Analytical Solution of Contact Problem for Nanomaterial with Surface Tension

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Abstract. This paper proposes an application of surface elasticity theory in the analysis of contact problem at nano-scale. The Fourier integral transform method is adopted to derive the fundamental solutions for contact problem with surface tension effects. As a special case, the deformation induced by normal triangle distribution force is discussed in detail. The results indicate some interesting characteristics in nano-mechanics, which are distinctly different from those in classical contact problem. The results show that the hardness of material depends strongly on the surface tension.

Introduction

For solids with large characteristic dimensions, the volume ratios of surface region to the bulk material is small, the effect of surface then can be neglected because of its relatively tiny contribution. However, for micro-nano solids with large surface-to-bulk ratio the significance of surfaces is likely to be important. Form the viewpoint of continuum mechanics, this difference can be described by such concepts as surface tension, surface energy, and surface constitutive relations [1]. This is extremely true for nano-scale materials or structures. In such cases, the surface residual tension plays a critical role and thus has been adding its appeal to many researchers. For example, Miller and Shenoy [2] first probed the size-dependent elastic properties of nanoplates and beams. Dingreville et al. [3] investigated the surface free energy and its effect on elastic behavior of the nanosized particles, wires, and films. For more recent developments in this field, the readers can refer to a review article by Wang et al. [4].

To study the mechanical behavior of an immediate neighborhood of material surfaces through a continuum-based model, Gurtin and Murdoch [5,6] developed a mathematical framework, known as the theory of surface elasticity. In the study of nano-scale problems, all material constants appearing in that constitutive model were commonly calibrated with data obtained from either experimental measurements [7] or atomistic simulations [2,8]. Therefore, the surface effect has been widely adopted to investigate the mechanical phenomena at nano-scale. Cammarata et al. [9] considered the size-dependent deformation in thin film with surface effects, Wang et al. [10] studied the response of a half-plane subjected to normal pressures with constant residual surface tension. Long and Wang [11] studied the effect of the residual surface stress on the two dimensional Hertz contact problem. Wang [12] derived the general analytical solution of nano-contact problem with surface effects by using the complex variable function method. In this paper, Fourier integral transform method is used to solve the non-classical boundary value problems with surface tension effects.

Basic Equations

In the absence of body force, the equilibrium equations in the bulk are as follows

\[
\sigma_{ij} = 0, \quad \sigma_{ij} = 2G\left(\varepsilon_{ij} + \frac{\mu}{1-2\mu}\delta_{ij}\right) \quad (1)
\]

where \(G\) and \(\mu\) are the shear modulus and Poisson’s ratio of the bulk material, \(\sigma_{ij}\) and \(\varepsilon_{ij}\) are the
stress tensor and strain tensor in the bulk material, respectively.

On the surface, the generalized Young-Laplace equation, surface constitutive relation and strain-displacement relationship can be expressed as

\[
\sigma_{\beta\alpha} n_{\beta} + \sigma_{\beta\alpha}^{s} = 0
\]

\[
\sigma_{ij} n_{i} n_{j} = \sigma_{\beta\alpha}^{s} K_{\beta\alpha}
\]

\[
\sigma_{\beta\alpha}^{s} = \tau^{s} \delta_{\beta\alpha} + \frac{\partial \tau^{s}}{\partial \varepsilon_{\beta\alpha}}
\]

where \( n_{i} \) denotes the normal to the surface, \( K_{\beta\alpha} \) the curvature tensor of the surface, \( \sigma_{\alpha\beta}^{s} \) and \( \varepsilon_{\alpha\beta}^{s} \) the surface stress and surface strain tensor, \( \tau^{s} \) is the residual surface tension under unstrained conditions.

**General Solutions**

For the considered plane problem, the equilibrium equations and Hooke’s law in the bulk reduce to

\[
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} = 0, \frac{\partial \sigma_{xx}}{\partial z} + \frac{\partial \sigma_{zz}}{\partial x} = 0
\]

\[
\varepsilon_{xx} = \frac{1}{2G} [(1-v)\sigma_{xx} - v\sigma_{zz}], \varepsilon_{zz} = \frac{1}{2G} [(1-v)\sigma_{zz} - v\sigma_{xx}], \varepsilon_{xx} = \frac{\sigma_{xx}}{2G}
\]

The strains are related to the displacements by

\[
\varepsilon_{xx} = \frac{\partial u}{\partial x}, \varepsilon_{zz} = \frac{\partial w}{\partial z}, \varepsilon_{xz} = \frac{1}{2} \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)
\]

As in classical theory of elasticity, the Airy stress function \( \chi(x, z) \) is defined by

\[
\sigma_{xx} = \frac{\partial^{2} \chi}{\partial z^{2}}, \sigma_{zz} = \frac{\partial^{2} \chi}{\partial x^{2}}, \sigma_{xz} = -\frac{\partial^{2} \chi}{\partial x \partial z}
\]

Then the equilibrium equations in Eq. (6) are satisfied automatically, and the compatibility equation in Eq. (12) becomes

\[
\left( \frac{\partial^{2}}{\partial x^{2}} + \frac{\partial^{2}}{\partial z^{2}} \right) \left( \frac{\partial^{2} \chi}{\partial x^{2}} + \frac{\partial^{2} \chi}{\partial z^{2}} \right) = 0
\]

To solve the boundary value problem, the Fourier integral transformation method is adopted to the coordinate \( x \). Then, the Airy stress function \( \chi(x, z) \) and its Fourier transformation \( \tilde{\chi}(\xi, z) \) can be expressed as

\[
\tilde{\chi}(\xi, z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \chi(x, z) e^{i\xi z} d\xi, \chi(x, z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\chi}(\xi, z) e^{-i\xi z} d\xi
\]

Substituting Eqs. (8) into Eq. (7) and considering the condition that the stresses vanish at infinity, one obtains

\[
\tilde{\chi}(\xi, z) = (A + Bz) e^{-|\xi|}
\]

where \( A \) and \( B \) are generally functions of \( \xi \) as yet to be determined by boundary conditions.

Substituting Eq. (9) and Eqs. (8) into Eq. (6), the stresses can be written as
\[ \sigma_{xx} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[ A(\xi) + (z - 2|\xi|)B(\xi) \right] \xi e^{-i\xi z - i|\xi|} d\xi \]
\[ \sigma_{zz} = -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[ A(\xi) + zB(\xi) \right] \xi^2 e^{-i\xi z - i|\xi|} d\xi \]
\[ \sigma_{xz} = \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \xi \left[ (1 - |\xi|)B(\xi) - |\xi|A(\xi) \right] e^{-i\xi z - i|\xi|} d\xi \]

By substituting the stresses into the Eq. (4) and using Eqs. (5), the displacements are derived as

\[ u(x, z) = \frac{i}{2G\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[ (2 - \nu)|\xi|A(\xi) + (z|\xi| - 2(1 - \nu))B(\xi) \right] e^{-i\xi z - i|\xi|} d\xi + C_1 \]
\[ w(x, z) = \frac{1}{2G\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[ |\xi|A(\xi) + (1 - 2\nu + z|\xi|)B(\xi) \right] e^{-i\xi z - i|\xi|} d\xi + C_2 \]

**Elastic Solution under a Normal Triangle Distribution Force**

As a particular example, let us consider the effect of a normal triangle distribution force \( p(x) \) over the region \( |x| \leq a \), while the normal force form zero (\( O_1 \) and \( O_2 \)) uniformly increased to maximum \( p_0 \) (O), while remainder of the boundary \( y = 0 \) being unstressed.

\[ p(x) = \frac{p_0}{a} (a - |x|), \quad |x| \leq a \]  

(12)

If the change of the atomic spacing in deformation is infinitesimal, the contribution from the second term Eq. (3) to the surface stresses is negligibly small compared to the residual surface tension [8]. In what follows, we keep only the first term in Eq. (3). Then, the surface stresses are given by

\[ \sigma_{\beta\alpha}^s = \tau^s \delta_{\beta\alpha} \]  

(13)

In this case, the boundary conditions (2) on the contact surface \( (z = 0) \) are simplified to

\[ \sigma_{xz}(x) = 0, \quad p(x) + \sigma_{zz}(x) = -\tau^s / R(x) \]  

(14)

Substituting Eqs. (14) into Eqs. (10), one obtains

\[ B = A|\xi| \]  

(15)

On the surface, the radius of curvature due to deformation is given by

\[ 1/R(x) = \partial^2 w(x, 0)/\partial x^2 \]

(16)

By substituting Eqs. (15) and (16) into the surface condition Eqs. (14), \( A(\xi) \) is determined

\[ A(\xi) = \frac{\tilde{p}(\xi)}{\left(1 + s|\xi|\right)\xi^2} \]  

(17)

where

\[ \tilde{p}(\xi) = \frac{p_0}{a} \sqrt{\frac{2}{\pi}} \frac{1 - \cos(a\xi)}{\xi^2}, \quad s = \frac{\tau^s(1 - \nu)}{G} \]

(18)
Therefore $A(\xi)$ is given by

$$A(\xi) = \frac{p_0}{a} \sqrt{2} \frac{1 - \cos(a \xi)}{\pi (s + \xi)} \xi^4$$

(19)

Substituting Eq. (19) into Eqs. (10) and (11), the stresses component and displaces component are obtained as

$$\sigma_{xx} = \frac{2q_0}{\pi a} \int_0^\infty \left( \frac{z \xi - 1}{1 + b \xi} \right) \cos \left( \frac{z \xi}{\xi} \right) \left[ 1 - \cos \left( a \xi \right) \right] e^{-iz \xi} d\xi$$

$$\sigma_{zz} = -\frac{2q_0}{\pi a} \int_0^\infty \left( \frac{z \xi + 1}{1 + b \xi} \right) \cos \left( \frac{z \xi}{\xi} \right) \left[ 1 - \cos \left( a \xi \right) \right] e^{-iz \xi} d\xi$$

$$\sigma_{xz} = -\frac{2q_0}{\pi a} \int_0^\infty \left( \frac{z}{1 + s \xi} \right) \sin \left( \frac{z \xi}{\xi} \right) \left[ 1 - \cos \left( a \xi \right) \right] e^{-iz \xi} d\xi$$

(20)

$$u(x, 0) = \frac{p_0}{\pi G a} \int_0^\infty \frac{1 - \cos t}{t^r} \left( 1 + \frac{s}{t} \right)^{-1} \cos \left( \frac{x}{a} t \right) dt$$

(21)

If the normal displacement is $w$ specified to be zero at a distance $r_0$ on the contact surface, that is, $w(r_0, 0) = 0$, the displacement on the surface is derived as

$$w(x, 0) = \frac{2p_0(1 - \nu) a}{\pi G} \int_0^\infty \left( 1 - \cos(t) \right) \left( \frac{s}{a} + 1 \right)^{-1} \left[ \cos \left( \frac{x}{a} t \right) - \cos \left( \frac{r_0}{a} t \right) \right] dt$$

(22)

Assuming that the origin has no displacement in the $x$ direction, that is, $u(0, 0) = 0$ one obtains

$$u(x, 0) = -\frac{p_0(1 - 2\nu) a}{\pi G} \int_0^\infty \left( 1 - \cos(t) \right) \left( \frac{s}{a} + 1 \right)^{-1} \sin \left( \frac{x}{a} t \right) dt$$

(23)

As show in Figure 1, The actual normal stress $\sigma_{zz}$ is smaller than the classical value in the loading zone and is larger outside of the zone. If the residual surface tension is ignored ($s/a=0$), the values of $\sigma_{zz}$ reduce to the classical values.
Due to the different residual surface stress value, the horizontal displacement is displayed in Figure 2, where we set \( r_0 = 5a \), and \( K_s = (1-2v)/\pi G \). It is seen that the horizontal displacement is continuous everywhere on the deformed surface. The indent depth is plotted in Fig. 3 with \( K_s = 2(1-\nu)/\pi G \), which also shows that the slope of the deformed surface for \( a > 0 \) is continuous everywhere. It is also found the indent depth decreases with the increase of residual surface tension.
To elucidate the size dependence of hardness on indenter size in nanoindentation, the following parameter is $H$ defined by

$$ H = \frac{2p_o a}{w(0,0)} = \pi G \int_0^\pi \left( \frac{1 - \cos(t)}{t^2} \right) \left( \frac{s}{a} + 1 \right)^{-1} \left[ 1 - \cos \left( \frac{r_o a}{s} t \right) \right] dt \quad (24) $$

To stand for the hardness of material subjected to the normal triangle distribution load. The variation of $H / H_0$ with respect to the indenter size $a$ is shown in Fig. 4, where $H_0 = \pi G (1 - \nu)$. The numerical results illustrate that the size effect becomes remarkable. At the nano-scale, the smaller the contact region, the larger the contact stiffness compared with the classical result.

**Conclusions**

In this paper, we consider the two-dimensional contact problem in the light of surface elasticity theory. The general analytical solution is derived by using the Fourier integral transform method. For a particular loading case of normal triangle distribution force, the results are analyzed in detail and compared with the classical linear elastic solutions. A series of theoretical and numerical results show that the surface elasticity theory illuminates some interesting characteristics of contact problems at nano-scale, which are distinctly different from the classical solutions of elasticity without surface effects. Therefore the effects of surface tension should be considered for nanocontact problems.

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**References**


