MOLECULAR ADHESIVE CONTACT FOR INDENTERS OF NON-IDEAL SHAPES

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Summary The JKR and the DMT theories of adhesive contact are developed to describe contact between an indenter and an elastic sample, when the distances between the surfaces are described as monomial functions of arbitrary degrees. The results are applied to depth-sensing nanoindentation of soft and hard materials by indenters of non-ideal shapes.

Usually adhesion between contacting bodies has a negligible effect on surface interactions at the macro-scale, while it becomes significant as the contact size decreases, in particular adhesion becomes an important issue at nanoscale. Hence, adhesion of dry surfaces plays a key role in the development of various technologies, especially in such applications as nanoindentation, contact of clean surfaces, information storage devices and microelectromechanical systems (MEMS).

The mechanics of adhesion is well established for contact between homogeneous elastic solids having spherical surfaces [1]. Three theories of adhesion of elastic spheres are now in common use. They were introduced by Johnson, Kendall, and Roberts (JKR) in 1971, by Derjaguin, Muller, and Toporov (DMT) in 1975, and by Maugis (JKR-DMT transition) in 1992 [1]. However, solids in contact may often have more general shape, in particular the shape functions f can be monomial functions of radius ρ

$$f(\rho) = B_d \rho^d, \tag{1}$$

where B_d is a shape constant. For example, it was shown [2] that nanoindenters can be well approximated by monomial functions of degrees d in the range $1 < d < 2$. Here the JKR and the DMT theories of contact in the presence of surface forces are developed to describe contact between an indenter and an elastic sample, when the distances between the solids are described as monomial functions of arbitrary degrees.

It was assumed by Tabor and showed precisely by Muller [3] that the JKR and DMT theories apply to the opposite ends of the range of the non-dimensional parameter

$$\mu = \frac{32}{3\pi}\left(\frac{2w^2 R}{\pi (E^*)^2 z_0}\right)^{1/3}$$

where $w = 2\gamma$ is the work of adhesion, γ is the surface energy, z_0 is the equilibrium separation between surfaces, R is the radius of the sphere, and E^* is the reduced Young's modulus that can be obtained from the following formula $(E^*)^{-1} = (1-\nu_1^2)/E_1 + (1-\nu_2^2)/E_2$. Here E_i and ν_i $(i = 1, 2)$ are the Young's modulus and the Poisson ratio of the first and the second solid respectively. Roughly speaking, the DMT model is applicable to hard materials (μ is less than 0.1 say), while the JKR model should be used for soft materials (μ is greater than 5 say).

First we consider the JKR theory. Using Galin's solution [4], it was obtained by the authors (see, e.g. [5]) independently from each other that there is an exact formula giving relation between the load P and the radius of the contact region a

$$P = C(d)E^* B_d a^{d+1} - \sqrt{8\pi w E^* a^3}, \quad C(d) = \frac{d^2}{d+1} 2^{d-1} \frac{[\Gamma(d/2)]^2}{\Gamma(d)}. \tag{2}$$

Here $\Gamma(d)$ is the Euler gamma function. Evidently, (2) coincides with the classic JKR formula [1]

$$P = (4E^*/3R)a^3 - \sqrt{8\pi w E^* a^3}$$

in the case $d = 2$. When d is an even integer, (2) coincides with the solution obtained independently by Carpick *et al.* [6]. However, an exact solution for pressure within the contact region exists only in the Hertzian case $d = 2$. Hence, we use a numerical approach to obtain the pressure for monomial indentors.

Note that the DMT model shows a smooth change in contact radius a until the point contact, while it follows from the JKR model that the detachment of the spheres is accompanied by an abrupt change in the contact radius. Indeed, it follows from (2) that the radius a_0 of the contact region at $P = 0$ is

$$a_0 = (\sqrt{8\pi w E^* a^3}/C(d))^{2/(2d-1)}.$$

In general, one cannot obtain an analytic solution in the case of the DMT theory. Hence, an integral equation was derived. The integral equation the DMT theory is solved numerically. To perform the numerical simulations, we apply the method of non-linear boundary integral equations (NBIE) developed by Galanov (see, e.g. [7, 8]). To solve the Hertzian contact problem for indenters of non-ideal shapes, we consider not a traditional formulation of contact problem, but rather the following NBIE with an unknown function $v(\mathbf{x})$ [8]

$$\alpha v^-(\mathbf{x}) + \beta \int_\Omega K(\mathbf{x}, \mathbf{y}) v^+(\mathbf{y})\, d\mathbf{y} = g(\mathbf{x}), \quad \mathbf{x}, \mathbf{y} \in \Omega \tag{3}$$

where

$$v^+(\mathbf{x}) = \sup\{v(\mathbf{x}),\, 0\}, \qquad v^-(\mathbf{x}) = \inf\{v(\mathbf{x}),\, 0\},$$

α is an arbitrary positive fitting parameter, $\beta = (\pi E^*)^{-1}$, $g(\mathbf{x}, P) = h(p) - f(\mathbf{x})$, and K is the standard kernel (see for details [8]). Ω is an arbitrary bounded domain containing the closure of Ω_0, and $\Omega_0 \subset \mathbb{R}^2$ is a bounded domain such that

$$g(\mathbf{x}, P) > 0 \quad \text{for} \quad \mathbf{x} \in \Omega_0, \qquad g(\mathbf{x}, P) \leq 0 \quad \text{for} \quad \mathbf{x} \notin \Omega_0 \tag{4}$$

The domain Ω_0 may be multiply connected or consist of non-connected sub-domains. Evidently, $G \subset \Omega_0$.

The mechanical meaning of the solution v to the NBIE (3) is the following

(i) for $\mathbf{x} \in G$, $v^+(\mathbf{x})$ is the contact pressure, i.e. $v^+(\mathbf{x}) = \sigma(\mathbf{x})$;

(ii) for $\mathbf{x} \in \Omega \backslash G$, the function $(-\alpha v^-(\mathbf{x}))$ defines the gap between the punch and the half-space after deformation.

To solve the adhesive contact problem for indenters of non-ideal shapes, we approximate Lennard-Jones potential F as

$$F(x) = Ax^{-m} - Bx^{-n}, \quad m > n > 0, \quad A > 0, \quad B > 0$$

and write the following integral equations for pressure σ

$$\sigma(\mathbf{x}) = F\left\{\left[g(\mathbf{x}) + 2\beta \int_\Omega K(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})d\mathbf{y}\right]^+ + c\right\}, \quad \mathbf{x}, \mathbf{y} \in \Omega \tag{5}$$

and for displacements

$$v(\mathbf{x}) = \left[g(\mathbf{x}) + 2\beta \int_\Omega K(\mathbf{x}, \mathbf{y}) F\left[v^+(\mathbf{y}) + c\right] d\mathbf{y}\right]^+, \quad \mathbf{x}, \mathbf{y} \in \Omega. \tag{6}$$

Solving (5), we obtain the pressure σ within the contact region, and solving (6), we obtain the function v and the vector of displacements.

For the Maugis theory, there are some exact results [9] obtained for $d = 2n$ where n is an integer. Evidently, the adhesive problem for arbitrary d for the Maugis theory can be solved numerically using the same approach.

The results are applied to depth-sensing nanoindentation of soft and hard materials by indenters of non-ideal shapes. Nanoindentation techniques are commonly used to obtain mechanical properties of materials of very small volumes [10]. The interpretation of nanoindentation tests is usually based on the main assumptions of the Hertz contact theory and formulae obtained for ideally shaped indenters. Evidently, molecular adhesion may affect the observed relations. For example, one can obtain using the DMT theory that the slope S

$$S = \frac{dP}{dh} = \frac{2}{3}\frac{2\sqrt{A}}{\sqrt{\pi}}E^*, \tag{7}$$

where A is the contact area ($A = \pi a^2$), and h is the indentation depth of the indenter tip. Hence, the slope is 2/3 of the slope without accounting molecular adhesion.

Thus, both the adhesive molecular interaction and non-ideality of the shape may affect the results obtained using the standard Hertzian approach.

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