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Detailed modelling of delamination buckling of thin films under global tension

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Abstract

Tensile specimens of metal films on compliant substrates are widely used for determining interfacial properties. These properties are identified by the comparison of experimentally observed delamination buckling and a mathematical model which contains the interface properties as parameters. The current two-dimensional models for delamination buckling are not able to capture the complex stress and deformation states arising in the considered uniaxial tension test in a satisfying way. Therefore, three-dimensional models are developed in a multi-scale approach. It is shown that, for the considered uniaxial tension test, the buckling and associated delamination process are initiated and driven by interfacial shear in addition to compressive stresses in the film. The proposed model is able to reproduce all important experimentally observed phenomena, like cracking stress of the film, film strip curvature and formation of triangular buckles. Combined with experimental data, the developed computational model is found to be effective in determining interface strength properties.

Keywords: Buckling; Delamination; Finite elements; Mechanical testing; Thin film

1. Introduction

The interface properties of thin, brittle films on compliant substrates are of great interest in applications such as hard protective coatings, gas barrier coatings, thin film transistors, flexible electronics and sensors. In these applications, interfacial adhesion dominates the mechanical performance where high adhesion is desired over poor adhesion. While there are several techniques available to measure the interfacial properties of thin films on rigid substrates, including nanoindentation [1,2], four-point bending [3] and spontaneous buckle delamination [4], it can be difficult to apply the same techniques to compliant polymer substrate systems [5]. Currently, the most commonly used techniques to assess interface properties of a thin film on a compliant substrate is to use bending experiments [6] or uniaxial tensile straining to induce film fracture and delamination in the form of buckles [7–9]. The tensile straining technique is based on the fragmentation test and described by shear lag theory [10]. Both adhesion measurement approaches (bending and tensile straining) rely on accurate mathematical models of the experimental process to determine the interface properties.

Many theoretical models have been developed over the years to describe brittle thin film fracture [4,11–15]. These models have been able to explain the failure criteria of thin films on a range of substrates due to thermal or mechanical strain. Another set of modelling efforts has focused on the buckling phenomena of films on rigid, i.e. very stiff, substrates [4,16,17]. The most successful theory is that of Hutchinson and Suo [4] to measure the interfacial adhesion

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using only the dimensions of the buckle and the elastic properties of the film. In this case, the buckles form spontaneously due to high residual stresses in the film or can be triggered by indentation. With respect to films on elastomer substrates, the wrinkling of films [18–20] is of great interest due to the possibility of providing more "stretchability" to flexible electronics [21]. The combination of models to take into account the fracture and buckling of brittle thin films on compliant polymer substrates under tensile strain and to help describe interfacial properties, as in this work, is relatively new. The existing approaches are based on two-dimensional (2-D) models [7] or shear-lag theory [9], and are thus limited in applicability. Particularly in the case of the uniaxial tensile test, as considered in this paper, 3-D effects play a dominant role that never can be achieved by 2-D models.

An analytical model based on an energy balance is able to relate measured buckle geometries from a tensile straining experiment to the adhesion energy of the interface [7]. However, this model was developed as a 2-D model and does not accurately capture the real interface failure or, consequently, buckling behaviour. Experiments have shown [7,8] that buckling and the associated delamination process are initiated and driven by interfacial shear in addition to compressive stresses in the film. Motivated by the deficiencies of the current 2-D models, the goal of this paper is to demonstrate a computational multi-scale 3-D finite element simulation of the experimental process. This new approach uses a two-stage model, which is able to capture all of the important experimentally observed effects, i.e. correct load transfer between film and substrate before and after cracking of the film, shear-stress-induced local out-of-plane deformation of the film and mixed mode delamination. Careful consideration of these 3-D effects is required for a sufficiently accurate determination of initial fracture stress and strain, initial buckling strain, etc. A macromodel comprising the tensile test specimen is analysed first, delivering boundary conditions for the micromodel of a single localized buckle. The modelling strategy involves cohesive zone elements to model the interface between the film and the substrate. The determination of interface properties, i.e. parameters of the cohesive elements, from the finite element model together with experiments is therefore an inverse problem that can be solved by conducting a parameter study.

2. Finite element modelling of the experimental process

In the uniaxial tension tests performed by Cordill et al. [7,22], specimens of a 100 nm chromium film, subsequently called "film", on a 50 μm polyimide substrate, subsequently called "substrate", with effective dimensions of 10 mm times 20 mm, were strained with a constant strain rate in a low-load tensile straining device (Kammrath & Weiss, Dortmund, Germany) and observed inside a scanning electron microscope. Channel cracks transverse to the straining direction initiate at a global strain of 0.4% and, with increasing strain, cracks continue to form until saturation spacing is obtained. The saturation crack spacing is 2.8 ± 0.9 μm (Fig. 1a). The different elastic properties of the two laminate layers lead to an observable curvature of the specimen. Additionally, due to the mismatch of the Poisson's ratio between the film ($\nu_f = 0.21$) and substrate ($\nu_s = 0.34$), uniaxial straining leads to compressive stresses transverse to the tensile direction in the film. At a global strain level of 10%, where both materials are in the plastic regime, buckles form in the film strips, causing interfacial failure between the film and the substrate. Buckles generally form in two shapes, rectangular (Fig. 1b) and triangular (Fig. 1c). The buckles will also form cracks at their apex (the top of the buckle) due to the brittle nature of the film and tensile bending stresses. This study will only address non-cracked buckles as the buckles initially form without cracking.

2.1. Macromodel

Macromodels are used to determine the cracking stress in the film and to gain boundary conditions for a micromodel. For these purposes, two different macromodels are required. In both models shell elements are used to represent a quarter of the symmetric tension test specimen (see Fig. 2). Symmetry boundary conditions are used on the edges in the symmetry planes. The loading edge is clamped and translated in the x-direction, modelling the global straining of the test specimen. The analysis is displacement controlled and starts from an undeformed, stress-free initial state, not taking into account any residual stresses, which might be present in the specimen due to the deposition process.

The first macromodel is used to determine the cracking stress of the film, which is the stress state at the global strain level at which cracking is experimentally observed, being 0.4%. At this strain level both materials, substrate and film, are assumed to be in the elastic regime. The specimen is modelled by composite shell elements with bilinear interpolation functions and a total of 11 integration points over the thickness; one integration point represents the film material and the rest represents the substrate. The determined maximum principal stress in the film at the global strain level of 0.4% is the determined cracking stress.

After the film has cracked transversely to the global straining direction, it loses its stiffness in this direction. Therefore, in a second macromodel, the film strips separated from each other by the cracks perpendicular to the global straining direction can be modelled by truss elements on the shell node lines in the y-direction. Truss and shell elements use shared nodes located on the shell reference surface. To accurately model the bending stiffness of the composite, an offset of $(h + t)/2$ is used for the truss elements (see Fig. 2). Comparisons of the results achieved from this model with the results obtained from a model, in which the cracked film is modelled as an orthotropic shell with no stiffness in the x-direction, have confirmed the correctness of the "truss" model. The analysis is started from an undeformed, initially stress-free state. This is