On Sneddon's boundary conditions used in the analysis of nanoindentation data

GUANGHUI FU*
Lam Research Corporation, 4540 Cushing Parkway, Fremont, CA 94538, USA
E-mail: guanghui.fu@lamrc.com

ANTHONY C. FISCHER-CRIPPS
CSIRO Division of Telecommunications & Industrial Physics, P.O. Box 218, Lindfield, NSW, 2070 Australia

Sneddon's solution [1] on the indentation of an elastic half-space with a rigid conical indenter has been the basis of nanoindentation data analysis for more than a decade [2]. In their finite element simulation, Hay, Bolshakov, and Pharr find that Sneddon's solution is not an exact representation of the actual contact [3]. Both the indenter shape and Sneddon's solution have to be modified before it can be used in the interpretation of nanoindentation data. We find that this happens due to the fact that Sneddon's boundary conditions do not represent the actual contact. Because the points of the half-space surface in the contact region move only along the indenter surface in a real contact, the r-displacement and z-displacement of those points are coupled. However, Sneddon's boundary conditions only specify the z-displacement. Sneddon's way of specifying boundary conditions is common in contact mechanics: people only specify the z-displacement for rigid punch problems and take it for granted that the final surface shape of the contact area is the same as that of the punch [4]. The correct boundary conditions for the actual contact are presented in this paper. These boundary conditions can be changed exactly to Sneddon's boundary conditions if there is no radial surface displacement. They can also be changed approximately to Sneddon's boundary conditions if the half-included angle of the cone is near 90°, i.e., within the limit of the linear elasticity. Similar conclusions can be drawn for rigid smooth frictionless axisymmetric indenters.

Sneddon's boundary conditions for the indentation of an elastic half-space by a rigid frictionless cone are at $z = 0$ (see Fig. 1):

$$\tau_{zr} = \tau_{z\theta} = 0, \quad (0 \le r < \infty) \tag{1}$$

$$\sigma_{zz} = 0, \quad (r > a) \tag{2}$$

$$u_z(r, 0) = h - r\cot\phi, \quad (0 \le r \le a) \tag{3}$$

where ϕ is the half-included angle of the cone and $\phi < 90°$.

Using the linear elasticity theory, Sneddon gives the radial displacement of the half-space surface within the contact region as [5]

$$u_r(r, 0) = \frac{(1-2\nu)}{4(1-\nu)}\frac{r}{\tan\phi}\left[\ln\frac{r/a}{1+\sqrt{1-(r/a)^2}} - \frac{1-\sqrt{1-(r/a)^2}}{(r/a)^2}\right], \quad (0 \le r \le a) \tag{4}$$

According to Equations (3) and (4), any point of the half-space surface within the contact region will have a vertical displacement and a radial displacement. If there is no radial displacement, the deformed surface within the contact region will be a cone described by Equation (3). However, for most materials, $\nu \neq 0.5$, and according to Equation (4), the radial displacement will not be zero. The non-zero radial displacement will lead to a curved surface within the contact region, which will not conform to the rigid cone. From this point of view, Sneddon's boundary conditions do not describe a real contact between a rigid cone and a half-space. In a real contact, the surface points of the half-space within the contact region move only along the rigid cone surface, which implies that in the r-z plane, z-displacement and r-displacement at any surface point of the contact area are coupled. However, Sneddon's boundary conditions only specify the z-displacement.

For a real contact, the boundary conditions at $z = 0$ should be (see Fig. 2):

$$\tau_{zr} = \tau_{z\theta} = 0, \quad (0 \le r < \infty) \tag{5}$$

$$\sigma_{zz} = 0, \quad (r > a') \tag{6}$$

$$\tan\phi = \frac{r + u_r(r, 0)}{h - u_z(r, 0)}, \quad (0 \le r \le a') \tag{7}$$

where a' is the radius of the future contact region before the deformation, and it will become a after the deformation (a is the radius of the final contact area after the deformation). Equation (7) guarantees that the deformed surface of the contact area in the r-z plane is straight. The unknown a' can be solved through the condition that the pressure on the indenter surface will drop to zero at the edge of the contact area. After a' is solved, a is given by $a = a' + u_r(a', 0)$.

*Author to whom all correspondence should be addressed.

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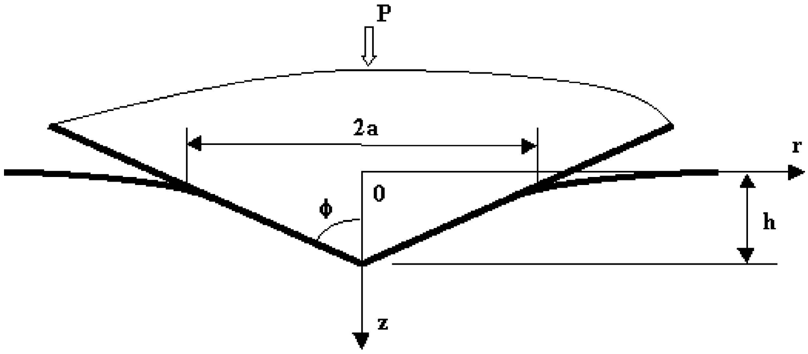

Figure 1 Normal indentation of an elastic half-space with a rigid cone.

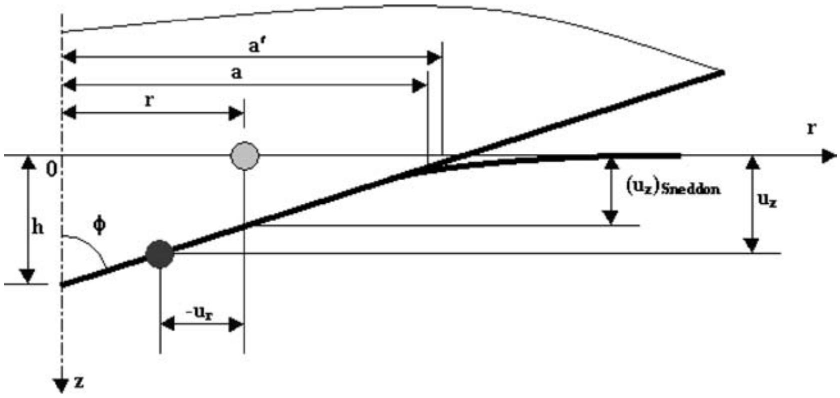

Figure 2 Displacements in a real contact.

If $u_r(r, 0) = 0$, we have $a = a'$ and Equations (5)–(7) will become Equations (1)–(3). Thus, Sneddon's boundary conditions represent the actual contact only when $u_r(r, 0) = 0$. Referring to Equation (4), which is based on the linear elasticity theory, this happens when $\nu = 0.5$ for incompressible materials.

In the following discussions, we show Sneddon's boundary conditions are approximately correct if it is used within the limit of linear elasticity, i.e., small deformations. The real z-displacement for a rigid cone—half-space contact problem is (see Fig. 2)

$$u_z = (u_z)_{\text{Sneddon}} + (-u_r)\cot\phi, \quad (0 \le r \le a') \tag{8}$$

For small deformations, i.e., $\phi \to 90°$, no matter what u_r is, we will always have $u_z \to (u_z)_{\text{Sneddon}}$. Thus, within the limit of linear elasticity, Sneddon's boundary conditions are approximately correct and his solutions, which are based on the linear elasticity theory, are valid.

In the nanoindentation theory [3, 6], Berkovich and Vickers indenters are modeled as conical indenters with a half-included angle $\phi = 70.32°$. A cube-corner indenter is modeled as a cone with $\phi = 42.28°$. For these conical indenters, the half-space deformation in the contact region at the indentation loading stage is out of the range of linear elasticity theory, e.g., the change of the surface normal direction corresponding to a cube-corner indenter is 47.72° and for a Berkovich or Vickers indenter, it is 19.68°. Sneddon's boundary conditions are no longer valid for those indenters. This explains why Sneddon's solution, which is based on his boundary conditions and the linear elasticity theory, is not consistent with the finite element result of the contact between a rigid cone ($\phi = 70.32°$) and an elastic half-space by Hay *et al.* [3].

We have the following conclusions on Sneddon's boundary conditions:

1. Within the limit of linear elasticity theory, Sneddon's boundary conditions are an approximation of the actual contact if the Poisson's ratio for the half-space, ν, is not equal to 0.5. They are an exact representation of the actual contact if $\nu = 0.5$.
2. For large deformations, Sneddon's boundary conditions are no longer valid unless the surface radial displacement within the contact area is zero.

In the following discussions, we show that similar conclusions can be drawn for rigid smooth frictionless axisymmetric indenters.

In the linear elasticity theory, boundary conditions for the indentation of an elastic half-space by a rigid smooth frictionless axisymmetric indenter are given as at $z = 0$ [4]:

$$\tau_{zr} = \tau_{z\theta} = 0, \quad (0 \le r < \infty) \tag{9}$$

$$\sigma_{zz} = 0, \quad (r > a) \tag{10}$$

$$u_z(r, 0) = h + f(r), \quad (0 \le r \le a) \tag{11}$$

where $f(r)$ describes the indenter shape and h is the indentation depth. $f(r)$ is a smooth function and $f(0) = 0$.

Using the integral transform method [5], we derive the radial displacement of the half-space surface within the contact region and it can be expressed as

$$u_r(r,0) = -\frac{1-2\nu}{1-\nu}\left\{\frac{h}{\pi}\frac{1-\sqrt{1-(\frac{r}{a})^2}}{\frac{r}{a}} + \frac{1}{2\sqrt{\pi}}\int_0^\infty\left[\sum_{n=1}^{\infty} a^n \frac{\Gamma\left(\frac{2+n}{2}\right)}{\Gamma\left(\frac{3+n}{2}\right)}\frac{f^{(n)}(0)}{n!} \times \Phi_n(p) J_1\left(\frac{r}{a}p\right)\right]dp\right\}, \tag{12}$$

where, $J_1(x)$ is the Bessel function of the first kind;

$$\Phi_n(x) = \frac{n+1}{x}\left[\sin(x) + \frac{n}{x}\cos(x) - \frac{n}{x}\Phi_{n-2}(x)\right]$$
$$\text{with } \Phi_{-1}(x) = 1 \quad \text{and} \quad \Phi_0(x) = \frac{\sin(x)}{x}.$$

Following the same argument for conical indenters, we need to have $u_r(r,0) = 0$ $(0 \le r \le a)$ in order to represent the real contact with boundary conditions (9), (10), and (11). According to Equation (12), it happens when $\nu = 0.5$ for incompressible materials.

If $u_r(r,0) \neq 0$, the correct boundary conditions for the real contact are

$$\tau_{zr} = \tau_{z\theta} = 0, \quad (0 \le r < \infty) \tag{13}$$

$$\sigma_{zz} = 0, \quad (r > a') \tag{14}$$

$$u_z(r,0) = h + f(r + u_r(r,0)), \quad (0 \le r \le a') \tag{15}$$

Because $f(r)$ is a smooth function, Equation (15) can be rewritten as

$$u_z(r,0) = h + f(r) + f'(r + \theta u_r(r,0))u_r(r,0),$$
$$(0 \le r \le a' \text{ and } 0 < \theta < 1) \tag{16}$$

If only small deformation is considered, the direction change of the surface normal vector within the contact area should be negligible, i.e., $f'(r + \theta u_r(r,0)) \approx 0$ $(0 \le r \le a'$ and $0 < \theta < 1)$. Equation (16) will become

$$u_z(r,0) \approx h + f(r), \quad (0 \le r \le a') \tag{17}$$

Thus, within the limit of linear elasticity theory, Equation (11) is an approximation of the real contact. It is an exact representation of the real contact if the half-space media is incompressible materials.

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