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Adhesive behavior of micro/nano-textured surfaces

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ABSTRACT

A numerical model of the adhesive contact between a rigid smooth sphere and an elastic textured surface based on the Lennard–Jones interatomic potential law and the Hamaker summation method is established. Textures are considered by introducing the texture height distribution into the gap equation. Simulation results show that the pull-off force on textured surfaces decreases compared to that on smooth surfaces. Furthermore, effects of sphere-shaped textures on reducing adhesion are more obvious than cylinder-shaped or cube-shaped textures when the coverage area ratio, maximum height and interval of textures are fixed. For surfaces with sphere-shaped textures, variation trends of the mean pull-off force with texture density are not monotonous, and there exists a certain range of texture densities in which the mean pull-off force is small and its variation is insignificant. In addition, the pull-off force depends also on the maximum height and radius of textures. On one hand, if the texture radius is fixed, larger maximum height results in smaller pull-off force, and if the maximum height is fixed, the pull-off force tends to increase almost linearly with increases in texture radius. On the other hand, if the height-diameter ratio of textures is fixed, the pull-off force reaches a minimum at an optimum texture radius or maximum height.

1. Introduction

As the size of devices shrinks to micro- and nano-scales, the surface-to-volume ratio increases obviously [1,2], and thus some unwanted adhesion failures due to surface forces occur frequently in micro/nano-devices such as micro switches [3]. To reduce this kind of adhesion-induced failure, micro/nano-texturing techniques are used to produce textured surfaces with nanoparticles [4], micro/nanometer-sized pillars [5] or grooves [6]. Early efforts on experimental studies have demonstrated that adhesive contact behaviors of textured or rough surfaces greatly depend on the pattern shape, distribution form, density, height and radius [4,7–9].

As far as the theoretical analysis of adhesive contact between textured or rough surfaces is concerned, three kinds of analytical models are often employed. The first kind is based on integrations of van der Waals interactions but neglects elastic responses of multi-asperities, such as the models introduced by Dejeu et al. [10], DelRio et al. [11], Katainen et al. [12] and Laitinen et al. [13]. The second kind introduced by Liu et al. [9] and Li et al. [14], combines both the approach of integrations of van der Waals interactions and the surface energy approach used in JKR [15] or DMT [16] theories so that elastic deformations can be taken into account. But in this kind of models, a single average asperity with a radius related to the RMS surface roughness is used to represent close-packed multi-asperities. The third kind is established according to the statistical method [17,18] which combines the GW theory [19] or the MB fractal theory [20] with JKR [15], DMT [16] or M-D [21] models, but sphere/substrate interactions are neglected. Apart from the respective problems of the above three kinds of models, common problems of them are that interactions between adjacent asperities and variations of the pull-off force with contact locations between rough surfaces [22] are not considered. However, when designing micro/nano-textured surfaces, the interval and height of textures may be varied in a large range, and thus interactions between adjacent textures and pull-off force data scatters may become significant. Consequently, the above analytical models fail to accurately describe the adhesive contact between textured surfaces with different designing parameters.

As for the numerical method, the existing models are mainly based on the Hamaker summation method [23] but only limited to studies of the adhesive contact between smooth surfaces. The Hamaker summation method is based on a microscopic theory which obtains the interaction force between macroscopic bodies by the pairwise additivity of molecular interactions. According to this method, Argento et al. [24] has proposed a surface formulation, in

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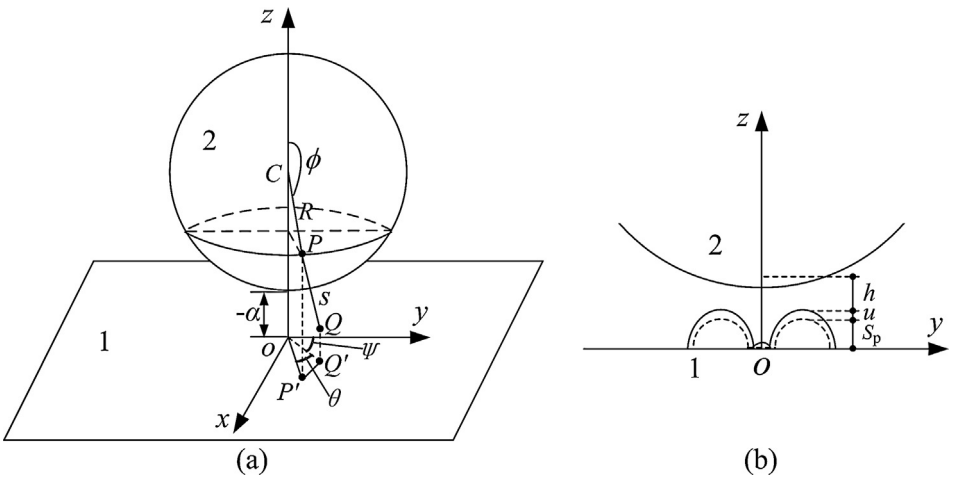

Fig. 1. Adhesive contact between an elastic substrate 1 including surface textures and a rigid sphere 2. (a) 3D plot, and (b) enlarged cross-sectional profile.

which the volume-integrated intermolecular force between bodies is partitioned to obtain a distribution of effective surface tractions. The widely used Derjaguin approximation [25] can be considered as a simplification of Argento's surface formulation when radii of spheres are larger than their separation [26,27]. Recent studies based on Argento's approach [28,29] have further suggested that the Hamaker summation method is more precise than the Derjaguin approximation when spheres approach the nano-scale. For textured surfaces designed to modulate the adhesive performance, the size of textures may be very small, and thus the Hamaker summation method has more potential to be extended to analyze the adhesive contact between textured surfaces if the texture geometry is considered.

This work is undertaken to establish a numerical adhesive contact model for textured surfaces and provide insight into effects of the texture shape, density, maximum height and radius on the adhesive performance. To do this, the texture height distribution is introduced to the surface gap, and the interaction force is calculated based on the Hamaker summation method and the Lennard–Jones interatomic potential law.

2. Theoretical model

A schematic drawing of the adhesive contact between an elastic substrate 1 including surface textures with the height of $S_p(x, y)$ and a rigid smooth sphere 2 is shown in Fig. 1. It is assumed that the contact scale under investigation is small enough so that adhesive effects need to be considered, but sufficiently large for the continuum theory to be valid. The gap h between the bottom of the sphere and the substrate surface can be expressed as:

$$h(x, y) = -\alpha - S_p(x, y) + u(x, y) \tag{1}$$

where α is the approach between the bottom of the rigid sphere and the undeformed substrate. $u(x, y)$ denotes the elastic deformation of the substrate and can be calculated by using the Boussinesq integral [30]:

$$u(x, y) = \frac{1}{\pi E^*} \iint_{\Omega} \frac{p(\xi, \eta)\,\mathrm{d}\xi\mathrm{d}\eta}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} \tag{2}$$

where E^* denotes the effective elastic modulus. $p(x, y)$ is the local pressure distribution caused by molecular interactions between the sphere and the substrate.

The total interaction force on substrate 1 exerted by sphere 2 can be obtained by integrating the Lennard–Jones interatomic potential $w(s)$ with all molecules in the body and converting the double volume integral into the surface integral with an intersurface stress tensor [24], which can be expressed as:

$$\begin{aligned} F &= \rho_1\rho_2 \int_{V_2}\int_{V_1} \nabla_2 w(s)\,\mathrm{d}V_1\,\mathrm{d}V_2 \\ &= \rho_1\rho_2 \int_{\bar{S}_2}\int_{\bar{S}_1} \mathbf{n}_2(\mathbf{G}\cdot\mathbf{n}_1)\,\mathrm{d}\bar{S}_1\,\mathrm{d}\bar{S}_2 \end{aligned} \tag{3}$$

where ρ_1, ρ_2 and $\mathbf{n}_1$, $\mathbf{n}_2$ are number densities of molecules and unit normal vectors of surfaces, respectively. V_1, V_2 and $\bar{S}_1$, $\bar{S}_2$ denote the volume and surface of 1 and 2, respectively. s is the distance between two molecules and $\mathbf{G}$ is a defined intersurface force kernel which can be obtained as:

$$\begin{aligned} \mathbf{G} &= \frac{\mathbf{x}_2 - \mathbf{x}_1}{s^3}\int_s^\infty w(t)t^2\,\mathrm{d}t = \frac{\mathbf{x}_2 - \mathbf{x}_1}{s^3}\int_s^\infty 4e[(\sigma/t)^{12} - (\sigma/t)^6]t^2\,\mathrm{d}t \\ &= 4e(\mathbf{x}_2 - \mathbf{x}_1)\left(\frac{\sigma^{12}}{9s^{12}} - \frac{\sigma^6}{3s^6}\right) \end{aligned} \tag{4}$$

where e is the minimum potential, and σ is the distance at which the potential is zero.

From Eq. (3), the interaction force per unit area on the surface element of substrate 1 by the surface of sphere 2 can be written as:

$$\begin{aligned} \mathbf{f} &= (\rho_1\rho_2 \int_{\bar{S}_2} \mathbf{n}_2\mathbf{G}\mathrm{d}\bar{S}_2)\cdot\mathbf{n}_1 = \mathbf{b}\cdot\mathbf{n}_1 = \begin{bmatrix} b_{xx} & b_{xy} & b_{xz} \\ b_{yx} & b_{yy} & b_{yz} \\ b_{zx} & b_{zy} & b_{zz} \end{bmatrix}\begin{bmatrix} n_{1x} \\ n_{1y} \\ n_{1z} \end{bmatrix} \\ &= \begin{bmatrix} b_{xx}n_{1x} + b_{xy}n_{1y} + b_{xz}n_{1z} \\ b_{yx}n_{1x} + b_{yy}n_{1y} + b_{yz}n_{1z} \\ b_{zx}n_{1x} + b_{zy}n_{1y} + b_{zz}n_{1z} \end{bmatrix} \end{aligned} \tag{5}$$

where $\mathbf{b}$ is the intersurface stress tensor.

As the elastic deformation of substrate 1 is small, only the vertical component of $\mathbf{f}$ is considered in the present problem, which is:

$$f_z = b_{zx}n_{1x} + b_{zy}n_{1y} + b_{zz}n_{1z} \tag{6}$$