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Fracture mechanics investigation on crack propagation in the nano-multilayered materials

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ABSTRACT

A set of new investigation method is proposed for the fracture mechanics experiments and analyses of nano-multilayered materials. The crack propagation behavior in a SiN/Cu nano-cantilever is investigated by fabricating a crack-like notch in the SiN layer. Two types of crack propagation behaviors are observed, including crack propagation in SiN layer and crossing-interface crack propagation through SiN/Cu interface. The interaction integral method combined with energy analyses is adopted for numerical simulation of the crack propagation behavior. The kinetic energy of the crack propagation is discussed. It is found that for the present brittle fracture process, the traditional Griffith criterion is not suitable and a new hypothesis based on the kinetic energy of the crack propagation is proposed that the crack will keep propagating until the accumulated kinetic energy is consumed totally to form new crack surface. Moreover, the hypothesis is consistent with the experimental results. It provides a significant thought for the analysis and prediction of nanoscale crack propagation behavior.

1. Introduction

Many advanced micro-mechanical and electronic devices are made from multilayers of different materials, and the size is even on the nanoscale. The investigation of fracture behavior is very significant to the design and safety analysis of nano-multilayered structures. However, the fracture mechanics experiments and the related analysis of this type of materials are still very limited.

The experiments of fracture behavior on the nanoscale are usually difficult to conduct. Previous works (Hirakata et al., 2007; Takahashi et al., 2008; Sumigawa et al., 2010b, 2010c; Yan et al., 2012) investigated the crack initiation at the edge of Cu/Si interface due to nanoscale stress concentration by developing a nano-cantilever bending specimen of the silicon/copper/silicon nitride (Si/Cu/SiN) multilayered materials. Sumigawa et al. (2010a, 2011) carried out a cyclic bending experiment by using a nano-specimen to investigate the interface fatigue strength. Moreover, the plasticity of a copper nano-component sandwiched between Si layer and SiN layer was experimentally evaluated by a cantilever beam specimen (Takahashi et al., 2008; Sumigawa et al., 2010b). Recently, a new fracture mechanism was revealed to investigate the crack propagation by *in situ* straining in nanocrystalline Au thin films, i.e. atomic migration (Wang et al., 2011). Even though more and more attentions have mainly been paid to the nanoscale fracture issues recently, we can see that, in the above experimental works, nearly no fabricated crack has been introduced into these nano-specimens, and the observations of nanoscale crack propagations are still rarely reported due to the difficulties from experimental aspects.

In addition to experimental investigations, the analysis methods of the fracture behavior of nanoscale specimens are also important. At present, continuum mechanics can be adopted to explain the fracture behavior in bulk (Rice, 1988; Hutchinson and Suo, 1992; Huang et al., 2004; Arai et al., 2007; Guo et al., 2012). However, its validity for nanoscale structures still needs to be further studied. The fracture behavior of nanoscale structures (such as some nano-film structures) with interfaces can be often met. Because of the mismatch of mechanical properties between the dissimilar materials, the bi-material interfaces are usually the weakest sites of delamination (Evans and Hutchinson, 1995). Taking advantage of a cohesive zone model (CZM), Yan et al. (2011) simulated the observed crack initiation and propagation along the Cu/Si interface with nanoscale stress concentration in the experiments conducted by Hirakata et al.

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(2007) and Sumigawa et al. (2010c) and examined the reliability of the CZM fracture model for nanoscale components. However, they have never investigated the fracture behavior of nanoscale structures with fabricated crack(s) previously. Using molecular dynamics (MD) simulations, Adnan and Sun (2010) investigated the crack formation process of a defective (with missing atoms) nanostructured material (NaCl), finding that single line Schottky defects would evolve into a planar crack under tensile loads. Zhang et al. (2011) conducted a series of atomic-scale simulation to investigate the influence of α/γ-iron phase boundary on crack propagation. Utilizing a combined atomistic-continuum approach, Chowdhury et al. (2013) developed a model for fatigue crack growth to address the physical processes contributing to crack advance. To investigate the atomic mechanism of the rarely seen nanoscale crack bridging behavior, molecular dynamics simulations were performed to show that during crack propagation twin boundaries are impinged upon by numerous dislocations from the plastically deforming matrix (Kim et al., 2012).

Besides, it is a tough issue to investigate crack propagation in rapid brittle fracture, especially on the nanoscale. A series of correlative works have been reported (Kalthoff et al., 1977; Freund, 1979; Broberg, 1989; Gao, 1996; Rosakis et al., 1999; Abraham and Gao, 2000; Guozden et al., 2010; Jia et al., 2012). Kalthoff et al. (1977) has experimentally investigated measurements of dynamic stress intensity factors for fast running and arresting cracks in double-cantilever-beam specimens, and observed a speed deceleration of the crack prior to arrest. Based on continuum mechanics, the Rayleigh wave speed is widely accepted to be the limiting speed of crack propagation (Freund, 1979; Broberg, 1989). Gao (1996) developed a concept of local limiting speed for dynamic crack propagation stemming from the standard nonlinear continuum mechanics approach. Rosakis et al. (1999) presented the direct experimental evidence that the shear cracks can propagate at speeds faster than the material shear wave speed when steady-state conditions were attained. Abraham and Gao (2000) and Gao et al. (2001) performed atomic simulations of crack propagation along a weak interface, showing that a mode II shear dominated crack can accelerate to the Rayleigh wave speed and then nucleate an intersonic daughter that travels at the longitudinal wave speed, which contradicts the general belief that a crack can travel no faster than the Rayleigh speed. Guozden et al. (2010) studied cracks traveling along weak interfaces by molecular dynamic method, finding that supersonic cracks are more common than has previously been realized both in Mode I and Mode III. Via theoretical analysis and numerical simulations, Jia et al. (2012) demonstrated in a straightforward way that non-equilibrium disturbance (e.g. force, displacement, energy, and so on) can propagate at a supersonic speed in discrete systems. Although crack propagation speed has been studied by some researchers, the kinetic energy of crack propagation on the nanoscale has been rarely discussed.

Previously, very limited experimental investigations have been conducted on the crack propagation behavior of nano-multilayered materials due to the difficulties in fabricating specimen and loading process. In this paper, a set of investigation method is proposed for the fracture mechanics experiments and analyses of nano-multilayered materials. The crack propagation behavior in a SiN/Cu nano-cantilever is investigated by fabricating a crack-like notch in the SiN layer. Two types of crack propagations are observed, including crack propagation in a single SiN layer and crossing-interface crack propagation in SiN–Cu layers. The interaction integral method combined with energy analyses is adopted for numerical simulation of the crack propagation behavior. The kinetic energy of the crack propagation is discussed.

2. Specimen and experimental procedure

2.1. Fabrication of the specimens

The specimens examined in this study are nanoscale cantilevers cut from multilayered film materials Si/Cu/SiN/Pt/C/W by using the focused ion beam (FIB) technique (Hitachi, FB2200). After removing the native oxidized layer on a Si substrate by argon ion etching, a Copper (Cu) layer with the thickness of 200 nm and a silicon nitride (SiN) layer with the thickness of 1000 nm are deposited on the Si substrate at rates of 24 and 10.5 nm/min by magnetron sputtering, respectively. Deposition is performed at a chamber pressure of 0.67 Pa. Platinum (Pt), carbon (C), and tungsten (W) layers are also deposited on the SiN layer to protect the SiN layer during the subsequent FIB processing.

In this study, two typical specimens are investigated. The geometric configurations and the loading conditions of Specimen 1 and 2 are shown in Fig. 1(a) and (b), respectively. The geometric parameters are provided in Table 1. The Cu layer is deposited between the hard Si and SiN layers with the thickness of 200 nm. The Si substrate is thick and tough enough to support the cantilevers without obvious deformation. In order to investigate the crack propagation behavior in the SiN layer, an initial crack-like notch is carved in the cantilever by FIB technique. Two typical specimens are fabricated successfully: one will be utilized to study the crack propagation behavior in the single SiN layer, and the other will be applied to study the crossing-interface crack propagation behavior in the SiN and Cu layers. It should be mentioned that it is very difficult to fabricate an ideal specimen with a crack which can be used to conduct the crack propagation experiment successfully.

2.2. Experimental procedures

The load P is applied to the SiN layer away from the Cu film by a diamond pyramid tip where the accuracy of the load system is 0.1 μN. The loading apparatus (Nanofactory Instruments AB, SA2000N) consists of a sample stage which can move in three orthogonal directions and a diamond loading tip with a micro-electromechanical system (MEMS) load sensor, as shown in Fig. 2. The moving speed of the stage is 5 nm/s. It is built in a transmission electron microscopy (TEM) specimen holder for experimental observation which is carried out with an accelerating voltage of 200 kV under a vacuum of 1.5×10^{-5} Pa. The displacement of the loading tip is precisely measured by means of the TEM observation.

3. Analysis method for the nano-cantilevers

In this paper, an interaction integral method will be adopted to obtain the crack-tip stress intensity factors (SIFs). The interaction integral, the 'cross terms' in the J-integral under superimposed load of the actual state and an auxiliary state, can be defined as (Yu et al., 2012)

$$I = \lim_{\Gamma \to 0} \int_{\Gamma} \left[\frac{1}{2} (\sigma_{jk}^{aux} \varepsilon_{jk} + \sigma_{jk} \varepsilon_{jk}^{aux}) \delta_{1i} - (\sigma_{ij}^{aux} u_{j,1} + \sigma_{ij} u_{j,1}^{aux}) \right] n_i d\Gamma, \qquad (1)$$

where u_j^{aux}, σ_{jk}^{aux} and ε_{jk}^{aux} are the auxiliary displacements, stresses and strains, respectively, and their definitions can be found in Yu et al. (2009), n_i is the unit outward normal vector to the contour Γ, the symbol δ_{ij} is Kronecker delta, and a comma denotes a partial derivative with respect to the coordinates.

The crack faces are traction-free for both the actual state and the auxiliary state. Therefore, as shown in Fig. 3, by defining an arbitrary weight function q with values varying smoothly from 1