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Parametric computational analysis of indentation-induced shear band formation in metal-ceramic multilayer coatings

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ABSTRACT

Shear band formation in multilayer thin-films subject to nanoindentation is studied numerically. The material system analyzed here is composed of alternating aluminum (Al) and silicon carbide (SiC) nanolayers, above a silicon (Si) substrate. Finite element models are developed to investigate system parameters that influence behavior of the shear band phenomenon. By introducing strain softening into the material model for the relatively hard ceramic layers, shear bands can be seen to emerge from the indentation site in the computational analyses. Effects of post-yield material parameter variations on the initiation of plastic instability are examined. Several geometric variations are also investigated, including the effect of relative layer thicknesses, homogeneity, layer order, and number of layers. The chain events that lead to shear band nucleation are postulated. Broad implications are noted, along with possible directions for future work.

1. Introduction

Multilayer thin-film coatings offer mechanical property advantages over homogeneous material films. Alternating metal and ceramic nanolayers to create a composite structure of relatively softer and harder materials, respectively, yields benefits including improved strength and toughness, increased wear and fatigue resistance, and more favorable damage tolerance characteristics. These advantages generate a wide application space from tooling to electronics [1–8]. At present, the leading methods for characterizing thin-film mechanical properties rely on nanoindentation techniques, most commonly to derive Young's modulus and hardness [9]. However, these methods were established to characterize homogeneous materials. Multilayered structures are inherently more complex, introducing complicated internal deformation and damage behaviors which may affect the derived mechanical property or interpretations in ways not currently understood. For example, historical nanoindentation techniques assume that elastic recovery occurs during the indentation unloading phase, devoid of further plastic deformation. Study has revealed this assumption to be untrue of metal-ceramic multilayered thin films, which exhibit plastic deformation during the unloading phase [10]. Prior work in this area has also investigated elastic modulus, hardness, imperfect layer geometry, and delamination [3,5,10–12].

Fig. 1 shows a scanning electron micrograph, which exposes shear bands within the structure of a nanoindented and sectioned aluminum (Al) and silicon carbide (SiC) multilayer coating [10]. The shear bands appear to initiate near the tip of the indentation and propagate downward on both sides. The localization of deformation was strong enough to sever the hard ceramic layers. Similar phenomena were observed in other post-indented cross sections of the same material system [11], as well as in other multilayers such as Al/Si_3N_4 [13].

This localization of plastic strain in the form of banded structure has not been analyzed in previous finite element models of Al/SiC multilayers. In these prior cases, the SiC material is modeled as elastic-perfectly-plastic [3,10,14,15]. In contradiction, the experimental work of Deng et al. [1] implies that the thin SiC layers, when subject to uniaxial loading, exhibit strain softening after yielding. Our exploratory work illustrated that the nucleation of shear bands can be facilitated by incorporating SiC strain softening behavior into the finite element model [16]. The present study therefore builds on and expands the previous work in great detail. The background information from the preliminary work is also included in this paper. The primary objective of the present systematic study is to investigate the effects of material parameters, softening characteristics, and layer geometry on indentation-induced shear bands through parametric computational analyses.

2. Numerical model

A finite element model of nanoindentation was created and performed using ABAQUS (Version 6.14, Dassault Systemes Simulia Corp., Providence, RI, USA). See Fig. 2 for the model configuration schematic. While a Berkovich nanoindenter was used in previous experimental

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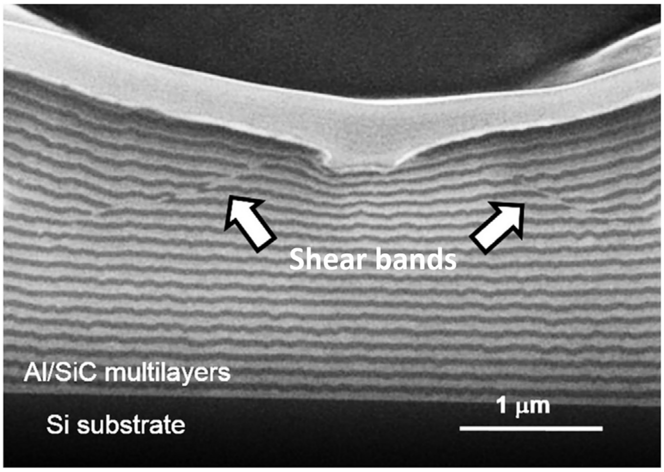

Fig. 1. Cross-sectioned scanning electron micrograph showing shear bands (highlighted by arrows) in Al/SiC thin-film multilayers after nanoindentation [10].

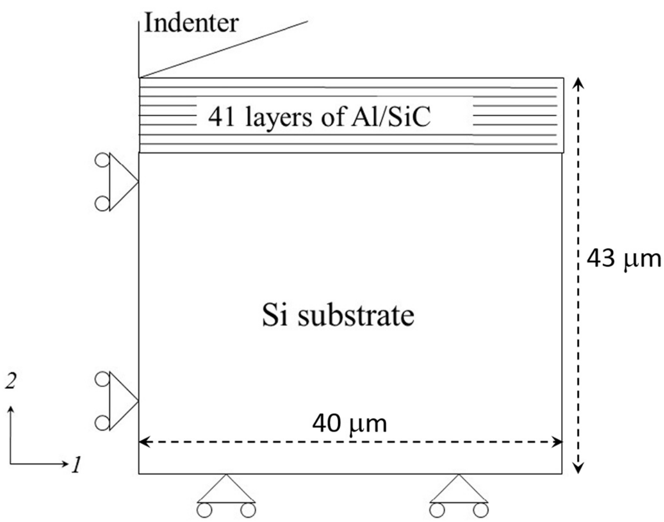

Fig. 2. Schematic of the axisymmetric finite element model, with symmetry axis and boundary conditions shown for the 41 alternating Al/SiC laminates on a Si substrate. The individual Al and SiC layers are 50 nm thick.

work [10], the model employs a conical diamond indenter in order to allow for a two-dimensional, axisymmetric representation of the setup. The 1-axis represents the radial direction and the 2-axis represents the axial direction along which the indenter moves. The conical indenter had a semi-angle of 70.3° to achieve the same projected contact area as a Berkovich nanoindenter. Note that some detailed geometric features occurred in an actual 3D experiment may not be fully captured with the current approach. However, the axisymmetric assumption is still able to represent the overall deformation pattern well, including the shear band configuration observed in Fig. 1. The model contained 41 total alternating layers of Al and SiC, with Al being the topmost layer, mimicking the configuration of the experimental film. The bilayer period was 100 nm, with equal individual layer thicknesses of 50 nm unless otherwise specified herein. The multilayers were situated atop a silicon (Si) substrate. The interfaces were modeled as perfectly bonded; no initial defects were included in the model. The radius of the total structure (Al/SiC film and Si substrate) was 40 μm, with an overall height of 43 μm. The left edge of the model was the axis of symmetry, with constraints allowing freedom of displacement solely in the 2-direction. The bottom edge of the substrate was constrained to allow displacement solely in the 1-direction. The remaining two edges were free in both directions. Frictional contact was assumed for contact between the indenter and the top Al layer. The coefficient of friction was 0.1 [17,18]. At minimum, 184,000 axisymmetric linear elements were used in the model when layers were of equal thicknesses, and minimum of 210,000 when layer thicknesses were unequal. The finest mesh resolution was near the indentation site (square shaped elements with side length 5 nm), with coarser elements located relatively far from the area of deformation. The mesh convergence was checked through the converged indentation response resulting from meshes with different extents of refinement [10].

The Young's modulus values utilized for Al and SiC layers were 59 GPa and 277 GPa, respectively, based on experimental measurements of the respective thin films [1,19]. The Al modulus is on the order of 20% lower than that of bulk Al, which is likely due to defects introduced by the vapor deposition technique used to fabricate the layers, including microcracks in the grain boundaries [20]. The SiC modulus is on the order of 40% lower than that of its crystalline bulk counterpart [2,19], which may be caused by the amorphous structure generated through the vapor deposition process [1,3]. Poisson's ratio for Al and SiC were 0.33 and 0.17, respectively. The plastic response of Al was derived from experimental loading data [1,10], and can be seen in Fig. 3a. Rate-independent isotropic elastic-plastic response was assumed, with plastic yielding adhering to the von Mises criterion with isotropic hardening and incremental flow theory. The Si substrate and diamond indenter are assumed as elastic materials. The Young's

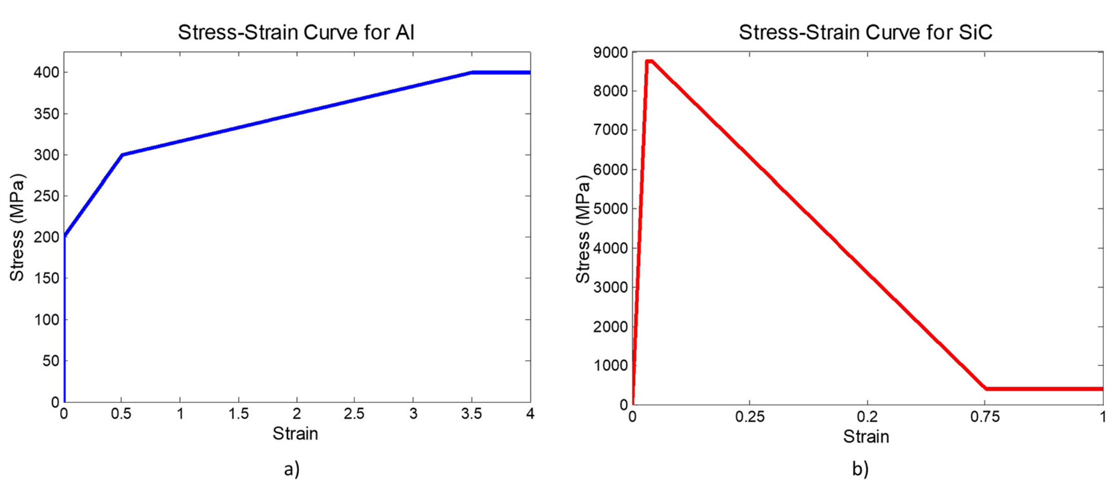

Fig. 3. Stress-strain input curves for a) the Al material model, and b) the strain softened SiC material model [16].