Interface effect on failure of ceramic coating/alloy substrate systems

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Abstract

The interface cohesive zone model is usually used in the finite element method to describe the damage and fracture of interfaces between two layers, two kinds of materials, or two segments in one kind of material or a layer. An introducing of interface cohesive elements in one layer should not affect the layer's properties, that how to take the thickness and stiffness of the interface cohesive elements is studied firstly and the related criterion is given. A finite element model of ceramic coating/alloy substrates under three-point bending loading with the interface cohesive elements inserted into coatings is developed, and the transverse crack evolution of coatings is studied. The simulation results indicate that the coating cracking is later and the crack length decreases with increasing interface toughness, i.e., the damage, defined by a total crack length, is slower with increasing fracture toughness. It can explain the experimental results that damage rate of nanostructured thin coatings with smaller cohesive energy is larger than that of conventional coatings with microscale microstructure, because the fracture toughness is proportional to the cohesive energy of coatings. The effect of cohesive strength on coating damage changes at a critical strength, when the cohesive strength is larger than the critical value, the crack length and damage rate increase with decreasing interface strength.

Keywords: **Interface cohesive element, coatings, cohesive strength, fracture toughness.**

Introduction

Ceramic coatings are widely used in mechanical, electronic, chemical engineering fields due to its better properties such as wear resistance, erosion resistance, and thermal protection. Once ceramic coatings crack, their function will lose. Therefore, the study on cracking behavior and mechanism of coating/substrate systems attracts great attention [1-5]. Crack density of thin films under tensile stress was predicted based on fracture mechanics model [2] or by developing an elastic-plastic shear-lag model [3]. Crack distribution of ceramic coatings was observed in the in-situ bending experiments by scanning electron microscope [4]. In order to study systematically crack and damage evolution of coating systems, finite element method (FEM) is a good choice. Interface cohesive zone model (CZM) is an effective tool to characterize cracking and is often introduced in FEM [5]. However, the introduction of CZMs should not affect the original mechanical properties of materials before cracking.

In this paper, the stiffness criterion of CZM with finite thickness is given firstly, then which is used to simulate cracking of ceramic coatings bonded on alloy substrates under three-point bending loading. Interface cohesive strength and fracture toughness effects on cracking

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damage and fracture behavior of coatings are characterized and the related mechanism is revealed.

Selection of cohesive element

In order to ensure that the insertion of cohesive elements does not affect original mechanical properties, the elastic constant E_{eq} of the equivalent continuous medium should be equal to that of the matrix material E_m correspondingly. A representative volume element (RVE) can be selected for the system is in tension, as shown in Fig. 1(a). Due to the introduction of cohesive elements, the length of the RVE increases from L to $L' = L + t_0$, t_0 is thickness of the cohesive element and interface stress-displacement relation is showed in Fig. 1(b). The elongation of the RVE can be divided into two parts: elongation of the matrix material and elongation of cohesive element. The normal strain of the RVE in the *x* direction and thus the equivalent Young's modulus E_{eq} can be expressed. Since it is required that $E_{eq} = E_m$, we obtain

$$k_n t_0 = E_m \tag{1}$$

where k_n is the stiffness of interface cohesive model as shown in Fig. 1(b).

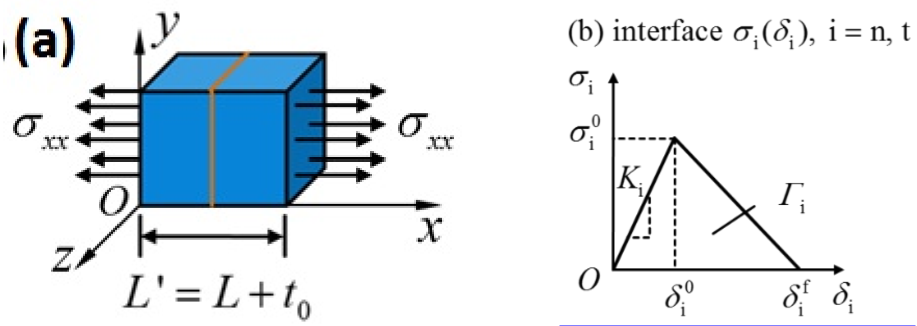

Figure 1. (a) Representative volume element of the system composed of matrix material and cohesive elements in uniaxial tension; (b) Interface cohesive zone model as cohesive elements.

It should be noted that Eq. (1) can be rewritten in the form of the ratio of two lengths: $t_0 / \delta_n^0 = E_m / \sigma_n^0$ with interface cohesive strength σ_n^0 and the corresponding critical displacement δ_n^0 as shown in Fig. 1(b), Γ_n is interface fracture toughness with the subscript n denoting normal direction and t tangential direction. Since the ratio of strength and Young's modulus is about $E_m / \sigma_n^0 \approx 10^2–10^3$, the thickness of cohesive elements is two or three orders of magnitude larger than the critical displacement. When thickness of cohesive elements is very small, a large stiffness should be selected based on Eq. (1).

Finite element model of ceramic coating/alloy substrate systems

Ceramic coating/substrate systems are assumed to be under the plane strain condition and the 2D FEM analysis is carried out using the commercial software ABAQUS. Due to symmetry, only the left half of the model is considered, as shown in Fig. 2. The model includes two layers: substrate with thickness h_s of 1.2 mm and ceramic coating with thickness h_c of varying a range compared with the experimental samples. The span length is 16 mm. The vertical loading displacement *w* is applied on the indenter. Ceramic coating is considered as linear elastic material with Young's modulus of E_c and Poisson's ratio of ν_c [4]. Superalloy substrate is assumed to be elastic-plastic material with Young's modulus of E_s and Poisson's ratio of ν_s, and its constitutive relation can be referred to Ref. [4]. The four-node plane strain reduced integration elements (CPE4R) are selected to mesh substrate and coating.

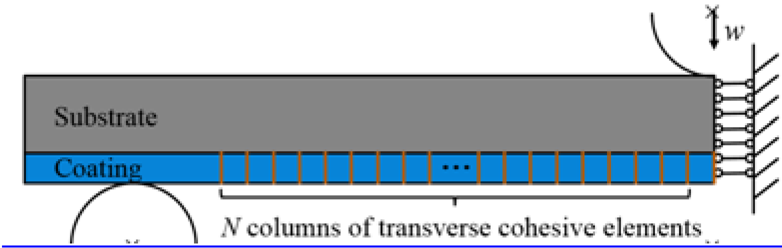

Figure 2. Coating/substrate model under three-point bending loading.

Only transverse cohesive elements with thickness of $t_0^{(T)}$ are inserted into the coating, as shown in Fig. 2. The four-node cohesive elements (COH2D4) are inserted into the coating. The strength and fracture toughness of transverse cohesive elements actually refer to coating strength and coating fracture toughness respectively as shown in Fig. 1(b). For simplicity, values of strength and fracture toughness of cohesive elements in normal and tangential directions are assumed to be the same [6], i.e., $\sigma_n^{0(T)} = \sigma_t^{0(T)}$, $\Gamma_n^{(T)} = \Gamma_t^{(T)}$. The thickness of cohesive elements is selected as $t_0^{(T)} / h_s = 1\times10^{-4}$. According to Eq. (1), dimensionless stiffness of transverse cohesive elements is selected as follows:

$$\begin{cases} \dfrac{K_n^{(T)} h_s}{\sigma_Y} = \dfrac{E_c / \sigma_Y}{(1-\nu_c{}^2) t_0^{(T)} / h_s} = 2.34\times10^5 \\ \dfrac{K_t^{(T)} h_s}{\sigma_Y} = \dfrac{1-\nu_c}{2} \dfrac{K_n^{(T)} h_s}{\sigma_Y} = 9.38\times10^4 \end{cases} \tag{2}$$

Dimensionless coating strength and coating fracture toughness are $\sigma_n^{0(T)} / \sigma_Y = 0.03\text{–}0.34$ and $\Gamma_n^{(T)} / (\sigma_Y h_s) = (1.0\text{–}5.1)\times10^{-5}$, respectively, σ_Y = 800 MPa [4]. Each of the interface parameters of CZMs varies in the range while others remain unchanged to consider influence of corresponding interface parameter.

Simulation results

The cracking mode of ceramic coating is showed in Fig. 3. The interface cohesive strength and fracture toughness effects on fracture behavior of coatings are obtained as shown in Fig. 4. It can be seen that crack length decreases with increasing coating toughness as shown in Fig. 4(a) and cracking occurs later, too, i.e., damage defined by a total crack length is slower for coatings with higher toughness, which is consistent with the previous energy analysis [7]. For coating strength effect, when the strength is larger than a critical value, the crack length also decreases with increasing strength as shown in Fig. 4(b), i.e., there exists a critical value of strength for changing damage rate of coatings. It was found that the damage rate of nanostructured thin coatings was higher compared with that of corresponding microscale microstructure coatings in the previous experimental measurement [8], which implies the lower fracture toughness of nanostructured coatings based on the above simulation. The study also shows the cohesive energy decreases for nanostructured materials compared to corresponding bulk materials [9], the fracture toughness of materials should be proportional to the cohesive energy, therefore, the present simulation results can explain the experimental results.

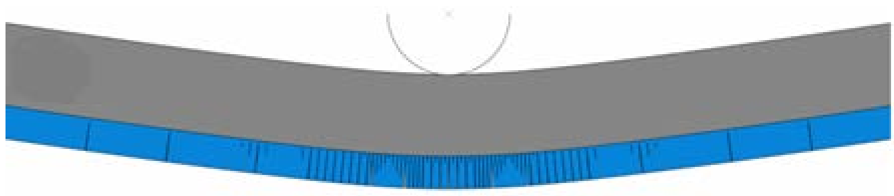

Figure 3. Cracking of coatings.

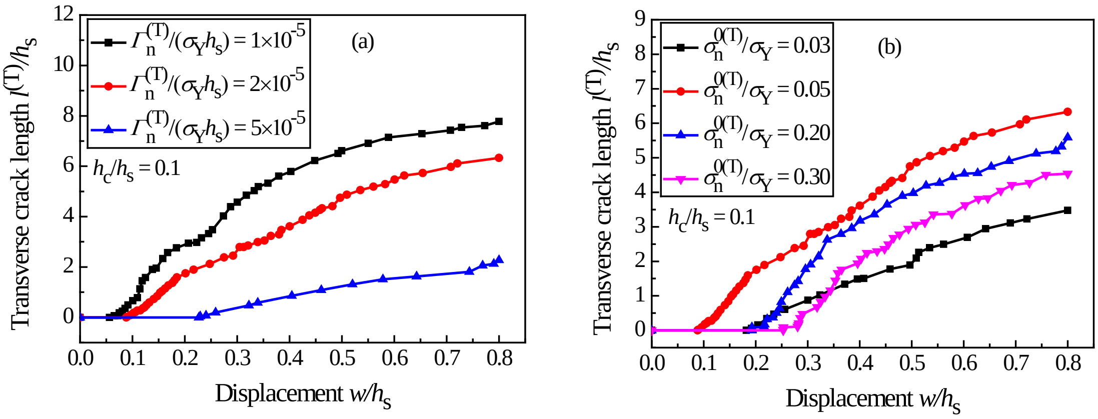

Figure 4. (a) Fracture toughness effect and (b) Strength effect of coating cracking.

Conclusions

In summary, interface effects on failure of ceramic coating/substrate systems are studied by using finite element method combining with interface cohesive zone model. The selection method of stiffness of interface cohesive elements is firstly proposed. Then cracking of coating systems under three-point bending loading is simulated. The results indicate that cracking is easier for the coating with lower interface toughness. For interface strength, there exists a critical value of changing damage rate of coatings.

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