Mechanics of Materials 49 (2012) 66–71

Contents lists available at SciVerse ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

Adhesive force between a spherical rigid particle and an incompressible elastic substrate

Shunping Yan, Linghui He *

CAS Key Laboratory of Mechanical Behavior and Design of Materials, University of Science and Technology of China, Hefei, Anhui 230026, PR China

ARTICLE INFO

Article history:
Received 22 March 2011
Available online 6 November 2011

Keywords:
Adhesive force
Derjaguin's approximation
Intermolecular interaction

ABSTRACT

Adhesion between a spherical rigid particle and an incomprssible elastic substrate is studied on the basis of the Lennard–Jones (L–J) potential, and the aim is to explore limitations of the well-known Derjaguin approximation. A new expression of the adhesive force is derived, in which the contribution from the elastic deformation of the substrate is incorporated naturally. Numerical results show that the Derjaguin approximation is valid down to particle radii of the order of the interaction range.

1. Introduction

Adhesion between elastic bodies induced by some types of interactions has been studied extensively in the past years. The early theoretical models commonly emphasize an explicit contact zone but differ substantially in the assumption of adhesive forces. For example, the Johnson–Kendall–Roberts (JKR) model (Johnson et al., 1971) assumed that adhesive force acts only within the contact zone, while the Derjaguin–Muller–Toporov (DMT) model (Derjaguin et al., 1975) accounted for adhesive force acting only outside the contact zone. As pointed out by Tabor (1977), the two theories applied to opposite extremes of a spectrum of a dimensionless parameter (called Tabor number). In the cases with intermediate Tabor number, the Lennard-Jones potential was adopted to model the adhesion force (Greenwood, 1977; Muller et al., 1980), under the Derjaguin approximation that the interaction energy between small areas of curved or slightly inclined solid surfaces is the same as the energy per unit area between infinite plane solids (Derjaguin, 1934). The analytical solution to the problem finally leads to the Maugis–Dugdale (MD) model (Maugis, 1992) which can give the transition between the JKR and DMT models.

The Derjaguin approximation is a useful tool in simplifying the calculation of adhesive force between solids with complicated shapes. However, less is known quantitatively about the limitations of this approximation (Greenwood, 2009). The difficulty arises from the fact that the adhesive force depends on the deformed configuration of the solids which is, reversely, determined by the force. For rigid bodies of unchanged shapes, the interaction can be transformed into certain surface tractions (Argento et al., 1997) or calculated by directly summing intermolecular interactions over the volume (Yao et al., 2008). Yet, for solids of finite stiffness, the problem becomes difficult to handle because both the adhesive force and deformed configuration are coupled with each other and are unknown a priori. Recently, Wu (2006) considered intermolecular adhesion between a rigid sphere and an elastic half-space based on the L–J potential. The study describes the adhesive force through its counterpart for rigid bodies (Argento et al., 1997) by adding the normal surface displacement of the substrate to the particle-substrate separation. Although the exact particle geometry is accounted for in comparison with the work by Greenwood (2009), the effect of substrate deformation is incorporated in the same way as before. The accuracy of such a treatment remains unclear.

The objective of this paper is to explore the limitations of the Derjaguin approximation. For simplicity and comparison, our attention is focused on adhesion between a

* Corresponding author.
E-mail address: lhhe@ustc.edu.cn (L. He).

0167-6636/$ - see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.mechmat.2011.10.005

spherical rigid particle and an incompressible elastic substrate. The fundamental L–J potential is utilized to characterize the intermolecular interaction. In this case we are able to derive the adhesive force via a variational method without introducing any other assumptions than small deformation of the substrate. Since the initial and deformed configurations of the substrate are distinguished, the adhesive force involves the contribution from substrate deformation naturally. Omitting the tangential components of the adhesive force, the adhesion behavior is investigated numerically for various particle sizes. A detailed comparison indicates that the Derjaguin approximation is of very high accuracy down to particle radii of the order of the equilibrium distance for the L–J potential.

2. Theoretical formulation

The problem we considered is sketched in Fig. 1. A rigid, sphere-shaped nanoparticle of radius R is fixed over an incompressible elastic substrate occupying the half space $x_3 < 0$. The center of the particle is at $(0,0,a)$, and the shear modulus of the substrate is μ. The particle and substrate are in close proximity, so that they interact with each other through intermolecular forces. A vertical external force F needs to be applied to the particle so as to maintain the mechanical equilibrium. We assume that the deformation of the substrate is small, and denote the displacement components by u_i ($i = 1,2$, and 3). Since the external force F does no work, the total energy U of the system is the sum of the intermolecular interaction energy U_I and the elastic deformation energy U_E of the substrate. We will derive the fundamental equations of the problem. The usual summation convention is adopted, where a repeating Latin subscript runs from 1 to 3 and a Greek one takes value of 1 or 2.

Our derivation is based on minimization of the total energy U, and thus requires the expressions of variations in U_I and U_E. The variational of the elastic deformation energy, δU_E, can be written simply as (Landau and Lifshitz, 1959)

$$\delta U_E = -\int_V \frac{\partial \sigma_{ij}}{\partial x_j}\delta u_i dV + \int_A \sigma_{i3}\delta u_i dA, \tag{1}$$

where σ_{ij} is stress component, V and A denote the volume and surface of the undeformed substrate, respectively. The stress σ_{ij} relates to the displacement u_i by $\sigma_{ij} = -p\delta_{ij} + \mu(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$, with p being the hydrostatic pressure, and δ_{ij} standing for the Kronecker's delta that equals 1 for $i = j$ and 0 for $i \neq j$. To involve the effect of substrate deformation in the interaction energy U_I, we have to distinguish the deformed and undeformed states of the substrate. The volume and surface of the former are denoted by $\widehat{V}$ and $\widehat{A}$, respectively, and a point $(\hat{x}_1,\hat{x}_2,\hat{x}_3)$ in $\widehat{V}$ relates to a point (x_1,x_2,x_3) in V by $\hat{x}_i = x_i + u_i$. To characterize the intermolecular interaction between the particle and substrate, the L-J potential $\psi_{L-J}(s) = 4\omega[(\sigma/s)^{12} - (\sigma/s)^6]$ is invoked, in which ω and σ are two parameters and s is the intermolecular distance (Israelachvili, 1991). The interaction energy between the particle and a volume element $d\widehat{V}$ centered at $(\hat{x}_1,\hat{x}_2,\hat{x}_3)$ in the deformed substrate can be evaluated by direct integration as $\rho_1\rho_2\Psi(l)d\widehat{V}$ with ρ_1 and ρ_2 being number densities of molecules per unit volume in the particle and deformed substrate, respectively,

$$\Psi(l) = \frac{16\pi\omega\sigma^3}{45n^9d^{12}}\left(\frac{128}{d^6}+\frac{216}{d^4}+\frac{108}{d^2}+15\right) - \frac{16\pi\omega\sigma^3}{3n^3d^6}, \tag{2}$$

$l = \sqrt{\hat{x}_1^2+\hat{x}_2^2+(\hat{x}_3-a)^2}$, d and n are dimensionless parameters defined by

$$d = \frac{\sqrt{l^2-R^2}}{R}, \quad n = \frac{R}{\sigma}. \tag{3}$$

From Eq. (2) it is known that the interaction energy between the particle and substrate reads $U_I = \int_V \rho_1\rho_2\Psi(l)d\widehat{V}$. Due to the incompressibility of the substrate, ρ_2 is a constant and U_I can be regarded as a functional $U_I = \int_V \rho_1\rho_2\Psi(l)dV$ defined in the undeformed volume V with $\hat{x}_i$ being the variable functions. Accordingly, in light of the relations $\partial(\delta\hat{x}_i)/\partial\hat{x}_i = 0$ and $\delta\hat{x}_i = \delta u_i$, the variational of U_I is calculated as follows

$$\begin{aligned}\delta U_I &= \int_V \rho_1\rho_2\frac{\partial\Psi(l)}{\partial\hat{x}_i}\delta\hat{x}_i dV = \int_{\widehat{V}} \rho_1\rho_2\frac{\partial\Psi(l)}{\partial\hat{x}_i}\delta\hat{x}_i d\widehat{V}\\ &= \int_{\widehat{V}}\left\{\frac{\partial}{\partial\hat{x}_i}[\rho_1\rho_2\Psi(l)\delta\hat{x}_i] - \rho_1\rho_2\Psi(l)\frac{\partial}{\partial\hat{x}_i}(\delta\hat{x}_i)\right\}d\widehat{V}\\ &= -\int_A f_i(\mathbf{x})\delta u_i dA,\end{aligned} \tag{4}$$

in which $\mathbf{x}$ denotes a point on the surface A, and $f_i(\mathbf{x})$ are defined by

$$\begin{aligned} f_\alpha(\mathbf{x}) &= \rho_1\rho_2\Psi(l_0)\frac{\partial u_3}{\partial x_\alpha},\\ f_3(\mathbf{x}) &= -\rho_1\rho_2\Psi(l_0)\left(1-\frac{\partial u_3}{\partial x_3}\right),\end{aligned} \tag{5}$$

with $l_0 = \sqrt{(x_1+u_1)^2+(x_2+u_2)^2+(u_3-a)^2}$. In passing through the last result in Eq. (4), we have used the divergence theorem as well as the Nanson's formalism $\hat{n}_i d\widehat{A} = (\delta_{3i} - \partial u_3/\partial x_i)dA$, where $\hat{n}_i$ are the components of the unit vector normal to the deformed surface $\widehat{A}$. Substituting Eqs. (1) and (4) into $\delta U_I + \delta U_E = 0$ and then making use of the arbitrariness of δu_i, we arrive at

$$\begin{aligned}&\frac{\partial\sigma_{ij}}{\partial x_j} = 0, \quad \text{in } V,\\ &\sigma_{i3} = f_i(\mathbf{x}), \quad \text{on } A.\end{aligned} \tag{6}$$

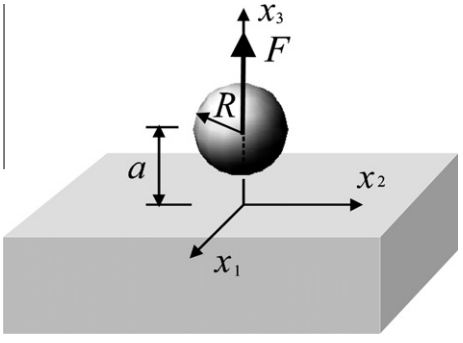

Fig. 1. A rigid nanoparticle located over an elastically incompressible semi-infinite substrate. An external force is applied to maintain the equilibrium.