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Adhesion mechanics of ivy nanoparticles

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ABSTRACT

Adhesion mechanism of ivy has been of major research interest for its potential applications in high-strength materials. Recent experimental studies demonstrated that nanoparticles secreted from ivy tendrils play an important role in adhesion. In this work, we investigate how various factors such as van der Waals interaction, capillarity, and molecular cross-linking influence the adhesion mechanics of ivy nanoparticles. This paper provides guidelines in choosing different adhesive contact models. Understanding the mechanics of ivy adhesion could potentially inspire the design and fabrication of novel nano-biomaterials.

1. Introduction

Ivy is a fascinating climber. Using its tendrils, ivy can climb on walls, trees, and many other surfaces. Though very small in size, the tendrils can provide surprisingly large forces. For example, Darwin [1] showed that an ivy disc of weight 0.5 mg can produce about 2 *lb* pull-off force, which is over 1.8 million larger than the weight of adhering disc. Thus, understanding ivy adhesion mechanics may have important significance in material science. Using atomic force microscopy (AFM), Zhang et al. [2,3] observed ivy secretes nanoparticles through adhering discs of the ivy rootlets that allow the plant to affix to a surface (see Fig. 1). This observation suggests that the nanoparticles play a direct and important role for ivy surface climbing although the mechanics interpretation for the adhesion is still not completely known. This paper attempts to explore the adhesion mechanics of ivy nanoparticles using contact and fracture mechanics models. In particular, the computational work here is greatly inspired by the seminal work of Gao et al. in their research about the adhesion structures of gecko [4–8].

From mechanics point of view, adhesion is expressed in terms of the work of adhesion [9], the physical origins of which may include: van der Waals interaction, electrostatic forces, capillarity and chemical bond. The adhesion also undergoes cross-linking with a corresponding increase in adhesion strength, and roughness with a decrease in strength. Continuum mechanics models of the adhesion between spherical surfaces which deform within the elastic limit are well developed. The inter-atomic forces at interfaces were first explained by London [10], and soon after they were applied by Bradley [11], Derjaguin [12] and Hamaker [13] to the problem of the forces between small particles. In an attempt to characterize the adhesive contact between elastic spheres, three major theories have been developed. These theories include: Johnson–Kendall–Roberts (JKR) [14], Derjaguin–Muller–Toporov (DMT) [15], and Maugis-Dugdale (M-D) [16]. The JKR theory is applicable to large, soft, compliant materials with high surface energy. The adhesion forces outside the area of contact are neglected and elastic stresses at the edge of the contact are infinite. Contrary to the JKR theory, the DMT theory applies to smaller, stiffer, less compliant materials with a low surface energy. The interaction forces outside the contact area are taken into account, but these interaction forces are assumed not to deform the profile. The M-D theory is for materials with property between JKR and DMT regimes, and can be governed by a non-dimensional elasticity parameter defined as follows

$$\lambda \equiv \sigma_0 \left(\frac{9R}{2\pi w E^{*2}} \right)^{1/3} \tag{1}$$

where $E^* = \left[(1-\nu_1^2)/E_1 + (1-\nu_2^2)/E_2 \right]^{-1}$ is the combined effective elastic modulus of the two contacting objects, E_i and ν_i are Young's moduli and Poisson's ratios of the two materials, respectively. R is the equivalent radius of the two spheres given by $1/R = 1/R_1 + 1/R_2$, R_i are the radii of the two contacting spheres, w is work of adhesion, σ_0 the maximum attractive stress. This parameter may be interpreted as the ratio of the elastic deformation of the surfaces at the point of separation (pull off) to the effective range of action of the adhesive forces. The JKR theory and DMT theory are each appropriate to opposite extremes of the parameter λ. When λ increases from zero to infinity there is a continuous transition from the DMT approximation to the JKR approximation [16,17].

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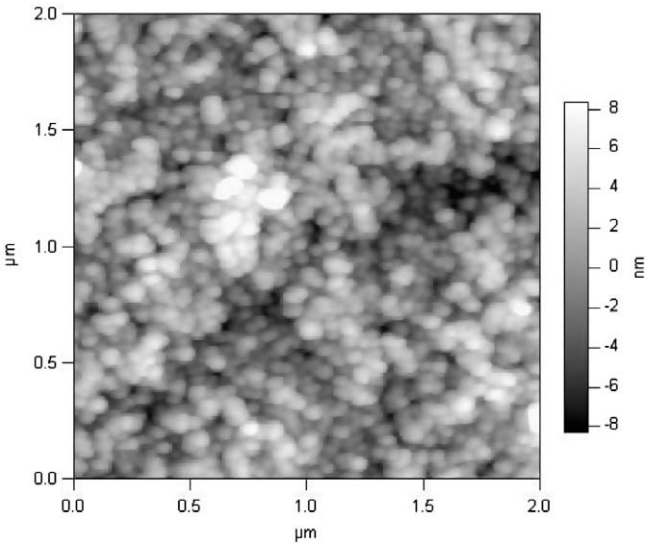

Fig. 1. An AFM image of nanoparticles secreted from the adhering discs of ivy on a silicon wafer surface.

2. Problem formulation

2.1. Geometry of a nanoparticle

Based on the observation of AFM topography images (see Fig. 1), we postulate that the ivy nanoparticles may not be perfect nanospheres, and assume that there are some irregular planes on the surface. To understand the nano scale adhesion mechanism, we consider a rigid/elastic spherical cap with a flat punch in contact with a smooth rigid substrate, as shown in Fig. 2. The radius of the actual contact area is $a = R\sin\alpha,\ 0^\circ \leqslant \alpha \leqslant 90^\circ$. Three models, generalized from DMT, JKR, and M-D theory to specified geometry, are presented to interpret the pull-off force.

2.2. DMT type model

In general, the surface force σ, defined as the force per unit area between two half-spaces separated by a distance z, can be obtained from the Lennard–Jones potential and is given by

$$\sigma(z) = \frac{8w}{3z_0}\left[\left(\frac{z_0}{z}\right)^3 - \left(\frac{z_0}{z}\right)^9\right] \tag{2}$$

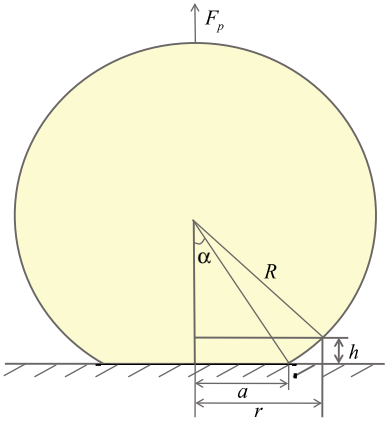

Fig. 2. Schematic diagram of the contact between a nanoparticle and a rigid substrate.

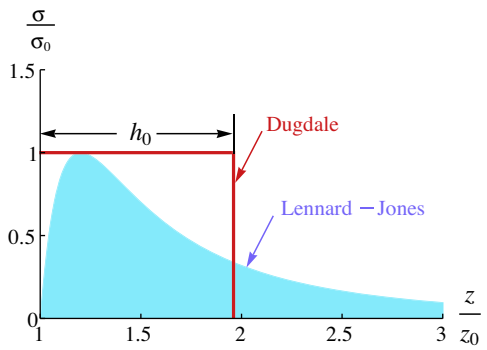

Fig. 3. Force-separation laws: Lennard–Jones potential; the Dugdale approximation, the work of adhesion $w = \sigma_0 h_0$, the cohesive zone is thus $h_0 = 0.97z_0$.

where z_0 is the equilibrium separation. To avoid self-consistent numerical calculations based on the Lennard–Jones interaction model, it is easier to representing the surface force by the Dugdale approximation [18], in which the attractive stress is assumed to be a constant σ_0 with a critical separation $h_0 = w/\sigma_0$ (called the cohesive zone) and zero beyond this distance, as shown in Fig. 3.

Using the Dugdale type interaction law, we consider a simple DMT type model in which the deformation of contact surfaces is neglected (rigid assumption) and assume a constant attractive stress σ_0 inside the contact area. The maximum adhesive force, i.e., the pull-off force to separate two rigid objects, can be calculated as follows:

$$F_p = \pi a^2\sigma_0 + \int_a^{r_0} 2\pi\sigma_0 r dr = \begin{cases} \pi a^2\sigma_0 + \int_0^{h_0} 2\pi\sigma_0(R\cos\alpha - h)dh, \\ \quad \text{if} \quad h_0 < R\cos\alpha \\ \pi a^2\sigma_0 + \int_0^{R\cos\alpha} 2\pi\sigma_0(R\cos\alpha - h)dh, \\ \quad \text{if} \quad h_0 \geqslant R\cos\alpha \end{cases}$$
$$= \begin{cases} F_0[1 - \cos^2\alpha(1-\zeta)^2], & \zeta < 1 \\ F_0, & \zeta \geqslant 1 \end{cases} \tag{3}$$

where r_0 is the radius of the cohesive zone, and

$$\zeta = \frac{h_0}{R\cos\alpha}, \quad F_0 = \pi R^2\sigma_0 \tag{4}$$

There is a saturation of adhesion strength below a critical size $R_0 = h_0/\cos\alpha(0^\circ \leqslant \alpha < 90^\circ)$ or a critical angle $\alpha_0 = \arccos(h_0/R)$. The contact achieves its theoretical strength F_0 when $R < R_0$ or $\alpha > \alpha_0$. The perfect shape is simply a hemisphere with $\alpha = 90^\circ$, under which condition the nanoparticle adhering to a flat rigid substrate would achieve the theoretical adhesion strength F_0 regardless of the particle size R.

2.3. JKR type model

Since biological contacts usually consist of compliant materials [19], elastic deformation should be considered in the analysis of adhesive contact.

Gao et al. proposed a JKR type model, which is consistent with linear elastic fracture mechanics (LEFM) approximation, to determine the pull-off forces of a cylindrical spatula [5]. Here we model the contact as an elastic spherical cap in contact with a rigid substrate, resembling a soft ivy nanoparticle in contact with a hard material. We assume that adhesion forces outside the area of contact are negligible and elastic stresses at the edge of the contact are infinite. The adhesive strength of such an adhesive joint can be calculated by treating the contact problem as a circumferential crack (see Fig. 4), in which case the stress field near the edge of the