturbation technique has been developed.
- The solution of the integral equation is evaluated analytically in terms of a power series.
- The expressions for the hoop stress in the zero-order and first-order approximations were obtained. In contrast with [22], the solution is built without the use of conformal mapping.

- The size effect as a dependence of the stress state on the size of the hole has been demonstrated.

ACKNOWLEDGEMENT

The work was supported by the Russian Foundation for Basic Research under the grant 14-01-00260.

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