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A numerical analysis of flexure induced cylindrical cracks during indentation of thin hard films on soft substrates

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Abstract

In this paper, the fracture behavior of a thin hard film, perfectly bonded to a soft substrate, containing circumferential (cylindrical) cracks subjected to spherical indentation is studied using the finite element method. These cracks emanate upwards from the film–substrate interface and are driven by the flexure of the film over the soft substrate under indentation. The film is taken to be linear elastic while the substrate obeys an elastic–plastic constitutive model with linear strain hardening. Three values for the substrate yield strength are considered in the analysis. The variation of energy release rate and mode mixity are examined as functions of crack length and load, for cracks located near and away from the indentation axis. The results show that, when the crack length is small, predominantly mode I conditions prevail due to tensile radial stresses near the interface. As the crack length increases, the mode mixity gradually changes from mode I to II. For cracks located near the axis, the crack growth process is stable over a range of crack lengths up to about a third of the film thickness and thereafter becomes unstable. The role of the substrate yield strength on the above issues is investigated.

Keywords: Thin hard films; Substrate plasticity; Indentation fracture; Finite elements

1. Introduction

Surface coatings are used in modern technological applications, especially in situations where the substrate needs protection against the operating environment due to extreme thermal, chemical or erosive conditions. In particular, thin (hard) brittle films deposited on soft substrates may be subjected to various types of loading such as contact tractions. Thus, the use of hard coatings for enhancing the performance of components is usually accompanied by the risk of brittle failure. Hence, it is imperative to understand the mechanics of deformation and fracture of thin films, especially in response to contact loads, to design better coating systems.

In view of the dimensional smallness of thin films, depth sensing nanoindentation has become a popular technique in recent times to provide quantification of the mechanical properties of the film and the interface. Thus, determination of the elastic modulus and hardness of a coated sample from nanoindentation load–displacement characteristics is now well established [1], given the area function associated with the indenter tip. However, methods for obtaining the fracture toughness of the film or interface from these test results are not well developed. Since in most structural applications, the film is brittle, this persists as an important obstacle to thin film design.

One of the earliest approaches to resolving this problem was due to Marshall and Lawn [2] who gave a semi-empirical formulation for estimating the fracture toughness from data obtained during indentation by a Vickers indenter. In several experimental studies [3–5], steps or kinks in load–displacement curves have been observed and also shown to be associated with the formation of circumferential cracks around the indented zone. These cracks grow along cylindrical surfaces through the thickness in films having a columnar grain structure with the axes of the elongated grains being perpendicular to the film surface [4]. The nature of the crack systems that form during indentation of columnar TiN coatings on steel substrates has been investigated in some recent experimental studies [6,7]. Sriram et al. [8] performed a finite element simulation of spherical indentation of elastic films on elastic–plastic substrates to understand the mechanics of cylindrical cracks

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extending inward from the film surface. The role of substrate yield strength on stability of these cracks was investigated. The authors also proposed a method to combine the steps observed in experimental load–displacement data with simulation results to estimate the fracture energy of the film.

In a series of investigations, Lawn and co-workers [9–11] have reported the formation of different crack systems during spherical indentation of hard coatings bonded to soft substrates. These include circumferential cracks around the contact zone [9,10] on the film surface as well as circumferential or radial cracks which initiate from the film–substrate interface [9,11] and extend upward into the film. The latter occur due to the flexure of the film as a thin plate on the plastically deforming substrate, inducing tensile radial and circumferential stresses at the interface [11]. Indeed, Lee et al. [11] noted from their spherical indentation experiments on silicon nitride (Si_3N_4) bilayers that an increase in boron nitride (BN) content enhances quasi-plastic damage in the substrate, which results in increased flexure as well as higher transverse crack population in the film. In a very recent paper, Chai and Lawn [12] studied fracture mode transitions among the above crack systems by employing the stress fields prevailing in the indented film.

However, a systematic fracture mechanics analysis of flexure induced transverse cracks emanating upwards into the film from the interface during indentation has not been undertaken. Only such an analysis will enable understanding the role of substrate plasticity on the initiation of these cracks as well as their propagation behavior. To this end, finite element analyses of spherical indentation of a thin brittle film perfectly bonded to a ductile substrate and containing circumferential (cylindrical) cracks as mentioned above are performed in this paper. The film is taken to be linear elastic while the substrate obeys an elastic–plastic constitutive model with linear strain hardening. Attention is focused on the effect of substrate yield strength and crack location on the crack driving force as well as mode mixity prevailing near the tip.

2. Modeling aspects

A schematic of the model used for the analysis is shown in Fig. 1. The illustration depicts an axisymmetric section of a thin elastic film of thickness t_f resting on an elastic–plastic substrate being indented by a spherical indenter of radius R_i. The film contains a transverse cylindrical crack of length c located at a radial distance R_c from the axis of indentation, which emanates upwards from the film–substrate interface. The reason for assuming the crack surface to be vertical in Fig. 1 is due to its relevance to the important class of films with columnar grain structure such as TiN, wherein cracks can grow along vertical grain boundaries [4,6,7]. Further, even in other types of films like Si_3N_4, the flexure induced cracks propagating upwards from the film–substrate interface underneath the indenter do not show significant inclination to the normal to the interface [10,11].

The axisymmetric model is used in the finite element analysis which is based on an updated Lagrangian formulation [13]. The ratios of the radial dimension of the film–substrate system and the substrate thickness to the indenter radius, R_s/R_i and t_s/R_i, are both chosen as 75, so that boundary effects do not influence the stress distribution near the indented region. The indentation load, displacement and contact radius are denoted as P, h and a, respectively (see Fig. 1). The ratio t_f/R_i is taken as 1.5 and two normalized radial locations, $R_c/R_i = 0.045$ and 0.45, are chosen for introducing the cylindrical cracks. These locations were selected so that, at the maximum indentation load considered here, the cracks would lie inside the zone of contact as observed in the experiments of [7,10,11]. It is understood [12] that these cracks are primarily driven by radial and transverse shear stresses prevailing in the indented film–substrate system (see Fig. 2(A) and (B) below). The fracture analysis is performed for a range of crack lengths varying from $c/t_f = 0.03$ to 0.6 for each radial location R_c. The objective is to compute the energy release rate as a function of crack length and load. This will enable understanding the stability of propagation of these cracks, as well as predicting the crack growth history (i.e., crack length as a function of load) during the stable crack extension regime [14].

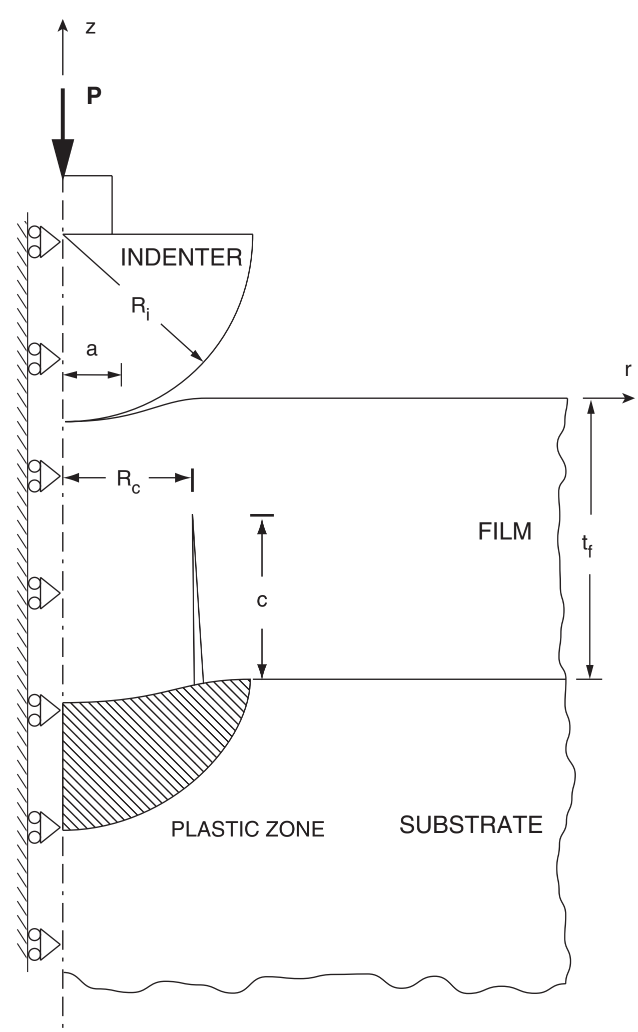

Fig. 1. Schematic of the model used in the fracture analysis. The illustration shows an axisymmetric section of a flexure induced transverse crack of length c emanating upwards from the interface at a radial location R_c.