



**ANALYTICAL SOLUTION
OF CONTACT PROBLEM FOR NANOMATERIAL WITH SURFACE TENSION**

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ABSTRACT

Consideration the effects of surface tension on the elastic field of solid material has applications in several modern problems in solid mechanics. 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. This study is helpful to characterize and measure the mechanical properties of soft materials through nanoindentation.

Key words: *Surface tension, nano-scale, contact problem, normal triangle distribution force, Fourier integral transform method.*

1. INTRODUCTION

In the recent years, many new nano-materials have been developed by utilizing the fact that, at a nano-scale, materials begin to exhibit unique mechanical properties, which significantly differ from those at a larger scale. To take most advantages of these novel properties on the development of powerful nano-devices, profound understanding on their behavior and characterization of material properties at such very small scale is essential for various researchers.

The surface of solids is a special region with very small thickness (a few times of atom-spacing). Since the equilibrium lattice spacing in the surface is different from that in the bulk, surface effect appears. 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. From 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. Hang *et al.* [3] explained the size dependent phenomenon by the strain gradient continuum theory. Sharma *et al.* [4] and Sharma and Ganti [5] studied the effect of surface/interfacial energy on the Eshelby's inclusion and inhomogeneity problems. Dingreville *et al.* [6] investigated the surface free energy and its effect on elastic behavior of the nanosized particles, wires, and films. Yang [7] studied the size-dependent effective modulus of spherical nanocavities at dilute concentrations. There are a lot of work regarding the surface/interface energy effects on the nanostructures and solids, and we can only include a small part of them here. For more recent developments in this field, the readers can refer to a review article by Wang *et al.* [8].

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To study the mechanical behavior of an immediate neighborhood of material surfaces through a continuum-based model, Gurtin and Murdoch [9-12] developed a mathematical framework, known as the theory of surface elasticity. In their model, the existing surface is simply represented by an infinitesimally thin layer (or, mathematically, a layer of zero thickness) bonded perfectly to the bulk (i.e., an interior of the body) and its behavior is governed by a constitutive law different from that of the bulk. 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 [13] or atomistic simulations [2, 14]. Therefore, the surface effect has been widely adopted to investigate the mechanical phenomena at nano-scale. Cammarata *et al.* [15] considered the size-dependent deformation in thin film with surface effects. Wang *et al.* [16] studied the response of a half-plane subjected to normal pressures with constant residual surface tension. Long and Wang [17] studied the effect of the residual surface stress on the two dimensional Hertz contact problem, and later Long *et al.* [18] generalized their work to the three dimensional case. In fact, spherical indenters are even more widely used in indentation tests. Wang [19] derived the general analytical solution of nanocontact problem with surface effects by using the complex variable function method. In this paper, Fourier integral transform method is used to solve the nonclassical boundary value problems with surface tension effects.

The outline of the paper is organized as follows. In section 2, the present problem is described. The basic equations of surface elasticity theory are reviewed briefly in Section 3. In section 4, the Fourier integral transform method is adopted to solve the nanocontact problem with surface tension effects subjected to a normal triangle distribution loading. The detailed result for the cases of normal load is discussed in Sections 5. Finally, the main results of the present work are summarized in Section 6.

2. PROBLEM DESCRIPTION

Now we consider a material occupying the upper half-plane $z > 0$, we refer to a Cartesian coordinate system ($o-xyz$), as shown in Fig. 1, where the x axis is along the surface and the z axis perpendicular to the surface. It is assumed that the material is subjected to 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 at the point O . The plane-strain conditions are assumed to $\varepsilon_{2i} = 0$, and the contact is assumed to be frictionless.

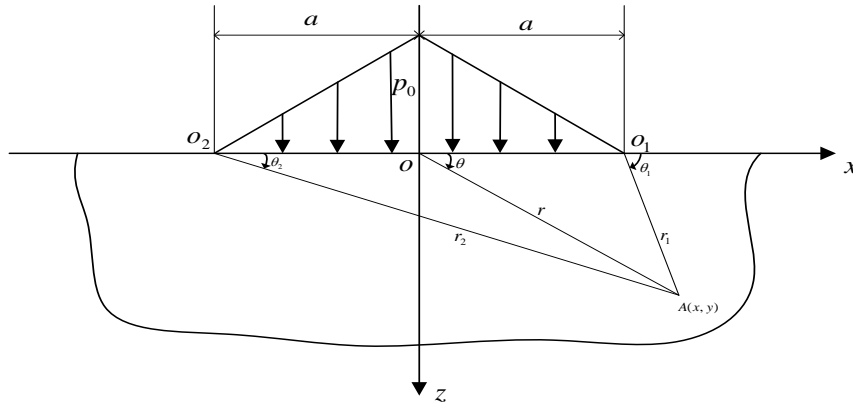


Figure-1: Schematic of contact problem under triangle distribution loads.

The problem statement is to determine the normal triangle distribution force exerted by the elastic field (e.g., displacement and stresses) with the half-plane for the influence of surface effects. The size-dependency behavior of the predicted solutions and the contribution of the surface residual tension to those solutions is to be fully investigated.

3. BASIC EQUATIONS

In the absence of body force, the equilibrium equations, constitutive law, and geometry relations in the bulk are as follows

$$\begin{aligned} \sigma_{ij,j} &= 0 \\ \sigma_{ij} &= 2G \left(\varepsilon_{ij} + \frac{\mu}{1-2\mu} \varepsilon_{kk} \delta_{ij} \right) \end{aligned} \tag{1}$$

where G and μ are the shear modulus and Poisson's ratio of the bulk material, σ_{ij} and ε_{ij} are the stress tensor and strain tensor in the bulk material, respectively. Throughout the paper, Einstein's summation convention is adopted for all repeated Latin indices (1, 2, 3) and Greek indices (1, 2).

The strain tensor is related to the displacement vector u_i by

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \quad (2)$$

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

$$\sigma_{\beta\alpha} n_\beta + \sigma_{\beta\alpha,\beta}^s = 0 \quad (3)$$

$$\sigma_{ij} n_i n_j = \sigma_{\beta\alpha}^s K_{\beta\alpha}$$

$$\sigma_{\beta\alpha}^s = \tau^s \delta_{\beta\alpha} + \frac{\partial \tau^s}{\partial \varepsilon_{\beta\alpha}^s} \quad (4)$$

$$\varepsilon_{\alpha\beta}^s = \frac{1}{2}(u_{\alpha,\beta}^s + u_{\beta,\alpha}^s) \quad (5)$$

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, τ^s is the residual surface tension under unstrained conditions.

4. GENERAL SOLUTIONS

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

$$\begin{aligned} \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} &= 0, \quad \frac{\partial \sigma_{zz}}{\partial z} + \frac{\partial \sigma_{xz}}{\partial x} = 0 \\ \varepsilon_{xx} &= \frac{1}{2G} [(1-\nu)\sigma_{xx} - \nu\sigma_{zz}] \\ \varepsilon_{zz} &= \frac{1}{2G} [(1-\nu)\sigma_{zz} - \nu\sigma_{xx}] \\ \varepsilon_{xz} &= \frac{\sigma_{xz}}{2G} \end{aligned} \quad (6)$$

The strains are related to the displacements by

$$\varepsilon_{xx} = \frac{\partial u}{\partial x}, \varepsilon_{zz} = \frac{\partial w}{\partial z}, \varepsilon_{xz} = \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \quad (7)$$

which satisfy the following compatibility condition

$$\frac{\partial^2 \varepsilon_{xx}}{\partial z^2} + \frac{\partial^2 \varepsilon_{zz}}{\partial x^2} = 2 \frac{\partial^2 \varepsilon_{xz}}{\partial x \partial z} \quad (8)$$

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

$$\sigma_{xx} = \frac{\partial^2 \chi}{\partial z^2}, \sigma_{zz} = \frac{\partial^2 \chi}{\partial x^2}, \sigma_{xz} = -\frac{\partial^2 \chi}{\partial x \partial z} \quad (9)$$

Then the equilibrium equations in Eq. (9) are satisfied automatically, and the compatibility equation in Eq. (12) becomes

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) \left(\frac{\partial^2 \chi}{\partial x^2} + \frac{\partial^2 \chi}{\partial z^2} \right) = 0 \quad (10)$$

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

$$\begin{aligned} \tilde{\chi}(\xi, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \chi(x, z) e^{ix\xi} d\xi \\ \chi(\xi, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\chi}(x, z) e^{-ix\xi} d\xi \end{aligned} \quad (11)$$

Substituting Eqs. (11) in to Eq. (10) and considering the condition that the stresses vanish at infinity, one obtains

$$\tilde{\chi}(\xi, z) = (A + Bz)e^{-z|\xi|}. \tag{12}$$

where A and B are generally functions of ξ as yet to be determined by boundary conditions.

Substituting Eq. (12) and Eqs. (11) in to Eq. (10), the stresses can be written as

$$\begin{aligned} \sigma_{xx} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} [A(\xi) + (z - 2|\xi|)B(\xi)] \xi e^{-ix\xi - z|\xi|} d\xi \\ \sigma_{zz} &= -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} [A(\xi) + zB(\xi)] \xi^2 e^{-ix\xi - z|\xi|} d\xi \\ \sigma_{xz} &= \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \xi [(1 - |\xi|z)B(\xi) - |\xi|A(\xi)] e^{-ix\xi - z|\xi|} d\xi \end{aligned} \tag{13}$$

By substituting the stresses into the Eq. (10) and using Eqs. (11), the displacements are derived as

$$\begin{aligned} u(x, z) &= \frac{i}{2G\sqrt{2\pi}} \int_{-\infty}^{\infty} [(2 - \nu)|\xi|A(\xi) + (z|\xi| - 2(1 - \nu))B(\xi)] e^{-ix\xi - z|\xi|} d\xi + C_1 \\ w(x, z) &= \frac{1}{2G\sqrt{2\pi}} \int_{-\infty}^{\infty} [|\xi|A(\xi) + (1 - 2\nu + z|\xi|)B(\xi)] e^{-ix\xi - z|\xi|} d\xi + C_2 \end{aligned} \tag{14}$$

5. 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 as shown in Fig.1.

$$p(x) = \frac{p_0}{a}(a - |x|), \quad |x| \leq a \tag{15}$$

Due to the second term in Eq. (4) indicates a variation of the surface energy density with respect to elastic strain, which is related to the stretching or compressing the atoms in the surface to accommodate to the bulk phase. If the change of the atomic spacing in deformation is infinitesimal, the contribution from the second term 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. (4). Then, the surface stresses are given by

$$\sigma_{\beta\alpha}^s = \tau^s \delta_{\beta\alpha} \tag{16}$$

In this case, the boundary conditions (3) on the contact surface ($z = 0$) are simplified to

$$\begin{aligned} \sigma_{xz}(x) &= 0 \\ p(x) + \sigma_{zz}(x) &= -\frac{\tau^s}{R(x)} \end{aligned} \tag{17}$$

Substituting Eqs. (17) into Eqs. (13), one obtains

$$B = A|\xi| \tag{18}$$

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

$$\frac{1}{R(x)} = \frac{\partial^2 w(x, 0)}{\partial x^2} \tag{19}$$

By substituting Eqs. (18) and (19) into the surface condition Eqs. (17), $A(\xi)$ is determined by

$$A(\xi) = \frac{\tilde{p}(\xi)}{(1 + s|\xi|)\xi^2} \tag{20}$$

where

$$s = \frac{\tau^s (1-\nu)}{G} \tag{21}$$

$$\tilde{p}(\xi) = \frac{p_0}{a} \sqrt{\frac{2}{\pi}} \frac{1 - \cos(a\xi)}{\xi^2} \tag{22}$$

Therefore $A(\xi)$ is given by

$$A(\xi) = \frac{p_0}{a} \sqrt{\frac{2}{\pi}} \frac{1 - \cos(a\xi)}{(1 + s|\xi|)\xi^4} \tag{23}$$

Substituting Eq. (23) into Eqs. (13) and (14), the stresses component and displaces component are obtained as

$$\begin{aligned} \sigma_{xx} &= \frac{2q_0}{\pi a} \int_0^\infty \left(\frac{z\xi - 1}{1 + s\xi} \right) \frac{\cos(x\xi)}{\xi^2} [1 - \cos(a\xi)] e^{-z\xi} d\xi \\ \sigma_{zz} &= -\frac{2q_0}{\pi a} \int_0^\infty \left(\frac{z\xi + 1}{1 + b\xi} \right) \frac{\cos(x\xi)}{\xi^2} [1 - \cos(a\xi)] e^{-z\xi} d\xi \\ \sigma_{xz} &= -\frac{2q_0}{\pi a} \int_0^\infty \left(\frac{z}{1 + s\xi} \right) \frac{\sin(x\xi)}{\xi} [1 - \cos(a\xi)] e^{-z\xi} d\xi \\ u(x, z) &= \frac{p_0}{\pi G a} \int_0^\infty \left[\frac{z\xi + 2\nu - 1}{\xi^3 (1 + s\xi)} \right] \sin(x\xi) [1 - \cos(a\xi)] e^{-z\xi} d\xi + C_1 \\ w(x, z) &= \frac{p_0}{\pi G a} \int_0^\infty \frac{z\xi + 2(1-\nu)}{\xi^3 (1 + b\xi)} \cos(x\xi) [1 - \cos(a\xi)] e^{-z\xi} d\xi + C_2 \end{aligned} \tag{24}$$

It is seen, when $s = 0$, that is, the surface influence is ignored in Eqs. (24), the stresses of the half-plane are consistent with those in the classical elastic results [20].

$$\begin{aligned} \sigma_{xx} &= \frac{p_0}{\pi a} \left[(x-a)\theta_1 + (x+a)\theta_2 - 2x\theta + 2z \ln(r_1 r_2 / r^2) \right] \\ \sigma_{zz} &= \frac{p_0}{\pi a} \left[(x-a)\theta_1 + (x+a)\theta_2 - 2x\theta \right] \\ \sigma_{xz} &= -\frac{z p_0}{\pi a} \left[\theta_1 + \theta_2 - 2\theta \right] \end{aligned} \tag{25}$$

where

$$r_1^2 = (x-a)^2 + z^2, r_2^2 = (x+a)^2 + z^2, r^2 = x^2 + z^2, \tan \theta_1 = \frac{z}{x-a}, \tan \theta_2 = \frac{z}{x+a}, \tan \theta = \frac{z}{x}$$

On the contact surface $z = 0$, the normal stress is given by

$$\sigma_{zz}(x, 0) = -\frac{2p_0}{\pi} \int_0^\infty \left(\frac{1 - \cos t}{t^2} \right) \left(1 + \frac{s}{a} t \right)^{-1} \cos\left(\frac{x}{a} t\right) dt \tag{26}$$

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

$$w(x, 0) = \frac{2p_0(1-\nu)a}{\pi G} \int_0^\infty \left(\frac{1 - \cos(t)}{t^3} \right) \left(\frac{s}{a} + 1 \right)^{-1} \left[\cos\left(\frac{x}{a} t\right) - \cos\left(\frac{r_0}{a} t\right) \right] dt \tag{27}$$

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

$$u(x, 0) = -\frac{p_0(1-2\nu)a}{\pi G} \int_0^\infty \left(\frac{1 - \cos(t)}{t^3} \right) \left(\frac{s}{a} + 1 \right)^{-1} \sin\left(\frac{x}{a} t\right) dt \tag{28}$$

It is instructive to examine the influence of the surface elasticity on the stresses and displacements of the contact surface and compare them with those in classical contact problem.

As show in Fig.2, the distribution of the normal stress σ_{zz} that is predicted by the classical theory experiences a singularity at the loading boundary and does not change smoothly; thus, this result appears unreasonable. The results that take into account the residual surface tension give a smooth distribution of the stress σ_{zz} and overcome the singularity at the loading boundary $x = \pm a$. The actual normal stress σ_{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 σ_{zz} reduce to the classical values.

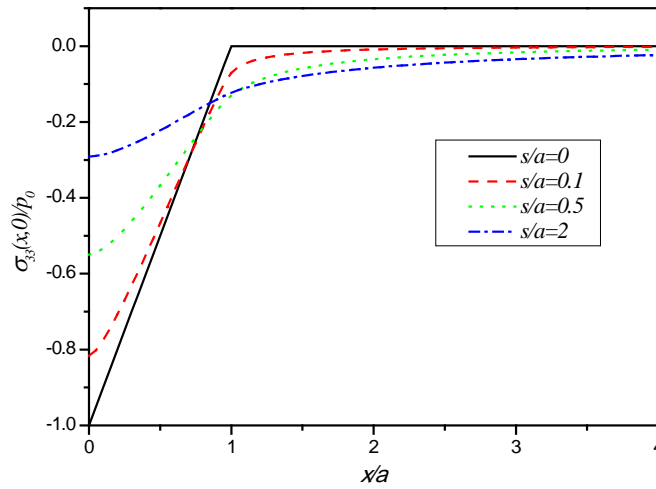


Figure-2: The distribution of contact normal stress σ_{zz} under normal triangle distribution load.

Due to the different residual surface stress value, the horizontal displacement is displayed in Fig.3, where we set $r_0 = 5a$, and $K_1 = (1 - 2\nu) / \pi G$. It is seen that the horizontal displacement is continuous everywhere on the deformed surface. However, the classical elasticity theory predicted unreasonably that the horizontal displacement of the deformed surface is discontinuously at the load boundary $x = \pm a$, as seen from the curve of $s/a=0$. The indent depth is plotted in Fig.4 with $K_2 = 2(1 - \nu) / \pi G$, 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. With the increase of residual surface tension, the indent depth decreases continuously.

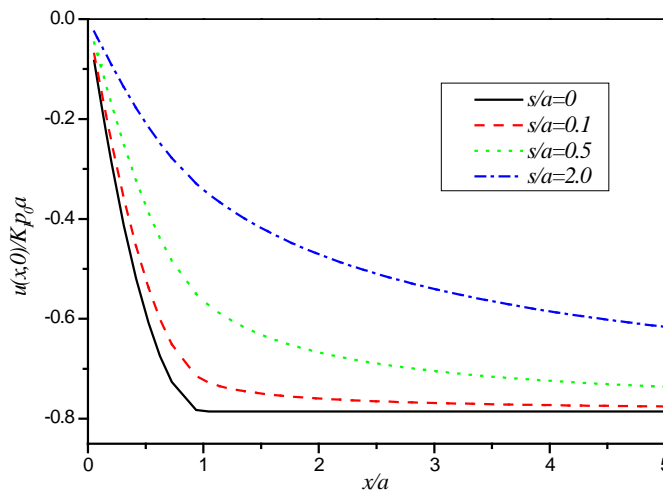


Figure-3: The distribution of surface displacement u under normal triangle distribution load.

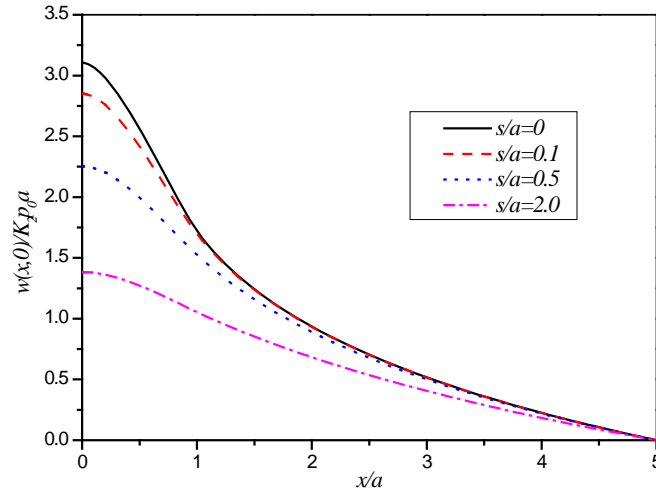


Figure-4: The distribution of surface indentation w under normal triangle distribution load.

To elucidate the size dependence of hardness on indenter size in nanoindentation, the following parameter is H defined by

$$H = \frac{2 p_0 a}{w(0,0)} = \frac{\pi G}{1-\nu} \left[\int_0^\infty \left(\frac{1-\cos(t)}{t^3} \right) \left(\frac{s}{a} + 1 \right)^{-1} \left[1 - \cos \left(\frac{r_0}{a} t \right) \right] dt \right]^{-1} \quad (29)$$

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. 5, 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. Additionally, we independently investigated the influences of the residual surface tension on the contact stiffness.

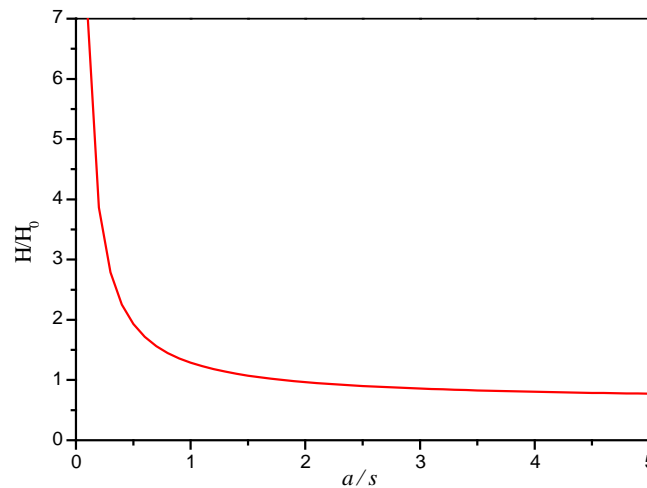


Figure-5: The variation of hardness H / H_0 with respect to the contact zone size.

6. 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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