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Indentation for evaluating cracking and delamination of thin coatings using finite element analysis

Yangyi Xiao*, Wankai Shi, Jing Luo

The State Key Laboratory of Mechanical Transmission, Chongqing University, Chongqing 400044, China

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ABSTRACT

The mechanics of indentation induced coating cracking and interfacial delamination in a typical weakly bonded brittle thin coating-substrate system (diamond-like carbon coating with low adhesion on steel substrate) is investigated by using finite element method. A bilinear cohesive zone model with prescribed cohesive strength and energy is applied to simulate evolutions of the crack and delamination. The effects of the cohesive zones, coating elastic modulus, and coating thickness on the indentation response are evaluated. It is found that increasing the cohesive strength/energy of coating reduces the probabilities of crack generation and propagation, whereas increases the susceptibility to interfacial delamination. At a critical value of the cohesive strength of the bonding layer, the resistance to interfacial delamination reaches its minimum. Nevertheless, the coating cracking is not sensitive to the interface adhesive properties. Moreover, a coating can receive better protection with lower coating elastic modulus. Additionally, increasing the coating thickness generally increases the critical load for coating/interface failures, but opposite effect occurs when the coating is thinner than a critical thickness. Numerical results have also been compared with other emulational or experimental works, and can establish a theoretical basis for improving the durability of brittle thin coatings.

1. Introduction

Thin hard coatings have been widely applied in mechanical components, such as gears, bearings, and joints, to reduce the coefficient of friction, improve the wear performance, and achieve excellent loading capacity of the surfaces. Although these coated mechanical components can realize perfect tribology performance, the major failure modes of thin hard coatings (usually brittle) on relatively softer substrates system are coating cracking and interfacial delamination [1–3], which we should highly regard. Physical vapor deposition (PVD) coatings, as a general rule, are hard and brittle, but cannot show good bonding performance with steels under some special conditions. For instance, an oxide layer on the substrate or rough surface of the substrate before deposition can result in an interfacial problem of low adhesive performance [4]. Furthermore, a PVD coating shows inferior adhesive performance at an elevated temperature operating condition [5,6]. Therefore, the selection of a typical weakly bonded brittle thin coating-substrate system is critical to the investigation.

Indentation test is an important way to assess failures of the coating [1,7–10]. Of course, mechanical behavior of coating-substrate system has more immediate concerns. For numerical simulation on indentation, the finite element method is often applied to analyze its mechanical behavior. In previous studies, for example, the stress characteristics of coating surface and bonding layer are analyzed to evaluate the coating failures [3,8–11]. Tilbrook et al. [12] obtained the damage mechanisms of hard TiN coatings based on a model by anisotropic property definitions and nodal coupling. The crack growth in thin elastic coatings bonded on elastic substrates was investigated by using the *J*-integral method [13,14]. These methods can only predict the failure locations or analyze the preexisting cracks. Moreover, the hard coating cracking under indentation was simulated by applying cohesive zones in the possible crack locations [15]. But Abdul-Baqi et al. [15] studied the circumferential coating cracks only by the method of step-by-step discerning analysis. In their research, the location of the $(n+1)$th crack can be found by stress analysis after the nth crack forms, and all coating cracks are assumed to initiate from the coating surface. Actually, this method has the shortcoming that it cannot simulate the crack behaviors if some coating cracks may form

* Corresponding author.
E-mail address: yyxiao@cqu.edu.cn (Y. Xiao).

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simultaneously. Also, some of the cracks initiate from the coating surface, and some initiate from the coating side of the interface. In addition to these works, the bonding layer was modeled by a cohesive surface to study the interfacial delamination [16–19]. Zhang et al. [19] obtained the effects of the interface adhesive properties and the thickness of the thin coating for cases of a perfect hard coating on a soft substrate on the onset and growth of interfacial delamination. In summary, there are three cases on the numerical models of indentation in previous works: perfect coating-substrate system, cohesive interface layer between perfect coating and substrate, and cracks on coating with perfect bonding layer. However, it has been shown that coating cracking often follows by interfacial delamination [15,16,20] under indentation, especially in a weakly bonded thin hard coating-substrate system. The method in neither case is going to be the best for evaluation on brittle thin coating failures. There are few studies that consider the interaction of coating cracking and interfacial delamination. Thus, these gaps will be the emphasis of the current paper.

Currently, the cohesive zone model (CZM) is one of the most modern evolutions in the area of fracture mechanics to simulate the cracks (between the coating neighbor segments) and delamination (between the coating and substrate) [15–23]. The major features of CZM is that it is able to adequately predict the behavior of uncracked structures, but also can be used to investigate the onset and growth of separations if damage occurs [18]. Additionally, the CZM does not represent any physical material, but describes the cohesive forces which occur when material elements are being pulled apart.

In the present paper, both the coating cracking and interfacial delamination are taken into account for brittle thin coatings by applying a cohesive zone finite element model during indentation simulation. A system consisting of a diamond-like carbon (DLC) coating on a steel substrate is investigated in this study. For simplicity, the residual stress is not considered in the coating-substrate system, which means the coating is assumed to be stress free prior to indentation. A spherical indenter is used in the indentation test. The radial cracking in the coating is not included in the study, because this type of indenter (spherical) is less likely to induce radial cracking, but rather ring cracking. Here, it is worth noting that the shapes of both the coating cracks (Hertzian ring cracks [8,21]) and the interfacial shear delamination are circumferential. The aim of this study is to offer an improved understanding of coating cracking and interfacial shear delamination during the loading stage of indentation and to improve the durability of brittle thin coatings by varying several parameters. The effects of the cohesive zones, coating elastic modulus, and coating thickness on the indentation response which includes initiations of coating cracking and interfacial delamination and their propagations are studied. Importantly, numerical results will be compared with other emulational or experimental works.

2. Indentation model description

2.1. Finite element model

During a loading step of the indentation test, the reaction force of indenter is continuously recorded as a function of the indenter displacement. Then the load–displacement (P–h) curves can be obtained. The quasi-static structural analysis (rate-dependent, but not involving inertia) is performed on the step. The indenter moves along the axis of symmetry and penetrates the coating-substrate system up to a prescribed depth (maximum value is equal to the coating thickness in the present paper) in loading stage.

In the simulation, the length and stress are respectively scaled by and Δ(substrate yield stress), which are respectively chosen as σ_{ys} and 1 μm for convenience. Fig. 1 describes the geometry of 1 GPa the simplified indentation model and its boundary conditions. The coating-substrate system has the shape of a cylinder and that the indentation is made just in the center of the coating surface. A two-dimensional finite element model is considered in the radial–axial (r–z) coordinate due to its symmetry along the axis, and the contact radius a can be obtained during indentation. As seen in Fig. 1, the parameters are defined as radius of spherical indenter of $R = 50\ \Delta$, coating thickness of $h_c = 2\Delta$, substrate thickness of $h_s = 200\Delta$, bonding layer thickness of $h_b = 0.1\Delta$, and system radius of $L = 200\Delta$. Roller-boundary conditions are applied along the axis of symmetry and fixed-boundary conditions are applied to the substrate base. In this finite element analysis, the indenter is considered as a rigid body for simplicity, because it is made of diamond which is much harder than the specimen. Then, a reference node located on the center of the spherical indenter is used as the reference point of the rigid indenter, and a specified displacement is applied to this reference node. In order to get accurate results and improve the convergent rate, different mesh densities are applied to the coating-substrate system. There is the highest mesh density near the contact and bonding areas.

The contact behavior between indenter and coating is divided into two parts: normal and tangential behaviors. The normal behavior applied to the model is “hard” contact. For tangential behavior, a penalty-type contact algorithm is carried out that places imaginary springs between the “master” surface and the “slave” surface. The coefficient of friction for contact between the indenter and coating is specified as 0.1. Cohesive zone models (CZMs) are applied on cracks and the bonding layer that can be found in the next section.

In continuum mechanics, the substrate is defined as homogeneous, isotropic, and elastic–plastic materials. It accords with the following uniaxial stress–strain law:

$$\sigma = \begin{cases} E\varepsilon & (\varepsilon < \sigma_y/E_s) \\ \sigma_y\left(\dfrac{\varepsilon}{\sigma_y/E}\right)^n & (\varepsilon \geq \sigma_y/E_s) \end{cases} \tag{1}$$

where, σ and ε are the stress and strain of the material, respectively.

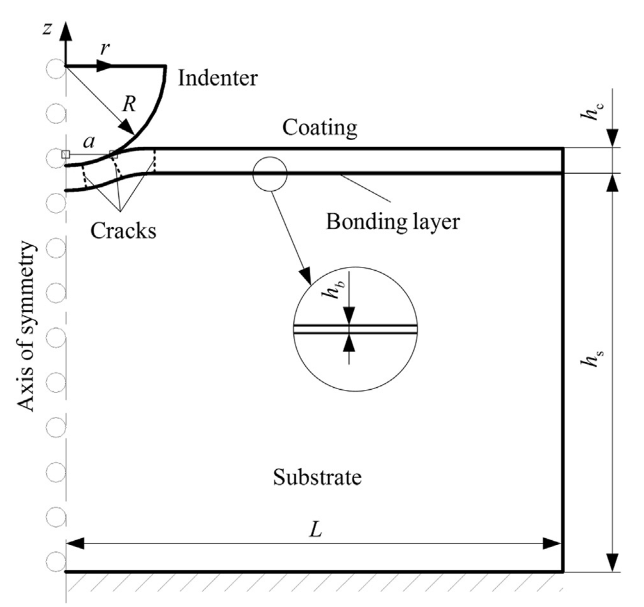

Fig. 1. Geometry of the simplified indentation model and boundary conditions.