DOUBLE COHESIVE ZONE MODEL AND PREDICTION FOR MICRO-SCRATCH TEST ALONG SOLID SURFACE

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ABSTRACT

A new double cohesive zone model describing the failure of ductile film in the micro-scratching test is presented in this paper. The failure behavior and adhesion work in the micro-scratch test is simulated and predicted based on the model. In the present analyses, the thin film is treated as the elastic-plastic material, and substrate is elastic material, and three-dimensional elastic-plastic finite element method is adopted. In order to simplify the analyses, the total problem will be divided into two sub-problems. One problem is that elastic-plastic large bend deformation of scratched film is considered, and an analytical solution can be obtained. Another problem is that the thin film is delaminated plastically along the interface with the elastic substrate, for which a special three-dimensional finite element method is used. The parameter relations of the horizontal driving force for the scratch test with the separation strength of thin film/substrate interface and the material shear strength, as well as the material parameters are developed. As an example of the application, the prediction result is applied to a scratch test for the Pt/NiO material system given in the literature, and both results are fairly agreement with each other.

KEYWORDS

Micro-scratch test, driving force, double cohesive zone model.

INTRODUCTION

The micro-scratch test is an important approach for determining the interfacial strength, toughness and adhesion properties for the thin film or coating layer on the substrate interface [1]. Its principle can be described as follows: On the material or specimen surface along the vertical direction an indentation force is exerted and indenter tip penetrates inside the material, then the indenter is moved in the horizontal and vertical directions simultaneously according to a fixed proportion. When the indenter tip moves near the film/substrate interface, a region of the thin film or coating layer near the indenter tip will be delaminated along the interface. Through measuring driving forces, the scratch depth, and the failure geometry, one will obtain the material or interface adhesion properties. According to usual experimental observations, there are two main kinds of failure characters in the scratch tests [1-5] depending on the material property of thin film or coating, whether ductile or brittle. One kind of failure character can be described as that for the ductile film case, a delaminated film strap is formed before the end of the scratch test and the delaminated film will be curved into a circular shape. The geometry of the delaminated area is fan shaped. Another failure character is that when film is brittle. A damage zone is formed near the indenter tip, inside which the film will be pressed to break into many small pieces and also delaminated from the substrate. In the present research, our attention will be focused on the metal film/ceramic substrate case. The ductile failure character will be simulated and analyzed in detail.

On the research of the material surface properties and adhesion work and strength of thin film or coating layer along the substrate interface, many experimental researches based on the scratch methods have been carried out in past decade [1-5]. However, theoretical analyses connected with the scratch experiments are very few [1]. This is because that any theoretical study must deal with on the complicated failure geometry of the scratch test. It is obvious that a three-dimensional elastic-plastic deformation problem must be solved, and a robust theoretical model for describing the scratch failure behavior is needed. Must theoretical researches have been based on the simple geometry of the scratch failure strap and the simple mechanics equilibrium to simulate the scratch failure behavior [1-5]. However, it is difficult to use a simple model to describe the strong influence of plastic deformation on the micro-scratch behavior. It is well known that plastic deformation has a strong shielding effect on the interface cracking [6-8]. So that in an elastic-plastic failure process more energy is dissipated than that in a pure elastic failure process. Therefore, it is important to develop a reasonable mechanics model for scratch test simulation.

The failure characteristics of the scratch test for ductile thin film materials[2-4] are somewhat similar with the thin film peeling problems. Therefore, in micro-scratch test research, the analytical method for the thin film peeling problem [8] is relevant. It is important to obtain a reasonable relation between the critical driving force and the parameters of the materials and scratch strap geometry.

In the present research, based on the three-dimensional character of failure strap, a new mechanics model describing the interface separation and the thin film shear failure, i.e., a double cohesive zone model will be presented. Using the new model, a relation between the scratch horizontal driving force and the parameters of the materials will be set up and used to predict the scratch work. Finally, the simulation results will be applied to an experimental result for Pt/NiO from [4].

FUNDAMENTAL DESCRIPTION AND SIMPLIFICATION

From failure characteristics for ductile film scratching, the scratch test process can be described by figure 1. This process can consist of two stages. One stage is a normal scratch before thin film delamination occurs along interface. With the indenter moving forward and downward with scratch depth increase, especially when indenter tip is near the interface, a region of thin film or coating layer near the indenter tip will be delaminated from interface. Thereby, the scratch process is transferred to another stage. The failure character changes from the indenter tunnel growth to the delaminated film strap formation and growth (or post-scratch process). For simplifying the analysis, the problem is divided into two sub-problems. One problem is "plate bend" under elastic-plastic large deformation for the delaminated thin film part BCD, see figure 1. This sub-problem has been solved successfully in [8]. Another problem is a three-dimensional delaminating problem for a part of thin film BA and jointed substrate. In the present research, our attention will focus on the latter problem. The solution of the former problem [8] will be taken as the boundary condition and exerted on the section B directly. For simplification, we present and adopt a new double cohesive zone model to simulate the film failure process and the scratch work for the post-scratch process. The new model is shown in figure 2. In this model, there are three cohesive zones, one is the separation-dominated cohesive zone and other two are shear-dominated cohesive zones.

DOUBLE COHESIVE ZONE MODELS AND MECHANICS DESCRIPTIONS

In figure 2, the thin film delaminates from interface of thin film/substrate (plane x_2=0), and this failure process can be simulated by a separation-dominated cohesive zone surface. Simultaneously, the curved film layer is cut off from two sides of the delaminated region (planes x_3=-W and 0). The cutting process for each plane can be described by the shear-dominated cohesive zone deformation. In figure 2, δ_{cn} and δ_{ct} are critic relative displacements for the separation and shear cohesive zone surfaces, respectively. The separation cohesive zone model under plane strain case has been widely adopted and completely formulated in [6-8]. In the following, we shall discuss and give a brief description and generalization for the two kinds of cohesive zone models for the three-dimensional case.

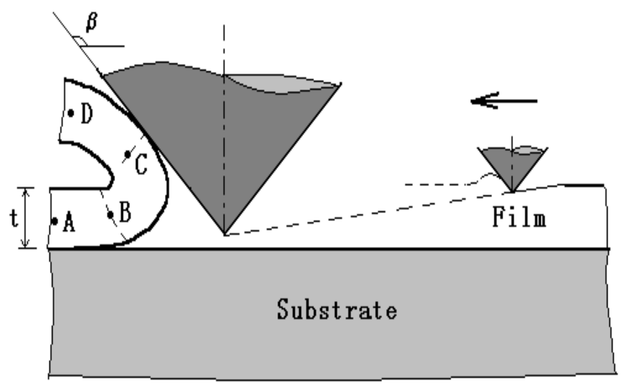

Figure 1: Scratch test geometry and ductile failure

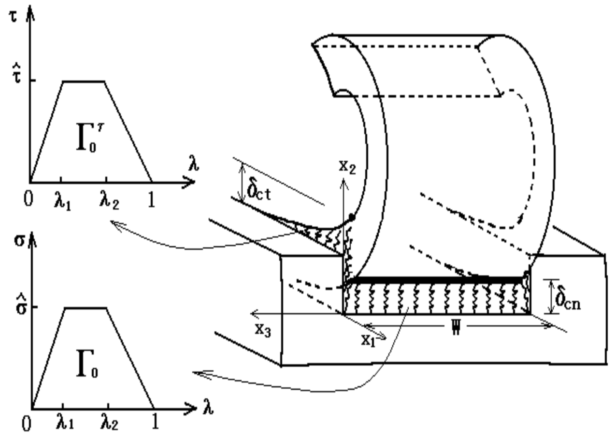

Figure 2: Double cohesive zone model

Let ($\delta_1, \delta_2, \delta_3$) be relative displacements at each cohesive surface along direction (x_1, x_2, x_3), respectively, and define a normalized displacement quantity

$$\lambda = \delta_c^{-1}\sqrt{\delta_1^2 + \delta_2^2 + \delta_3^2} \quad , \tag{1}$$

The critical condition for the cohesive zone is, $\lambda = 1$. For the separation-dominated cohesive zone case, $\delta_c = \delta_{cn}$, while for the shear-dominated cohesive zone case, $\delta_c = \delta_{ct}$. The traction relations, $\sigma(\lambda)$ and $\tau(\lambda)$, on the cohesive zone surfaces are sketched in figure 2.
The traction component expressions can be formulated in detail as follows. Define a potential function

$$\Pi(\delta_1, \delta_2, \delta_3) = \delta_{cn}\int_0^{\lambda} \sigma(\lambda')d\lambda' \tag{2}$$

then, one will derive out the traction expressions easily

$$(T_1, T_2, T_3) = (\frac{\partial \Pi}{\partial \delta_1}, \frac{\partial \Pi}{\partial \delta_2}, \frac{\partial \Pi}{\partial \delta_3}) = \frac{\sigma(\lambda)}{\lambda \delta_{cn}}(\delta_1, \delta_2, \delta_3) \tag{3}$$

Similarly, for the shear-dominated cohesive surface, one reads

$$(T_1, T_2, T_3) = \frac{\tau(\lambda)}{\lambda \delta_{ct}}(\delta_1, \delta_2, \delta_3) \tag{4}$$

Adhesion work per unit area along the cohesive surface can be written as

$$\Gamma_0 = \tfrac{1}{2}\hat{\sigma}\delta_{cn}(1 + \lambda_2 - \lambda_1) \tag{5}$$

for the separation zone, and

$$\Gamma_0^{\tau} = \tfrac{1}{2}\hat{\tau}\delta_{ct}(1 + \lambda_2 - \lambda_1) \tag{6}$$

for the shear cohesive zone. Earlier work has shown that the shape parameters (λ_1 and λ_2) of cohesive zone model have the secondary influence on the analytical results. In the present analysis, we take $(\lambda_1, \lambda_2) = (0.15,\ 0.5)$. Moreover, for reducing the number of governing parameters, we take $\delta_{cn} = \delta_{ct} = \delta_c$, then from (5) and (6), one have $\Gamma_0^{\tau} / \Gamma_0 = \hat{\tau}/\hat{\sigma}$.

ENERGY BANLANCE AND ELASTIC-PLASTIC MECHANICS METHOD

The double cohesive zone model has been sketched by figure 2. The variation equation for the total system can be written as

$$\int_V \delta\varepsilon_{ij}.\sigma_{ij}dV = \int_V \delta\varepsilon_{ij}.D^e_{ijkl}\varepsilon^e_{kl}dV = \int_V \delta\varepsilon_{ij}.D^e_{ijkl}(\varepsilon_{kl}-\varepsilon^p_{kl})dV$$

$$= \sum_{k=1}^{3}\{\int_{S_k^+}\delta u_i.t_i dS + \int_{S_k^-}\delta u_i.t_i dS\} + WQ.\delta|\varDelta_1| = -\sum_{k=1}^{3}\int_{S_k}\delta|u_i^+ - u_i^-|.|T_i|dS + WQ.\delta|\varDelta_1|$$

$$= -\sum_{k=1}^{3}\int_{S_k}\delta|\delta_i|.|T_i|dS + WQ.\delta|\varDelta_1| \qquad (7)$$

Where S_k ($k=1,3$) are cohesive surfaces, (u_i, t_i) are the displacement and traction components on the cohesive zone surfaces, (δ_i, T_i) are the relative displacement and traction on the cohesive surfaces, see formulas (1) to (4) . $\varDelta_1$ is the displacement of the point acted by horizontal driving force Q.

Based on (7), one can develop the finite element method for scratch test problem. The incremental constitutive relation of plasticity usually is expressed as

$$\dot\sigma_{ij} = \frac{E}{1+\nu}\left\{\delta_{ik}\delta_{jl} + \frac{\nu}{1-2\nu}\delta_{ij}\delta_{kl} - \frac{(3/2)\Omega}{[1+(2/3)(1+\nu)H/E]\sigma_e^2}\sigma'_{ij}\sigma'_{kl}\right\}\dot\varepsilon_{kl} \qquad (8)$$

σ'_{ij} is deviator stress, $\sigma_e = \sqrt{3\sigma'_{ij}\sigma'_{ij}/2}$ is effective stress; for plastic loading $\Omega = 1$, otherwise $\Omega = 0$. H is plastic modulus. In uniaxial tension the film material has

$$\varepsilon = \sigma/E, \text{ for } \sigma < \sigma_Y; \quad \varepsilon = (\sigma_Y/E)(\sigma/\sigma_Y)^{1/N}, \text{ for } \sigma \ge \sigma_Y \qquad (9)$$

so that
$$H = E\{(1/N)(\sigma_e/\sigma_Y)^{1/N-1} - 1\}^{-1} \qquad (10)$$

Strap advance is assumed to occur in steady-state such that the stress and strain increment components can be expressed as
$$(\dot\sigma_{ij}, \dot\varepsilon_{ij}) = V(\partial\sigma_{ij}/\partial x_1, \partial\varepsilon_{ij}/\partial x_1) \qquad (11)$$

where *V* is velocity of crack tip during film delamination in x_1 direction. The formula (8) is independent of *V*. Plastic strain components can be expressed by stress and total strain as

$$\varepsilon^p_{ij} = \varepsilon_{ij} - D^{e\,-1}_{ijkl}\sigma_{kl} \qquad (12)$$

A numerical method [9] which employs iteration to satisfy condition (11) is used to directly obtain the steady-state solution. Similarly, in the present analyses, adopting the fundamental relations of tensors and matrixes, (7) can be changed into the finite element relations. The steps of solving the problem can be described as follows: (1) Adopting a plastic strain distribution (in first step, take $\varepsilon^p_{ij} = 0$), find displacement and strain. (2) Find stress distributions in plastic zone and unloading zone using (8), (11) and yielding condition $\sigma_e = Y$ (Y is current flow stress). (3) Find plastic strain by (12). Repeat procedures until a convergent solution is obtained.

Consider that the substrate material is elastic and Young's modulus and Poisson ratio are E_s and ν_s respectively. For further simplification, neglect the effect of mismatch of film and substrate materials, so that we take $(E_s, \nu_s) = (E, \nu)$ in the present analysis. During the steady-state advance of delaminated film strap, total work per unit length is QW; dissipated work per unit length along the separation cohesive surface is $\varGamma_0 W$; and along two shear cohesive surfaces it is $2t\varGamma_0^\tau$. Let plastic dissipation work be $W\varGamma_P$. According to energy balance under steady-state advance, we have

$$Q = \varGamma_0 + \frac{2t}{W}\varGamma_0^\tau + \varGamma_P \qquad (13)$$

For elastic case, $\varGamma_P = 0$. In principle, the interface separation work (interface fracture toughness) $\varGamma_0$ and the material shear work (or material shear strength) $\varGamma_0^\tau$ could be determined by experimental measurement. The normalized horizontal driving force Q during the steady-state advance of failure strap can be expressed by the related independent parameters as follows

$$\frac{Q}{\Gamma_0} = 1 + \left(\frac{2t}{W}\right)\left(\frac{\hat{\tau}}{\hat{\sigma}}\right) + \frac{\Gamma_P}{\Gamma_0} = f\left(\frac{E}{\sigma_Y},\frac{\hat{\sigma}}{\sigma_Y},\frac{\hat{\tau}}{\sigma_Y},\frac{t}{R_0},\frac{t}{W},N,\nu,\beta\right) \tag{14}$$

In（14）a reference length parameter has been introduced, whose definition is $R_0 = E\Gamma_0/[3\pi(1-\nu^2)\sigma_Y^2]$, characterizing the plastic zone size in small scale yielding.

SOLUTIONS AND ANALYSES

Three-dimensional elastic-plastic finite element calculation for the scratch test problem is carried out based on the concepts implemented in previous sections. The results and analyses are shown in the following. Figure 3 shows the relation of the normalized horizontal driving force (or applied work per unit area) to the maximum strength of separation and shear for two kinds of cohesive zones. The driving force changes with shear strength and separation strength are very sensitive, especially for large values of separation strength or

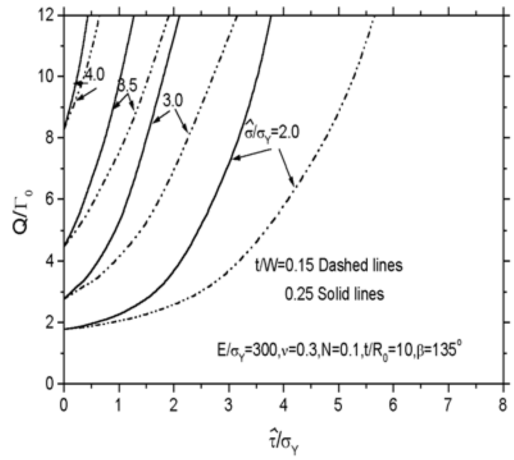

Figure 3: Scratch work vs. material parameters for low hardening film

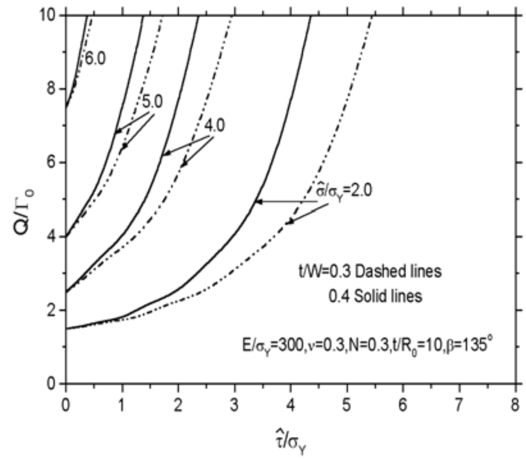

Figure 4: Scratch work vs. material parameters for high hardening film

shear strength. For the lower separation strength case, the horizontal driving force changes with the material shear strength slowly as shear strength increases, then sharply increases. For the higher separation strength, even a lower material shear strength will make the horizontal driving force increase very quickly. In the figure 3, the results of two different ratio of thin film thickness with the delaminated film width are compared. Clearly, the horizontal driving force changes sensitively with the ratios. The results correspond to the lower strain hardening exponent material, i.e., N=0.1. The separation cohesive energy along interface is taken as the normalized quantity. When the shear strength of material is zero and the elastic case is considered, the value of the normalized horizontal driving force (applied work per unit area) equals to unity. When the material shear strength is not zero, the normalized horizontal driving force will change linearly with the

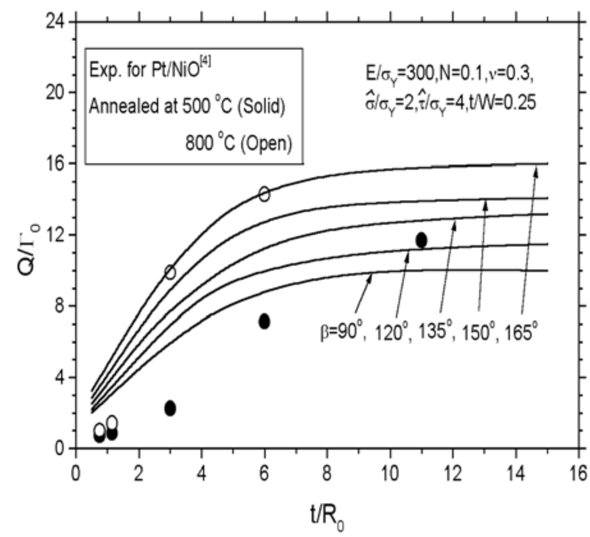

Figure 5: Scratch work vs. film thickness and indenter angles

shear strength from (14) for elastic case. Obviously, from figure 3, the energy contributed from plastic deformation is very high.

Figure 4 shows the results for the higher hardening thin film material case, N=0.3. The variations of the horizontal driving force with the material shear strength and the interface separation strength are similar to those of the lower hardening material. Clearly, the work dissipated in the plastic deformation for higher hardening material is lower than that for lower hardening material.

Figure 5 shows the relation of the driving force (applied work) changing with normalized thin film thickness. The curves are for different direction angles of indenter surface, $\beta = 90^o$, 120^o, 135^o, 150^o and 165^o. In the figure, the experimental results for the Pt/NiO film/substrate system and for the two kinds of techniques annealed at 500^{o}C and 800^{o}C from [4] are also shown. From figure 5, the horizontal driving force increases as thin film thickness increases and as the indenter angle increases. The indenter shape with the largest β corresponds to the high driving force. The simulation results are roughly consistent with the experiment results.

CONCLUDING REMARKS

By the detailed analyses in the present research, some important conclusions are obtained as follows: (1) Thin film plastic deformation has the important influence on the advance of delaminated film strap in the scratch test. (2) The interface separation strength and material shear strength have important influence on the failure of thin film/substrate system. (3) The horizontal driving force depends on the thin film or coating layer thickness. With the thin film thickness increase, the horizontal driving force increases and asymptotes to a stable value, which corresponds to the small scale yielding case.

When either the interface separation strength or the material shear strength is large, a strong shielding effect from plastic deformation can be produced when the failure strengths are increased. In other words, with any cohesive strength increase, it is difficult or even impossible to make a film failure strap advance due to the strong plastic shielding. Such a prediction from using the conventional elastic-plastic theory seems somewhat contradictory. Actually, for the strong separation strength of interface or for the high shear strength, or for both, a strong plastic strain gradient effect could dominate the crack tip fields [10]. A reasonable simulation for this behavior might be obtained by using the strain gradient plasticity theory. A success application of the strain gradient plasticity to the crack growth problem has been shown in [11].

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