Surface Effects and Problems of Nanomechanics

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Abstract: A boundary value problem on a circular nanometer hole in an elastic plane loaded at the boundary and infinity is solved. It is assumed that complementary surface stresses are acting at the boundary of the hole. Based on Goursat-Kolosov's complex potentials and Muskhelishvili's technique, the solution of the problem is reduced to a hypersingular integral equation in an unknown surface stress. The solution of the problem shows that, due to an existence of the surface stresses, the stress concentration at the boundary depends on the elastic properties of a surface and bulk material, and also on the radius of the hole.

Key words: nanometer circular hole; surface stress; hypersingular integral equation; stress concentration

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The theory of elasticity which takes into consideration the action of stresses at a surface of a body[1-4] is recently applied to the problems of nanotechnology. The surface stresses are supposed to be responsible for abnormal properties of nano-samples in comparison with macro-samples of the same mamerial. In particular, the surface stresses are directly related to the scale effect that means the material properties of a spesimen depend on its size[5-6]. Furthermore, unexpected effects not corresponding to our traditional representations become apparent. For example, Young's modulus of a cylindrical specimen increases significantly, when the cylinder diameter becames very small[7]. From these positions the classical problem concerning an elastic plane with a circular hole loaded at the boundary and infinity will be considered. It is assumed that complementary surface stresses act along the boundary of the hole.

1 The statement of the problem

According to the Laplace-Young law[1,4], the boundary conditions for the circular hole of radius a in a plane are given as follows

$$\sigma_{rr}-\frac{\sigma_{\theta\theta}^{s}}{a}=p_{rr},\sigma_{r\theta}+\frac{1}{a}\frac{\partial\sigma_{\theta\theta}^{s}}{\partial\theta}=p_{r\theta}, \tag{1}$$

here $\sigma_{\theta\theta}^{s}$ is the surface stress; $\sigma_{rr},\sigma_{r\theta}$ and $\sigma_{\theta\theta}$ are the classical stresses in the polar coordinates r,θ, with the center coinciding with that of the circular hole; p_{rr}, $p_{r\theta}$ are the external normal and tangential loads respectively.

The conditions at infinity are

$$\lim_{r\to\infty}\sigma_{jk}=s_{jk},\ \lim_{r\to\infty}\omega=0, \tag{2}$$

where σ_{jk} $(j,k=1,2)$ are the stresses in the Cartesian coordinates x_1 and x_2 ($x_1=r\cos\theta,\ x_2=r\sin\theta$), ω is a turning angle of the material particle.

The constitutive equations for the surface[1,4] and volume linear elasticity in the case of plane strain are reduced to the following

$$\sigma_{\theta\theta}^{s}=\sigma_{0}^{s}+(2\mu_s+\lambda_s-\gamma_s)\varepsilon_{\theta\theta}^{s},$$
$$\sigma_{33}^{s}=\sigma_{0}^{s}+(\lambda_s+\gamma_s)\varepsilon_{\theta\theta}^{s}, \tag{3}$$

and

$$\sigma_{\theta\theta}=(2\mu+\lambda)\varepsilon_{\theta\theta}+\lambda\varepsilon_{rr},\ \sigma_{rr}=(2\mu+\lambda)\varepsilon_{rr}+\lambda\varepsilon_{\theta\theta},$$

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$$\sigma_{r\theta}=2\mu\varepsilon_{r\theta},\ \sigma_{33}=\lambda(\varepsilon_{\theta\theta}+\varepsilon_{rr}). \tag{4}$$

In equations (3) and (4), $\varepsilon_{\theta\theta}^{s}$ is the surface strain; $\varepsilon_{rr},\varepsilon_{r\theta}$ and $\varepsilon_{\theta\theta}$ are the strains in the bulk material; λ_s,μ_s are the modules of the surface elasticity, similar to the Lamé constants λ,μ of the bulk material; γ_s is the residual surface stress under unstrained conditions.

2 Basic relations

First, we construct a solution for the hole of unit radius, therefore, introduce $a=1$ in equation (1). Then in the complex writing, the conditions (1) take the form

$$\sigma_{rr}+i\sigma_{r\theta}=t^{s}(\zeta)+p(\zeta),\ |\zeta|=1, \tag{5}$$

where $t^{s}=\tilde{\sigma}_{\theta\theta}^{s}-i\partial\tilde{\sigma}_{\theta\theta}^{s}/\partial\theta,\ \tilde{\sigma}_{\theta\theta}^{s}=\sigma_{\theta\theta}^{s}/a,\ p=p_{rr}+ip_{r\theta}$, i is the imaginary unit.

Introduce a local orthogonal system of coordinates n, t rotated anticlockwise with respect to the system x_1, x_2 by the angle $\alpha-\pi/2$. Then following Muskhelishvili's technique[8], one can derive the joint expression for the traction $\sigma_n=\sigma_{nn}+i\sigma_{nt}$ and the displacement vector $u=u_1+iu_2$ [9].

$$G(z,\bar{z})=\eta\Phi(z)+\overline{\Phi(z)}+\frac{\mathrm{d}\bar{z}}{\mathrm{d}z}(z\overline{\Phi'(z)}+\overline{\Psi(z)}), \tag{6}$$

where $G=\sigma_n$ for $\eta=1$ and $G=-2\mu\mathrm{d}u/\mathrm{d}z$ for $\eta=-\kappa=-(\lambda+3\mu)/(\lambda+\mu)$, Φ, Ψ are functions holomorphic for $r>1$. A quantity with the bar denotes complex conjugation and the prime denotes the derivative with respect to the argument. The increment $\mathrm{d}z$ is taken in the direction of the axis t. Thus in equation (6), $\mathrm{d}z=|\mathrm{d}z|e^{i\alpha}$, $\mathrm{d}\bar{z}=\overline{\mathrm{d}z}$. According to Muskhelishvili[8] we define function Φ holomorphic for $r<1$ by the formula

$$\Phi(z)=-\overline{\Phi(\bar{z}^{-1})}+z^{-1}\overline{\Phi'(\bar{z}^{-1})}+z^{-2}\overline{\Psi(\bar{z}^{-1})},\ |z|<1. \tag{7}$$

Using equality (7), we derive from (6) the following equation

$$G(z,\bar{z})=\eta\Phi(z)+\overline{\Phi(z)}+\frac{\mathrm{d}\bar{z}}{\mathrm{d}z}\left(\frac{1}{\bar{z}^{2}}\left(\overline{\Phi(z)}+\Phi\left(\frac{1}{\bar{z}}\right)\right)+\left(z-\frac{1}{\bar{z}}\right)\overline{\Phi'(z)}\right),\quad |z|>1, \tag{8}$$

we take the limit $z\to\zeta=e^{i\theta}$ in equation (8) and direct axis n towards the center $z=0$. Since in this case $\alpha=\theta+3\pi/2$ and $\mathrm{d}z=-i|\mathrm{d}z|e^{i\theta}$, by virtue of conditions (3) we obtain from (8)

$$\Phi^{+}(\zeta)-\Phi^{-}(\zeta)=-t^{s}(\zeta)-p(\zeta), \tag{9}$$

here $\Phi^{\pm}(\zeta)$ are the limiting values of function $\Phi(z)$ on the circumference of unit radius when $|z|\to 1\pm 0$.

The solution of the boundary problem (9) is given in [8] and can be written in the form

$$\Phi(z)=-I(z)-I_p(z)+S(z),\ |z|\neq 1, \tag{10}$$

where

$$I(z)=\frac{1}{2\pi i}\oint_{|\eta|=1}\frac{t^{s}(\eta)}{\eta-z}\mathrm{d}\eta,\ I_p(z)=\frac{1}{2\pi i}\oint_{|\eta|=1}\frac{p(\eta)}{\eta-z}\mathrm{d}\eta,$$

$$S(z)=c+c_1/z+c_2/z^{2}, \tag{11}$$

and

$$c=(s_{11}+s_{22})/4,\ c_2=(s_{22}-s_{11}-2is_{12})/2,$$

$$c_1=\frac{\kappa}{2\pi i(1+\kappa)}\oint_{|\eta|=1}p(\eta)\mathrm{d}\eta.$$

We impose the continuity constraint on the displacements vector under passing from the volume to the boundary

$$\lim_{\substack{z\to\zeta\\|z|>1}}u(z)=u^{s}(\zeta),\ |\zeta|=1, \tag{12}$$

where $u^{s}(\zeta)$ is the displacement vector of the boundary point ζ. From (12) follows the same for the volume deformations $\varepsilon_{\theta\theta}$ and the deformation on the boundary $\varepsilon_{\theta\theta}^{s}$, i.e.,

$$\lim_{\substack{z\to\zeta\\|z|>1}}\varepsilon_{\theta\theta}(z)=\varepsilon_{\theta\theta}^{s}(\zeta),\ |\zeta|=1. \tag{13}$$

The relations (11) – (13) result in the equation for the surface stress

$$\sigma_{\theta\theta}^{s}(\zeta)=\gamma_s+M_s\varepsilon_{\theta\theta}(\zeta),\ |\zeta|=1, \tag{14}$$

where $M_s=2\mu_s+\lambda_s-\gamma_s$.

To obtain expression for $\varepsilon_{\theta\theta}$, we find σ_{rr} and $\sigma_{\theta\theta}$ from equation (8) for $\mathrm{d}z=ire^{i\theta}\mathrm{d}\theta$ and $\mathrm{d}z=-e^{i\theta}\mathrm{d}r$ when $\eta=1$ and then use two first equations (4). This way yields the equation

$$2\mu\varepsilon_{\theta\theta}(\zeta)=\mathrm{Re}(\kappa\Phi^{-}(\zeta)+\Phi^{+}(\zeta)). \tag{15}$$

Introducing (15) into (14) and taking into account equations (10) and (11), we arrive at the following equation

$$\sigma_{\theta\theta}^{s}=\gamma_s-M\,\mathrm{Re}(\kappa I^{-}(\zeta)+I^{+}(\zeta))+M(\kappa+1)\cdot(S(\zeta)+\overline{S(\zeta)})-M\,\mathrm{Re}(\kappa I_p^{-}(\zeta)+I_p^{+}(\zeta)), \tag{16}$$

where $M=M_s/2\mu$.

Let $\sigma_s=\sigma_{\theta\theta}^{s},\ \tilde{\sigma}_s=\tilde{\sigma}_{\theta\theta}^{s}$. Since $\partial\sigma_s/\partial\theta=i\zeta\partial\sigma_s/\partial\zeta=i\zeta\sigma_s'(\zeta)$, the Sokhotskii-Plemelj formulas for the

Cauchy type integrals $I(z)$ and $I_p(z)$ acquire the forms

$$I^{\pm}(\zeta)=\pm\frac{\tilde{\sigma}_s(\zeta)}{2}\pm\frac{\zeta\tilde{\sigma}_s(\zeta)}{2}+\frac{1}{2\pi i}\oint_{|\eta|=1}\frac{\tilde{\sigma}_s(\eta)+\eta\tilde{\sigma}_s(\eta)}{\eta-\zeta}\mathrm{d}\eta,$$

$$I_p^{\pm}(\zeta)=\pm\frac{p(\zeta)}{2}+\frac{1}{2\pi i}\oint_{|\eta|=1}\frac{p(\eta)}{\eta-\zeta}\mathrm{d}\eta, \quad (17)$$

where the integral is understood in the sense of the Cauchy principal value.

Introducing (17) into (16) and taking into account the relations $\bar{\eta}=\eta^{-1}, \bar{\zeta}=\zeta^{-1}, \overline{\sigma_s(\eta)}=\sigma_s(\eta), \overline{\eta\tau'(\eta)}=-\eta\tau'(\eta), \mathrm{d}\bar{\eta}=-\eta^{-2}\mathrm{d}\eta,$ we obtain the following singular integro-differential equation

$$(2a-M(\kappa-1))\sigma_s(\zeta)+M(\kappa+1)\cdot\left(\frac{1}{2\pi i}\oint_{|\eta|=1}\frac{\sigma_s(\eta)+\eta\sigma_s'(\eta)}{\eta-\zeta}\mathrm{d}\eta-\frac{\zeta}{2\pi i}\oint_{|\eta|=1}\frac{\eta^{-1}\sigma_s(\eta)-\sigma_s'(\eta)}{\eta-\zeta}\mathrm{d}\eta\right)=2a\gamma_s+Ma(\kappa+1)(S(\zeta)+\overline{S(\zeta)})-2Ma\,\mathrm{Re}(\kappa I_p^-(\zeta)+I_p^+(\zeta)). \quad (18)$$

In (21) and (22) we denote $\eta=\eta_1/a, \zeta=\zeta_1/a$ where η_1,ζ_1 are points on the circumference of radius a.

It is clear that $\sigma_{\theta\theta}^s=\mathrm{const}$ if the external loads are absence. Let $s_{jk}=0, p=0$ and $\sigma_{\theta\theta}^s=\sigma_0^s$. We derive from equation (18) that surface stress σ_0^s at the boundary of the circular hole in the unloaded plane is

$$\sigma_0^s=\frac{a}{a+M}\gamma_s. \quad (19)$$

Using the regularization formula[10] and denoting $\tau=\sigma_s-\sigma_0^s$, we reduce equation (19) to the hypersingular integral equation in the unknown function $\tau(\zeta)$,

$$(2a-M(\kappa-1))\tau(\zeta)+\frac{M(\kappa+1)}{2\pi i}\cdot\oint_{|\eta|=1}\frac{(\eta+\zeta^2/\eta)\tau(\eta)}{(\eta-\zeta)^2}\mathrm{d}\eta=Ma(\kappa+1)\cdot(S(\zeta)+\overline{S(\zeta)})-2Ma\,\mathrm{Re}(\kappa I_p^-(\zeta)+I_p^+(\zeta)),\quad |\zeta|=1. \quad (20)$$

It is important to note that according to the construction of the equation (20), the homogeneous equation. corresponding to the equation (20) does not have non-trivial solution.

3 Solution for the circular hole with free boundary

For the case of a circular hole the boundary of which is free from the external load ($p=0$), the solution of the equation (20) has the simple form

$$\tau=d_0+d_2\zeta^2+\overline{d_2}\zeta^{-2}, \quad (21)$$

where

$$d_0=aH_1(s_{11}+s_{22}),\ 2d_2=aH_2(s_{22}-s_{11}+2is_{12}), \quad (22)$$

and

$$H_1=\frac{M(1+\kappa)}{4(a+M)},\ H_2=\frac{M(1+\kappa)}{2a+M(3+\kappa)}.$$

The expression for the hoop stresses we derive from equation (8) under $\mathrm{d}z=-e^{i\theta}\mathrm{d}r$ and $\eta=1$

$$\sigma_{\theta\theta}(\zeta_1)=\mathrm{Re}(3\Phi^-(\zeta)+\Phi^+(\zeta)),\ |\zeta_1|=a. \quad (23)$$

Taking into account (10), (11), (19), (21) and (22), we obtain from equation (23)

$$\sigma_{\theta\theta}\big|_{r=a}=-\frac{\gamma_s}{a+M}+(1-H_1)(s_{11}+s_{22})+(2-3H_2)(s_{22}-s_{11})\cos 2\theta-2(2-3H_2)s_{12}\sin 2\theta. \quad (24)$$

This formula coincides with the solution of Tian and Rajapakse[5] obtained by another way.

Particular cases

(1) Equibiaxial tension/compression $s_{11}=s_{22}=p$, $s_{12}=0$,

$$\sigma_{\theta\theta}\big|_{r=a}=-\frac{\gamma_s}{a+M}-\frac{M(1+\kappa)}{2(a+M)}p+2p. \quad (25)$$

(2) Uniaxial tension (the Kirsch problem) $s_{11}=p_1$, $s_{22}=s_{12}=0$,

$$\sigma_{\theta\theta}\big|_{r=a}=-\frac{\gamma_s}{a+M}+\left(1-\frac{M(1+\kappa)}{4(a+M)}\right)p_1-\left(2-\frac{3M(1+\kappa)}{2a+M(3+\kappa)}\right)p_1\cos 2\theta. \quad (26)$$

(3) Simple shear $s_{12}=q,\ s_{11}=s_{22}=0$,

$$\sigma_{\theta\theta}\big|_{r=a}=-\frac{\gamma_s}{a+M}-2\left(2-\frac{3M(1+\kappa)}{2a+M(3+\kappa)}\right)q\sin 2\theta. \quad (27)$$

The equalities (25) – (27) show that the presence of the surface stress decreases the stress concentration if $M>0$. The residual stress γ_s produces the same effect. Besides, the stress concentration depends on the radius of the hole (scale effect). According to theoretical calculations for cubic metals[11] and estimates produced in [6], the parameter $M = (2\mu_s+\lambda_s-\gamma_s)/(2\mu)$ in which the residual stress γ_s is negligible has an order $M \sim (10^{-10}-10^{-9})$ m, and $\gamma_s \sim 1\,\mathrm{N{\cdot}m^{-1}}$. In this case if $a \sim 10$ nm, the first member in (25) – (27) has the order $10^8\,\mathrm{N{\cdot}m^{-2}}$=100 MPa. So, for the values of remote loads p, p_1, q up to 100 MPa, the influence of the residual stress γ_s on the stress dis- tribution at the boundary and especially on the stress concentration is comparable with the influence of remote loads. Furthermore, the effect of the residual surface stress surpasses that of surface elasticity because the rest members in (25) – (27) con- taining parameter M are less than the first one. This phenomenon was recently ascertained by Goldstein et al[6].

4 Conclusion

The general analytical solution of the 2D problem on a circular nanometer hole in an elastic plane is constructed and reduced to the hypersingular integral equation in the surface stress. For the case of remote loading, the solution of this equation is obtained in a closed form. The effect of the surface stress and residual surface stress on the stress concentration is analyzed for the simplest kinds of loading.

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纳米力学中的表面效应及相关问题

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摘要：对载荷作用在边界和无穷远处的含有纳米圆孔弹性平面薄板问题进行了分析，给出了其边界值问题的解．假设全表面应力作用于孔的边界上，基于古沙－科洛索夫复势和 Muskhelishvili's 技术，问题可简化为一个未知表面应力的超奇异积分方程的解．结果表明：由于表面应力存在，边界上的应力集中取决于材料表面和体内的弹性性质，也与孔的半径相关．

关键词：纳米圆孔；表面应力；超奇异积分方程；应力集中

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