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Numerical study of interfacial crack growth effects on nanoindentation mechanical properties in presence of pre-existing defect

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ABSTRACT

Accurate calculation of the mechanical properties of the coatings needs finding out the sources of errors. One of the important sources of errors is the presence of pre-existing defect along the interface. In this study we consider elastic–plastic coating on elastic–plastic substrate system and the cohesive zone model embedded in the finite element code is used to simulate the interface between coating and its substrate. The aim of this paper is to investigate the effect of interfacial crack growth in the presence of a defect on deformation behavior and some mechanical properties such as hardness and modulus of elasticity in Cu/Si coating system. The results reveal that when the position of the defect is nearer to the shear stress concentration point, the crack will initiate sooner. Crack propagation results in some errors in calculation of the hardness and modulus of elasticity and according to the range in which the interfacial crack has grown, the amount of errors is different. The position of the pre-existing defect, even before any crack initiation, also has substantial effect on the distribution of shear stress along the interface during loading. Numerical study shows that the variance of the nanoindentation test results will significantly increase in specific range of indentation depth.

1. Introduction

Nanoindentation test is the preferred option for quantifying the mechanical properties of small volume materials. During the loading and unloading steps, the instrument directly measures the indentation force versus displacement of the indenter, from which the elastic modulus and hardness are estimated. However, the level of accuracy of the estimated hardness and Young's modulus values is always a question, since the method is very sensitive to several various parameters. Some sources of error has been addressed by some researchers in previous studies such as the effect of sample tilt [1], surface roughness of the specimen [2], sample compliance [3], residual stress [4], pile up [5–8], on nanoindentation results.

Since the application of coatings in industry has lately increased, accurate determination of the mechanical properties of coatings has become one of the most important concerns for scientists. Complete understanding of the mechanisms of crack initiation and growth seems necessary to determine the sources of error during nanoindentation test. To this end, failure mechanisms of coated systems have been investigated during recent years [9–19]. The main emphasis in such investigations has been to extract quantitative data about the coating and interfacial fracture energies and strengths. Being subjected to contact loading, coatings may confront a variety of failure mechanisms, such as, the ring cracks in coatings [11,20,21], the interface delamination of coating [22–24], and the combination of coating fracture and delamination [25]. Among many others, interfacial delamination is a particular concern and interfacial crack growth may lead to major damage to the coating/substrate system.

The interface between coating and its substrate plays an important role to protect the coating against delamination from its substrate. There are several publications on the mechanics and mechanisms of interfacial crack initiation and growth [10,12,13,16,26–29]. The interfacial delamination of ductile coating from elastic substrate [10,13], and elastic coating from ductile substrate [26,28], has been studied during recent years. In both types of material systems, in addition to the decrease of hardness (softening) envisaged in [29], there have been reports of ‘fingerprints’ on the load–displacement curves in the form of twists [16,27,28]. These kinks are one of the main sources of error in determining the mechanical properties of coating such as hardness and Young's modulus.

There are few publications in the literature on the mechanisms of interfacial crack growth in the presence of pre-existing defect [30]. Existence of pre-existing defect along the interface between the coating and substrate leads to sooner initiation of the interfacial crack [30]. One of the important issues that have not been mentioned in previous works is the position of the pre-existing defect and its effect on the failure mechanisms and mechanical properties. In this study we consider elastic–plastic coating on elastic–plastic substrate system and the

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cohesive zone model embedded in the finite element code is used to simulate the interface between coating and its substrate. The aim of this paper is to investigate the effect of interfacial crack growth in the presence of a defect on deformation behavior and some mechanical properties such as hardness and modulus of elasticity in Cu/Si coating system. The reason that we choose Cu/Si interface is that experimental results show that the interface between Cu and Si layers in Si/Cu/SiN/Pt/C multilayer coating stack is the most probable interface to delaminate during the test [31]. In this analysis, we assume that the other failure events such as through thickness coating crack, do not occur during the test.

2. Interface behavior

The interface behavior in this study is defined by the exponential cohesive zone model. The cohesive zone model has been introduced to overcome the limitation of Linear Elastic Fracture Mechanics (LEFM). LEFM method is on the basis of Griffith's criterion [32] and Irwin's modification [33] and first assumes that the material is isotropic and linear elastic. Based on this assumption, the stress field near the crack tip is calculated using the theory of elasticity. When the stresses near the crack tip exceed the material fracture toughness, the crack will grow. In LEFM, most formulas are derived for either plane stress or plane strain states, associated with the three basic modes of loadings on a cracked body: opening, sliding, and tearing. LEFM methods are troublesome when the nonlinear process zone is relatively large compared to the crack length. Also the process of crack nucleation cannot be described by LEFM. Moreover, the stress singularity introduced by LEFM at the crack tip makes the analysis more complicated. The origin of the cohesive zone models (CZMs) goes to the "Dugdale–Barrenblatt model" [34,35], and the "Leonov–Panasuk model" [36]. The cohesive zone is a fracture processing zone ahead of the crack tip. For most cohesive laws, the traction-separation curves used to model the material within the cohesive zone are phenomenological, and therefore are not directly related to the physical process in the damage zone which typically is difficult to determine experimentally. Nevertheless, the CZM approach has been greatly accepted as a computationally useful fracture analysis tool. If the CZM approach be used in a finite element analysis, the crack initiation, growth, and direction of growth can be automatically determined. Many different cohesive laws with variances in maximum traction, maximum separation, and shape have been proposed; like the linear softening cohesive law by Camacho and Ortiz [37], the exponential cohesive law by Needleman [38,39] and Xu and Needleman [40], the trapezoidal cohesive law by Tvergaard and Huchinson [41], and the polynomial cohesive law by Tvergaard [42]. Researchers found that these cohesive laws generally produce results that correlate well with experimental data such as the failure load and crack growth for cracked structures. The cohesive zone model directly introduces fracture mechanism by adopting softening relationships between tractions and the separations, which in turn introduces a critical fracture energy that is also the energy required to break apart the interface surfaces. The cohesive zone model consists of a constitutive relation between the traction T acting on the interface and the corresponding interfacial separation Δ (displacement jump across the interface). The definitions of traction and separation depend on the element and the material model. The general structure of different types of cohesive zone models is such that when the interfacial separation increases, the tractions across the interface increase to obtain a maximum, and then reduce, eventually disappearing with complete decohesion. Rate of convergence of the numerical simulation process for interface cracking is one of the advantages of exponential CZM in comparison with other types of CZM. As the tractions and their derivatives in the exponential CZM are continuous, the convergence rate enhances. Previous works show that exponential cohesive zone model can predict not only the crack initiation but also the crack spreading along the Cu/Si interface. In this paper we use the exponential cohesive zone model. The fundamental relations of exponential cohesive zone model are discussed below. For the exponential CZM, the interfacial potential is taken as

$$\phi(\Delta) = e\sigma_{max}\delta_n\left[1-\left(1+{}^{\Delta_n}/_{\delta_n}\right)\exp\left(-{}^{\Delta_n}/_{\delta_n}\right)\exp\left(-\left({}^{\Delta_t}/_{\delta_t}\right)^2\right)\right]. \quad (1)$$

Where e equals to 2.7182818; Δ is the interfacial separation, Δ_n and Δ_t are its normal and tangential components respectively; ϕ is surface potential; $\sigma_{max}$is maximum normal traction at the interface; δ_n is normal separation across the interface where the maximum normal traction is attained with $\Delta_t = 0$ and δ_t is tangential separation when the maximum shear traction is at $\Delta_t = \left({}^{\sqrt{2}}/_{2}\right)\delta_t$.

Hence, the normal and tangential tractions are defined as

$$T_n = e\sigma_{max}\left({}^{\Delta_n}/_{\delta_n}\right)\exp\left({}^{-\Delta_n}/_{\delta_n}\right)\exp\left(-\left({}^{\Delta_t}/_{\delta_t}\right)^2\right) \quad (2)$$

$$T_t = 2e\sigma_{max}\,{}^{\delta_n.\Delta_t}/_{\delta_t^2}\left(1+{}^{\Delta_n}/_{\delta_n}\right)\exp\left({}^{-\Delta_n}/_{\delta_n}\right)\exp\left(-\left({}^{\Delta_t}/_{\delta_t}\right)^2\right). \quad (3)$$

The normal and tangential works of separation are defined by

$$\phi_n = e\sigma_{max}\delta_n \quad (4)$$

$$\phi_t = \sqrt{2e}\tau_{max}\delta_t. \quad (5)$$

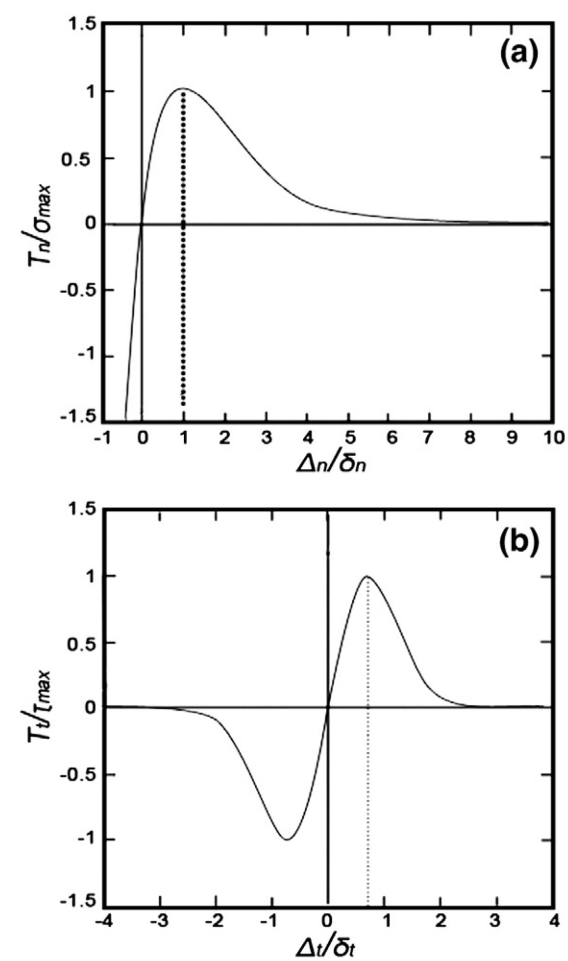

Fig. 1. (a) Normal traction, T_n vs. δ_n.for $\delta_t = 0$; (b) Shear traction, T_t vs. δ_t for $\delta_n = 0$.