



# Adhesive contact analysis for anisotropic materials considering surface stress and surface elasticity



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## ABSTRACT

In this study, an adhesive contact problem for anisotropic materials is analyzed by considering surface stress and surface elasticity. The displacement field on the surface is obtained from the surface Green's function considering the surface stress and surface elasticity. The displacement due to the adhesive force, i.e., the van der Waals force, calculated from the Lennard–Jones potential is used in the analysis. The adhesive force is calculated from the distance between two surfaces. First, an adhesive contact problem of a rigid spherical indenter and an isotropic substrate with various material properties is analyzed under a condition in which no surface mechanical property is considered, and the results are compared with the Johnson–Kendall–Roberts theory in order to validate the calculation algorithm of the analysis. Next, a substrate with orthotropic properties is subjected to adhesive contact analysis. When the elastic modulus in the normal direction to the substrate surface increases, the maximum adhesion force increases, similar to the case of the isotropic substrate. However, when the elastic modulus in the tangential direction of the substrate surface is varied, the maximum adhesion force does not vary much. Finally, an anisotropic half-substrate is subjected to adhesive contact analysis considering the surface mechanical property. This analysis reveals that when the values of the surface mechanical property are varied, the maximum adhesion force changes, similar to the case of varying the elastic modulus in the tangential direction of the surface.

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## 1. Introduction

Recent technological developments have led to the requirement of measuring the physical and chemical properties of a material surface. Specifically, it is necessary to measure the material properties in the nanoscale region for manufacturing extremely sensitive sensors. Gibbs (1928) introduced the concept of surface stress in solids. According to this concept, the energy of atoms near the free surface is different from that in bulk. Surface stress, related to surface energy, affects the mechanical behavior of the material surface in the nanoscale region. Gurtin and Murdoch (1975, 1978) developed a mathematical framework for studying the mechanical behavior of material surfaces. This framework takes into account the surface stress within continuum mechanics. Renault et al. (2003) showed that the surface of gold thin film is elastically stiffer than that of bulk gold. Muller and Saul (2004) reviewed the effects of surface stress and surface elasticity on surface phenomena in surface physics.

Nanoindentation and scanning probe microscopy (SPM) are used to estimate material properties on the nanoscale. These techniques can be used to evaluate material properties on the nanoscale on the basis of the relationship between the approach of an indenter and the contact force or adhesion force. Hertz (see Johnson, 1985) derived the contact theory between two elastic spherical bodies. Further, Bradley (1932) deduced that the adhesion force between two rigid spheres is  $4\pi\omega R$ , where  $\omega$  is the work of adhesion and  $R = R_1R_2/(R_1 + R_2)$ ,  $R_1$  and  $R_2$  being the radii of the two rigid spheres. Johnson et al. (1971) derived an adhesion theory, i.e., the Johnson–Kendall–Roberts (JKR) theory, between elastic spheres by using the Hertz theory and surface energy. In the JKR theory, the adhesion force outside of the contact area is assumed to be negligible. Derjaguin et al. (1975) derived an adhesion theory, i.e., the Derjaguin–Muller–Toporov (DMT) theory, by considering the molecular force between two surfaces. The pull-off forces according to the JKR theory and DMT theory are  $1.5\pi\omega R$  and  $2\pi\omega R$ , respectively. Tabor (1977) showed that the JKR theory and DMT theory represent two extreme cases of adhesion. Attard and Parker (1992) and Greenwood (1997) analyzed adhesion between an elastic sphere and a flat surface by using the van der Waals force obtained from the Lennard–Jones potential

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function. Recently, Medina and Dini (2014) investigated the adhesion problems of a rough surface by using the Lennard–Jones potential function. Further, Yamamoto et al. (2013) analyzed the adhesive contact between a cylinder and a rigid substrate by using the boundary element method (BEM). In recent years, contact and adhesive contact analyses of isotropic materials with surface properties have been performed. Koguchi (2005) solved the contact problems of an indenter and the substrate of an isotropic material in consideration of the surface energy and surface stress. Pinyochotiwong et al. (2013) analyzed the contact problem of an axisymmetric rigid indenter and an isotropic half-space by employing the Gurtin–Murdoch model for surface elasticity.

The mechanical behavior of nanoscale structures is related to the anisotropy of crystal structures in a substrate. The Stroh's formalism is frequently used in the analysis of anisotropic materials (Ting 1996). Ting and Lee (1997) and Yang and Pan (2002) derived Green's functions for general anisotropic elastic materials based on the Stroh's formalism. Similarly, Koguchi (2008) derived a surface Green's function for anisotropic materials considering the surface stress and surface elasticity. The displacement field obtained using the Green's function considering the surface stress and surface elasticity exhibited good agreement with that obtained by the molecular dynamics (MD) method. For the adhesive contact analysis of anisotropic materials, Chen and Gao (2007) developed an adhesive contact model for a rigid cylinder with a transversely isotropic material. They assumed that the contact region is symmetric with respect to the center of the cylinder. Further, Yao et al. (2009) developed a contact model without any assumption of the symmetry of the contact region. Hayashi et al. (2013) performed contact analysis of anisotropic materials considering the surface stress and surface elasticity; they used the surface Green's function derived by Koguchi and the conjugate gradient method for this analysis. With the aim of the adhesion analysis of anisotropic materials, Borodich et al. (2014) analyzed the adhesion problem of a transversely isotropic material. In their analysis, the distance between the two surfaces was described by a power-law function and the JKR theory was considered as an adhesion problem of a power-law indenter with an index of 2. Barber and Ciavarella (2014) derived a solution for the adhesive contact problem of two spherical indenters to consider the effect of anisotropic elasticity. They assumed that the contact area between the two indenters is elliptical and that the energy release rate at the contact edges on each axis is equal to the interface energy. However, the shape of the contact area between fully anisotropic spheres is not elliptical. For example, Hayashi et al. (2013) demonstrated that the contour plot for the displacement of the Cu(111) surface under a concentrated force is hexagonal in shape.

To the best of our knowledge, only a few studies have been conducted on adhesive contact problems of fully anisotropic materials considering surface properties. In the present study, we analyze the adhesive contact problem between rigid spherical indenter and anisotropic elastic half-space considering surface stress and surface elasticity. To calculate the surface displacement for the adhesive force, Green's function derived by Koguchi is used. We developed an iterative method in the adhesive contact analysis considering van der Waals force. We also conduct an adhesive contact analysis of a rigid spherical indenter against the flat surface of an anisotropic substrate for the adhesion and separation processes.

## 2. Theory and analysis method

### 2.1. Green's function for anisotropic material considering surface stress and surface elasticity

A more detailed derivation of the surface Green's function considering the surface stress and surface elasticity can be found

in Koguchi (2008). In the present study, we outline this derivation of the surface Green's function.

The equilibrium equation for anisotropic materials can be expressed in terms of the displacement  $u_i$  as follows:

$$C_{ijkl} u_{k,lj} = 0 \quad (1)$$

where  $C_{ijkl}$  is the elastic stiffness. The general solution of the equilibrium equation, Eq. (1), can be expressed as follows by applying two-dimensional (2D) Fourier transform:

$$\hat{\mathbf{u}}(\eta_1, \eta_2, x_3) = \mathbf{a}(\eta_1, \eta_2) e^{-ip\rho x_3} \quad (2)$$

where  $\eta_1 = \rho n_1$ ,  $\eta_2 = \rho n_2$ ,  $\rho$  is a parameter related to the Fourier transform and greater than or equal to zero, and  $p$  and  $\mathbf{a}$  satisfy the following eigenrelation:

$$\{\mathbf{Q} + p(\mathbf{R} + \mathbf{R}^T) + p^2\mathbf{T}\}\mathbf{a} = 0 \quad (3)$$

where,  $Q_{ik} = C_{ijks}n_j n_s$ ,  $R_{ik} = C_{ijks}n_j m_s$ , and  $T_{ik} = C_{ijks}m_j m_s$ , with  $\mathbf{n} = [n_1, n_2, 0] = [\cos\theta, \sin\theta, 0]^T$  and  $\mathbf{m} = [0, 0, 1]$ . Next, the boundary condition is expressed using an equilibrium relationship among the surface stress tensor  $\tau_{\alpha\beta}$ , the bulk stress  $\sigma_{ij}$ , and the traction vector  $t_i$  as follows:

On the tangential plane of the surface:

$$\sigma_{ix} v_i - \tau_{\alpha\beta} v_\beta = t_\alpha \quad (4)$$

In the normal direction to the surface:

$$\sigma_{i3} v_i - \tau_{\mu\beta} \kappa_{\mu\beta} v_\beta = t_3 \quad (5)$$

where  $\kappa_{\mu\beta} = \partial^2 u_3 / \partial x_\mu \partial x_\beta |_{x_3=0}$  is the curvature tensor of the deformed surface;  $v_1$  and  $v_2$  are unit vectors in the tangential direction of the surface;  $v_3$  is the unit normal vector of the surface;  $\alpha, \beta, \mu = 1, 2$  correspond to the rectangular coordinates on the surface; and  $i = 1, 2, 3$  corresponds to the rectangular coordinates.

The surface elastic modulus  $d_{\alpha\beta\gamma\lambda}$  relates the surface stress to the surface strain:

$$\tau_{\alpha\beta} = \tau_{\alpha\beta}^0 + d_{\alpha\beta\gamma\lambda} \epsilon_{\gamma\lambda}^s \quad (6)$$

where  $\tau_{\alpha\beta}^0$  is the surface stress tensor for zero surface strain induced by an external load and  $\epsilon_{\gamma\lambda}^s$  is the surface strain. The surface stress depends linearly on the surface strain. In the present study, the surface stresses and surface elastic moduli are calculated using the MD method. The calculation method is explained in Section 3.3.

By substituting Eq. (6) into Eqs. (4) and (5), we can express the boundary condition in matrix form as follows:

$$\hat{\mathbf{t}} = -i\rho(\mathbf{b} + i\rho\mathbf{F})e^{-ip\rho x_3} \quad (7)$$

where

$$\mathbf{b} = -\frac{1}{p}(\mathbf{Q} + p\mathbf{R})\mathbf{a} \quad (8)$$

and

$$\mathbf{F} = \begin{bmatrix} d_{1\beta 1\lambda} n_\beta n_\lambda & d_{1\beta 2\lambda} n_\beta n_\lambda & 0 \\ d_{2\beta 1\lambda} n_\beta n_\lambda & d_{2\beta 2\lambda} n_\beta n_\lambda & 0 \\ 0 & 0 & \tau_{\alpha\beta}^0 n_\alpha n_\beta \end{bmatrix} \quad (9)$$

The general solution is obtained by superposing three solutions of Eqs. (2) and (7) associated with  $p_j$  and  $\mathbf{a}_j$  ( $j = 1, 2, 3$ ), which are eigenvalues and the corresponding eigenvectors, respectively, as follows:

$$\hat{\mathbf{u}}(\eta_1, \eta_2, x_3) = \mathbf{A}(e^{-ip_j \rho x_3}) \mathbf{q} \quad (10)$$

$$\hat{\mathbf{t}}(\eta_1, \eta_2, x_3) = -i\rho(\mathbf{B} + i\rho\mathbf{F})(e^{-ip_j \rho x_3}) \mathbf{q} \quad (11)$$

where  $\mathbf{F}$  is a real matrix,  $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]$ ,  $\mathbf{B} = [\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3]$ ,  $\langle e^{-ip_j \rho x_3} \rangle = \text{diag}[e^{-ip_1 \rho x_3}, e^{-ip_2 \rho x_3}, e^{-ip_3 \rho x_3}]$ , and  $\mathbf{q}$  is a complex vector

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