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Effect of surface tension on the behavior of adhesive contact based on Lennard–Jones potential law

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ABSTRACT

The present study explores the effect of surface tension on adhesive contact behavior where the adhesion is interpreted by long-range intermolecular forces. The adhesive contact is analyzed using the equivalent system of a rigid sphere and an elastic half space covered by a membrane with surface tension. The long-range intermolecular forces are modeled with the Lennard–Jones (L–J) potential law. The current adhesive contact issue can be represented by a nonlinear integral equation, which can be solved by Newton–Raphson method. In contrast to previous studies which consider intermolecular forces as short-range, the present study reveals more details of the features of adhesive contact with surface tension, in terms of jump instabilities, pull-off forces, pressure distribution within the contact area, etc. The transition of the pull-off force is not only consistent with previous studies, but also presents some new interesting characteristics in the current situation.

1. Introduction

Surface adhesion is of significant importance not only in natural objects but also in many engineering systems, such as microelectromechanical, nanoelectromechanical devices and atomic force microscopy (AFM) where surface forces dominate bulk forces. In surface adhesion, the fundamental problem is the adhesive contact between two bodies. One of the precursive investigations on adhesive contact is ascribed to Bradley (1932), who adopted the Lennard-Jones potential to describe the adhesive forces between two rigid spheres. The studies on adhesive contact between two elastic spheres were initially performed by Johnson et al. (1971) who formulated the relation between applied load and the contact radius, known as JKR theory, and later the contact edge in the adhesive contact problem was treated as the cusp of an external crack.

Although the JKR theory has possessed success in predicting the adhesive contact behavior of elastic spheres, it is lately found that the adhesion-induced deformation of soft substrates, e.g. plasticized polystyrene (Rimai et al., 2000), hydrogels (Chakrabarti and Chaudhary, 2013) and silicone gels (Style et al., 2013) diverges significantly from that described by JKR theory. For example, Style et al. (2013) found that the relation between contact radius and sphere radius is analogous to that predicted by the Young–Dupre law rather than JKR theory, as either the sphere radius or the elastic modulus of substrate reduces. Style et al. (2013) ascribed this divergence to the exclusion of the substrate-air surface tension which also resists the adhesion-induced deformation by flattening the surface of soft solids.

Owing to this deviation, some recent studies began to investigate the effect of surface tension on the adhesive contact. Salez et al. (2013) probed the adhesive contact between an elastic sphere and a rigid plane under zero external load with

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surface tension, and they realized a continuous bridge between the JKR and Young-Dupre asymptotic regimes. Using the finite element method including the surface tension and hyperelasticity, Xu et al. (2014) simulated the adhesive contact between a rigid sphere and a neo-Hookean substrate in the absence of external load, and showed the transition between the classical Johnson–Kendall–Roberts (JKR) deformation and a liquid-like deformation. Cao et al. (2014) verified this transition via simulations realized by molecular dynamics. Hui et al. (2015) studied the impact of surface tension on the non-slip adhesive contact between a rigid sphere and an incompressible substrate, and proposed a single dimensionless parameter: $\omega = \sigma(GR)^{-2/3}(9\pi\Delta\gamma/4)^{-1/3}$ (σ, G, R and $\Delta\gamma$ denote surface tension, shear modulus of the substrate, sphere radius and the interfacial work of adhesion respectively) to characterize the transition between JKR theory and Young–Dupre law. Long et al. (2016) reconsidered the same problem studied by Hui et al. (2015), but without the requirement of non-slip and incompressibility of substrate material, and they presented an explicit relation between the contact radius and the indent depth in the absence of external load, which are more convenient in practical applications.

In all the experimental and numerical studies mentioned above, the surface adhesion is interpreted by short-range intermolecular forces (in fact, intermolecular forces are consider as a delta function in JKR theory), and thus the adhesive forces vanish outside the contact area. Since the short-range intermolecular forces are merely an approximation of their actual counterpart which are generally long-range, it is of great necessity to reconsider the effect of surface tension on the adhesive contact which is subject to more realistic molecular interactions, e.g. van der Waals forces. On the other hand, the success of Lennrad–Jones (L–J) potential in describing the adhesive contact behavior of elastic bodies without surface tension by Greenwood (1997) and Feng (2000) also provides us with sufficient fundamental technique to apply the L–J potential law to the current issue.

In the present study, we aim to explore the effect of surface tension on the behavior of adhesive contact where the adhesive interaction obeys the Lennard–Jones potential law. In the next section, we firstly reintroduce the Green's function of a point force acting on an elastic substrate with surface tension, and show that the current adhesive contact problem can be transformed into the solution of an integral equation. Section 3 presents computational techniques to solve this integral equation. Discussions are presented in Section 4. Concluding remarks are provided in Section 5.

2. Adhesive contact with surface tension

In the surface elasticity theory (Gurtin and Murdoch, 1975; Gurtin et al., 1998), the surface is treated as an inappreciably thin membrane ideally adhered to the bulk material. Analogous to classical theory of solid mechanics, the elastic surface also has its equilibrium and constitutive equations. For a flat surface, the equilibrium conditions are given by (Chen et al., 2006; Mogilevskaya et al., 2011):

$$t_\alpha + \sum_{\beta=1}^{2} \sigma^s_{\beta\alpha,\beta} = 0 \tag{1}$$

$$\sum_{i=1}^{3}\sum_{j=1}^{3} \sigma_{ij} n_i n_j = \sum_{\alpha=1}^{2}\sum_{\beta=1}^{2} \sigma^s_{\alpha\beta}\kappa_{\alpha\beta} \tag{2}$$

where t_α ($\alpha = 1, 2$) is the surface traction in x_α direction, n_i is the unit vector normal to the deformed surface, $\kappa_{\alpha\beta}$ is the curvature tensor of the surface and ${\sigma_{\alpha\beta}}^s$ is the surface stress tensor. Cammarata (1994) presented the relationship between the surface stress tensor ${\sigma_{\alpha\beta}}^s$ and surface energy density $\sigma(\varepsilon_{\alpha\beta})$, which could be viewed as the constitutive equations for surface elasticity, as

$$\sigma^s_{\alpha\beta}\left(\varepsilon_{\alpha\beta}\right) = \sigma\left(\varepsilon_{\alpha\beta}\right)\delta_{\alpha\beta} + \frac{\partial\sigma\left(\varepsilon_{\alpha\beta}\right)}{\partial\varepsilon_{\alpha\beta}} \tag{3}$$

where $\delta_{\sigma\beta}$ and $\varepsilon_{\alpha\beta}$ denote Kronecker delta function and surface strain tensor respectively. If the change of the atomic spacing in deformation is infinitesimal, the contribution of the second term in Eq. (3) to the surface stress tensor is negligibly small compared to the surface energy (Yang, 2004; Shenoy, 2005), and hence one has

$$\sigma^s_{\alpha\beta} = \sigma\left(\varepsilon_{\alpha\beta}\right)\delta_{\alpha\beta} \tag{4}$$

Since atomic simulation indicates that the surface energy of nanoparticles almost remains constant when the radius of nanoparticles is larger than 4 nm (Bian et al., 2012), we assume that surface energy density σ is constant on surface in the present study, resulting in a constant residual surface tension, which can capture the main surface effects in contact mechanics (Gao et al., 2013). It is worth noting that the surface elasticity theory by Gurtin and Murdoch (1975) (G–M model) remains as an open topic, and later it is followed by subsequent new studies by such as Huang and Wang (2006) who developed a hyperelastic surface model, and Chen and Yao (2014) who proposed the concept of surface energy density to characterize surface elasticity.

Based on the following hypotheses:

1. The surface tension σ in the membrane mentioned above is large enough such that it is not changed appreciably after being subject to small deformations.