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A numerical study on nano-indentation induced fracture of low dielectric constant brittle thin films using cube corner probes

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ABSTRACT

In this study, a finite element (FE) model of indentation induced fracture of brittle thin films on tough substrates using the cube corner probes is developed utilising the cohesive zone method. The model is specifically applied to brittle low dielectric constant (low-k) thin films and is corroborated by comparison to experimental results. It is shown that the model can decipher mechanisms of radial crack initiation and propagation during loading and unloading phases consistent with experiments. As such, the model lends itself to use as a platform for quantitative and mechanistic understanding of thin film mechanics and characterisation of their fracture properties.

1. Introduction

The implementation of ultra-low dielectrics constant (low-k) films has become essential for future technology nodes in the microelectronics industry. However, due to their lower mechanical strength, fractures and delamination are becoming major challenges faced by the semiconductor industry. Fracture mechanics paradigm has been widely applied to address some of the challenges related to thin film fracture. The classical fracture mechanics experiments including four point bending, double cantilever bending and end notched flexure tests have been widely applied to stacked films [1–7]. Nonetheless, as the technology requirements dictate the application of thinner films with inferior mechanical properties, conducting macroscopic fracture experiments becomes more and more cumbersome and also less relevant. Therefore, there is a need to develop more localised and robust methodologies such as indentation experiments that can be easily applied to thin films and inconvenient test sample configurations [8–9]. In this context, nano-indentation experiments constitute a robust methodology and have been applied successfully for estimation of various mechanical properties of thin films including elastic modulus and hardness [10–17], Poisson's ratio [18] and also fracture properties of thin films, including their cohesive fracture properties [19–21] and also adhesive properties relevant for film delamination [22,23]. Various types of pyramid shaped indentation probes have been employed for characterisation of thin film fracture toughness, including the Vickers, Berkovich and cube corner probes, all of which can potentially induce cohesive radial cracks in brittle thin films. One specific benefit of cube corner probes is that due to their more acute profile the influence of film plasticity is minimised and can be neglected in experiments [24–25]. In this context, the fracture toughness of compliant films coated on relatively rigid substrates, such as low-k films on silicon substrates, can be estimated empirically depending on the length of the radial crack, the indentation force and also the shape of the indentation probe [25].

Therefore, nano-indentation using cube corner probes constitutes a promising methodology for characterisation of cohesive fracture properties of low-k dielectric films which benefits from further investigation using numerical modelling approaches to help better understand the underlying mechanisms of crack initiation and propagation in low-k films. To this end, in the current study an FE model of thin film indentation using cube corner probes was developed and the influence of various mechanical and fracture properties related to the film and the substrate were investigated. In addition, the model was corroborated by comparison to experimental results on low-k films.

2. Materials and methods

2.1. Model geometry

An FE model of a cube corner probe indentation onto a brittle thin film coated on a relatively tough substrate was constructed using Abaqus 6.14 FEA package (Simulia, Dassault Systèmes) and analysed in Abaqus standard, see Fig. 1. A cube corner probe with a blunt edge (40 nm edge fillet radius) was constructed as a 3D discrete rigid part.

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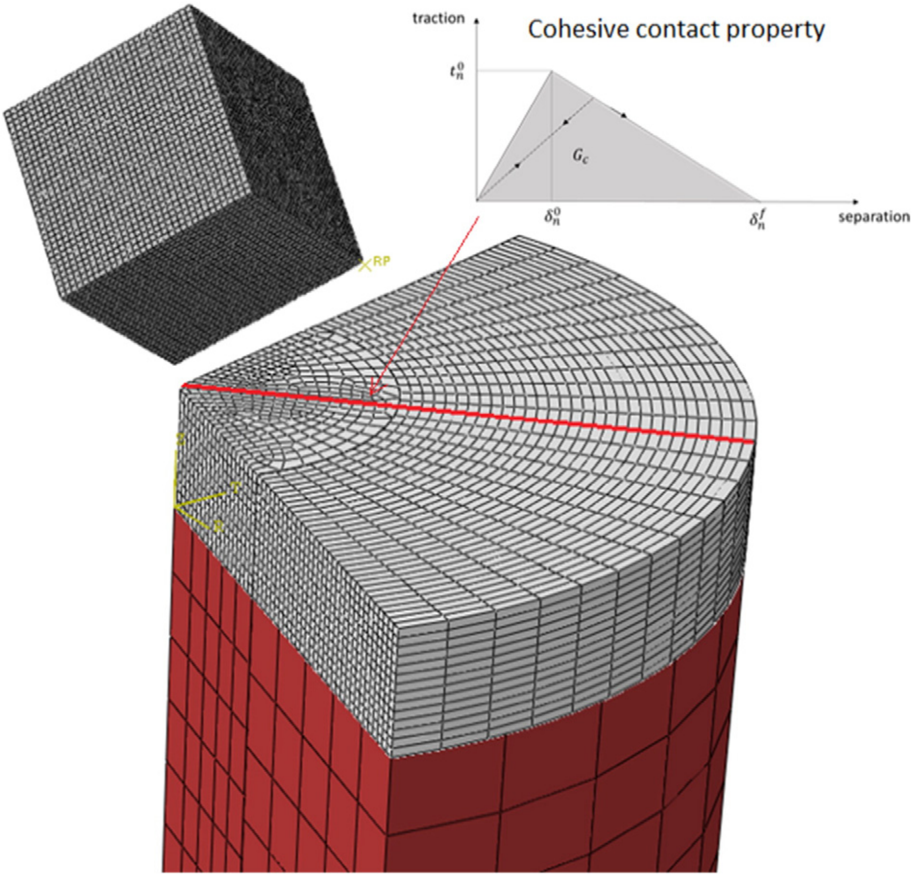

Fig. 1. The constructed FE model of thin film indentation with the cube corner probe. One third symmetry is used, (light grey) thin film (red) substrate. A cohesive contact property with linear traction–separation damage model is used to simulate the radial crack.

One third symmetry was employed to model the film-substrate assembly in order to minimise the computation cost. The film was modelled with a thickness of 600 nm and was composed of two half symmetry parts which were attached using a cohesive contact interaction at the plane of the radial crack and hence the radial fracture was modelled using the cohesive contact behaviour [26–29]. The film was assembled onto a 3 μm thick substrates using cohesive contact interaction in order to capture potential delamination of the film from the substrate. The radius of the film-substrate model was 2.6 μm and the element side length in the circumferential direction was as small as 14 nm at the centre of indentation where initial contact with the probe occurs. Element lengths in the radial direction were kept consistent however, so as to minimise any influence from the mesh size on the radial crack growth. The mesh size of the substrate was chosen relatively larger with a minimum element edge length of 180 nm. In total the film and substrate were discretized by 14,712 and 688 linear hexahedral incompatible mode elements of type C3D8I, respectively. Using the incompatible mode elements significantly improved the convergence and handling of the initial contact between the probe and the film when the sharp probe initiates the de-bonding process. The indenter probe was meshed with 6898 linear quadrilateral elements of type R3D4 and 38 Linear triangular elements of type R3D3. This discretization scheme was chosen based on a mesh sensitivity study and to ensure that potential element distortions did not occur at the contact region with the probe.

2.2. Material properties

Firstly, the property of 600 nm thick organo-silicate glass low-k film with a dielectric constant of 2.4 (OSG 2.4) which were known directly from nano-indentation experiments (i.e. Young's modulus = 8GPa, critical cohesive energy $G_C = 0.3$ J/m^2) were assigned to the film and mechanical properties of silicon (i.e. Young's modulus = 170 GPa) were assigned to the substrate and the model results were compared with the experiments to calibrate the cohesive damage model of the film for fracture simulations. As mentioned earlier, the cohesive contact property was used to simulate the radial cracks. The cohesive contact property allows simulating the degradation and failure of the bond between the two cohesive surfaces of the two half symmetry parts of the film by defining a contact property based on a cohesive damage traction-separation law. A damage initiation criterion and a damage evolution law need to be defined to capture crack initiation and propagation. A linear traction–separation damage model was employed for damage evolution together with a damage initiation criterion based on the maximum nominal contact stresses as shown in Fig. 1. The process of degradation begins when the contact stresses satisfy the maximum stress damage initiation criterion as follows:

$$\max\left\{\frac{\langle t_n\rangle}{t_n^0}\right\} = 1 \tag{1}$$

where, t_n^0 represents the peak values of the contact stress when the separation is purely normal to the interface. Given that the radial crack opening is mode I dominant, its response was found not to be sensitive to the choice of mode II and III initiation stress because of shear separation absence but it was found highly sensitive to the mode I initiation stress. This is why only the normal tractions are discussed herewith for the simulation of the radial crack. Of note, the compressive contact stresses are assumed not to initiate damage which is emphasized by