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Delamination mechanism maps for coatings/substrates system subjected to adhesive contact loads

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ABSTRACT

Previous delamination mechanism maps for coatings/substrates system cannot predict the critical conditions for delamination nucleation under adhesive contact loads, because the effects of surface adhesion on delamination are not considered. In this paper, the finite element simulation of a rigid sphere in adhesive contact with an elastic coating on an elastic-plastic substrate is undertaken to clarify interface crack initiation and growth, in which the surface adhesion of the indenter/coating contact system is modeled by nonlinear spring elements with a force-displacement relationship derived from a Lennard-Jones potential, and the coating/substrate interface is represented by an irreversible cohesive zone law. By conducting parametric studies, delamination mechanism maps considering surface adhesion are constructed. It is found that increasing the adhesion work will initiate delamination nucleation, and the critical indentation depth increases with increasing the interfacial cohesive energy in the presence of the surface adhesion. For relatively stronger adhesion, the higher the coating elastic modulus or the coating thickness is, the greater the critical indentation depth becomes. However, for relatively weaker adhesion, increasing the coating elastic modulus will decrease the critical indentation depth, and increasing the coating thickness will increase the critical indentation depth for lower indentation depths, but an opposite trend occurs for higher indentation depths.

1. Introduction

Hard coatings are widely applied in various mechanical components to improve friction, wear, and contact fatigue resistance of surfaces subjected to contact loads. However, coatings subjected to contact loading may generate a variety of failure mechanisms such as cracks in coatings [1,2], delamination at the coating/substrate interface [3–8], combination of coating fracture and delamination [9,10], and so on. As far as the delamination of subjected to contact loading from the substrate is concerned, the nanoindentation test is an efficient way to characterize the coating/substrate interface bonding behavior. Marshall and Evans [3] applied the clamped circular plate assumption to analyze the coating/substrate interface delamination induced by indentation and evaluated the interface facture toughness. Drory and Hutchinson [4] studied conical indentation of coated systems with compliant substrates and put forward a test method for evaluating the interfacial energy as well. However, due to the material and geometrical nonlinearities, it is quite difficult to theoretically analyze the delamination mechanism based only on the fracture mechanics approach. Therefore, numerical methods such as the finite element method (FEM) together with the cohesive model [11–13] based on Dugdale-Barenblatt cohesive zone approach [14,15] have been developed into an effective tool to simulate initiation and propagation of delamination during indentation. For example, Abdul-Baqi et al. [5,6] simulated spherical indentation of a ductile substrate coated with a hard thin film, with the interface modeled by means of a cohesive surface, and found shear delamination outside the contact area during loading and tensile delamination at the center of the contact during unloading. But convergence problems restricted their studies to a limited parameter space. To overcome these problems, Gao et al. [16] introduced a fictitious viscosity in the cohesive models. Based on the above-mentioned studies, Xia et al. [7] conducted detailed parametric studies and constructed delamination mechanism maps to show the critical indentation depth and load to initiate shear or tensile cracks. However, the effects of surface adhesion on the interface delamination have not been considered so far.

In fact, with the continuous miniaturization of devices, such as micro/nano electro-mechanical systems, adhesive contact problems induced by molecular interactions become remarkable [17–19]. However, there have been only a few researches related to adhesion-delamination issues. Muller et al. [20] first proposed the expression of adhesion force per unit area between two infinite parallel surfaces based on the Lennard-Jones (LJ) interatomic potential law [21]. Song et al. [22] analyzed adhesion-induced delamination at the coating/substrate interface, in which the surface adhesion is modeled by nonlinear springs obeying the law of LJ surface force, and the interface is represented by a bilinear cohesive zone law. They studied the interdependence of contact

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instabilities and interfacial damage encountered in layered media during adhesive contact loading and unloading. However, the delamination mechanism maps have not been constructed so that the critical conditions for delamination to occur under adhesive contact loads cannot be predicted yet. Actually it is of great significance that the relationship of interface delamination and relevant parameters under adhesive contact is described in the form of delamination mechanism maps, which can provide guidelines for design and engineering applications of coatings.

The aim of this paper is to offer a deeper understanding of adhesion-induced delamination, and construct the delamination mechanism maps which describe the effect of the adhesion work, the strength and toughness of the interface, the coating elastic modulus and the coating thickness on the initiation of delamination.

2. Model description and validation

2.1. Model description

Adhesion contact between an indenter and a coating on a substrate is simplified as an axisymmetric model illustrated in Fig. 1. The sphere indenter with radius R, indentation depth h and indentation force P is rigid. The coating with thickness t, Young's modulus E_c and Poisson's ratio ν_c is linearly elastic, and cracking of the coating is ignored. The substrate with yield stress σ_Y, Young's modulus E_s and Poisson's ratio ν_s is elastic-perfectly plastic, and the Von Mises criterion is selected to indicate the onset of substrate plastic deformation.

Surface adhesion between the indenter and the coating is represented by nonlinear spring elements obeying a traction-separation relation derived from LJ potential [20]. In Fig. 1, $z(r)$ describes the vertical distance between two surfaces, where r is the radial distance from the axis of symmetry. For surface interaction controlled by the LJ potential, the local traction distribution $p(r)$ can be expressed as

$$p(r) = \frac{8\Delta\gamma}{3\varepsilon}\left\{\left[\frac{\varepsilon}{z(r)}\right]^3 - \left[\frac{\varepsilon}{z(r)}\right]^9\right\} \tag{1}$$

where $\Delta\gamma$ is the work of adhesion and ε is the equilibrium distance. The first and the second item represent the attraction and repulsion, respectively. Thus, when $z(r) > \varepsilon$, $p(r)$ refers to surface attractive interaction.

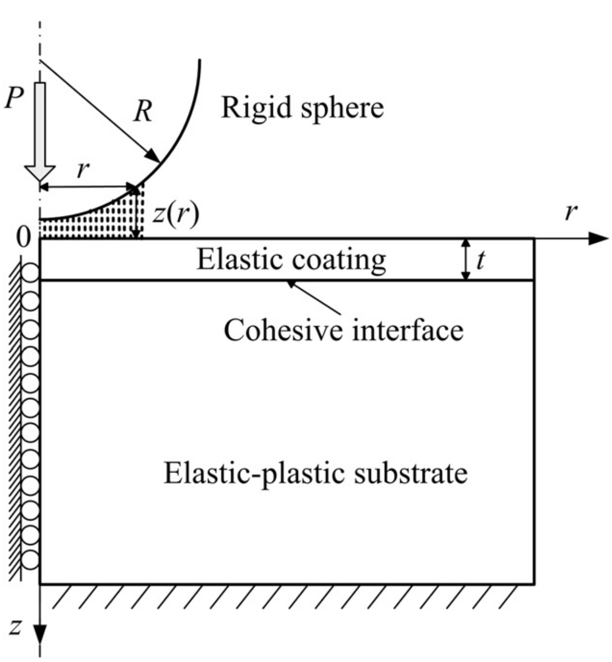

Fig. 1. A rigid sphere in close proximity with a coating on a compliant substrate.

The irreversible bilinear cohesive zone model developed by Repetto et al. [12] is used to simulate initiation and propagation of delamination at the coating/substrate interface. In the description of the interface as a cohesive surface, a small effective opening displacement $\delta = (\langle\delta_n\rangle^2 + \delta_t^2)^{1/2}$ between the coating and substrate is allowed, with normal and tangential components (δ_n, δ_t), where $\langle\,\rangle$ represents the Macaulay bracket and $\langle\delta_n\rangle = (\delta_n + |\delta_n|)/2$. The interfacial behavious is specified in terms of a constitutive equation for the corresponding traction components (T_n, T_t) at the same location. Thus, the bilinear traction-separation law is given by the following equations:

$$T_n = \begin{cases} T(\delta)\dfrac{\delta_n}{\delta}, \delta_n > 0 \\ k_c\delta_n, \delta_n < 0 \end{cases} \qquad T_t = T(\delta)\frac{\delta_t}{\delta} \tag{2}$$

where the function of $T(\delta)$ is illustrated in Fig. 2. Here, δ_{max} is the opening displacement for damage initiation within the cohesive zone, $\sigma_{max}/\delta_{max}$ controls the undamaged surface reversible elastic stiffness, δ_C is the opening displacement for interface failure, the critical cohesive energy for the interface is given by $\Gamma = (\sigma_{max}\delta_c)/2$, and the k_c is a contact stiffness that resists inter-penetration of the coating and substrate under compressive loading [7].

The above-prescribed cohesive zone model is performed through the user element subroutine in ABAQUS/Standard (Version 6.14-1), and the displacement-controlled indentation is used in the simulation. To improve convergence in computations, a technique based on viscous regularization (a generalization of the Duvaut-Lions regularization [23]) of the damage variables is implemented in the user subroutine. To accurately obtain numerical solutions, the mesh is mapped very fine locally near the contact and cohesive interface area with an element size of $t/10$. The full flow chart for obtaining the critical indentation depth h_{crt} is depicted in Fig. 3, where δ_o and σ_z represent coating-substrate separation at the symmetry axis and normal stress along the coating surface, respectively.

2.2. Model validation

Firstly, to validate the feasibility of the present cohesive zone model performed through the user element subroutine, indentation-induced delamination of a coating/substrate system is simulated in the absence of surface adhesion. The simulation results of the critical indentation depth for the initiation of both

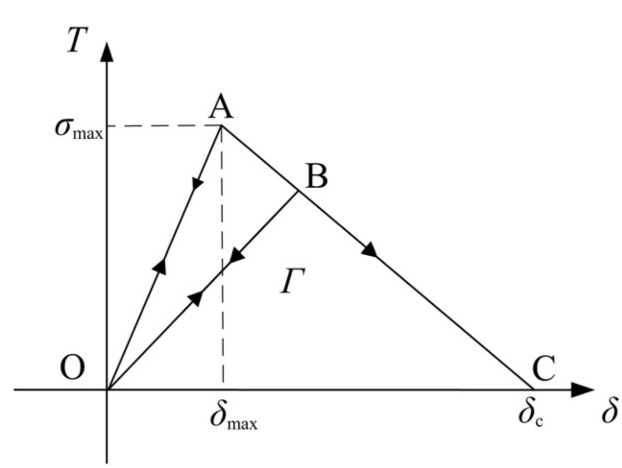

Fig. 2. An irreversible bilinear cohesive zone law $T(\delta)$.