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Indentation behavior of multilayered thin films: Effects of layer undulation

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ABSTRACT

The behavior of aluminum/silicon carbide multilayered thin films in response to nanoindentation loading is studied. The effect of undulating layer geometry on indentation derived hardness and modulus, and stress/strain field development, is investigated using the finite element method. Two regular waveforms that are 180° out-of-phase are used to represent the undulating features of the SiC layers. The derived hardness and modulus are shown to be sensitive to the undulating layers and the phase of the waveform used to describe these layers. Undulating layers create bands of tensile and compressive axial stress that is significantly different from the flat layers. The amount of equivalent plastic strain in the Al layers is increased. Lastly, the unloading-induced plasticity in the Al layers is amplified with the presence of undulating layers.

1. Introduction

Multilayer coatings consisting of alternating ductile metal and high-strength ceramic thin films can possess superior mechanical properties such as high toughness and high damage tolerance, and thus these coatings have been a subject of intensive research [1–11]. Mechanical characterization of thin-film and coating materials relies primarily on nanoindentation. However, complexity arises when the indentation technique is applied to multilayered thin films. This is due to the high degree of heterogeneity pertaining to the soft/hard arrangement along with the large interface areas. The deformation field will be different from that of a homogeneous thin film. Internal damage may also be induced by the indentation loading itself [10,12–14].

Numerical finite element analyses have been conducted on the aluminum (Al)-silicon carbide (SiC) nanolaminates, to examine the internal deformation field and its correlation with the overall indentation response [15,16]. It was found that layered thin-film structure responds to indentation loading in a complicated manner. Unique hardness and trustworthy elastic modulus values (derived from the indentation test) may not be obtained, even if the indenter penetrates deep into many layers [16]. Despite the predominant compressive stresses directly below the indentation contact, significant tensile stresses along the vertical direction were found to exist at certain locations, which can explain local fracture observed experimentally in post-indented specimens. Furthermore, plastic deformation in the Al layers continues to occur during the unloading phase of indentation modeling. This was attributed to the internal mechanical constraint resulting from the hard SiC layers in the composite, as well as the development of special stress pattern within the layers. Although the finding was based on numerical modeling, it serves to raise awareness that, in actual indentation testing the unloading process may no longer be considered simple elastic recovery as in a homogeneous material. The same study also concluded that, when performing numerical modeling of indentation loading, it is important to incorporate the explicit multilayered structure rather than using a homogenized approach.

The present study seeks to extend the previous work and examine the effect of imperfect layer geometry on the nanoindentation response. Specifically, we consider the undulating (wavy) appearance of the layers, which inevitably exists when the individual layer thickness is in the nanometer range. Fig. 1 shows an example of layered Al and SiC films above a silicon (Si) substrate, with the individual nominal film thickness of 50 nm [17]. The interfacial roughness is due to the newly deposited SiC following the surface contour of the underlying Al film, which has the columnar grain structure. How this layer undulation can quantitatively affect the indentation behavior is unknown and is the primary objective of this study. Specifically, we construct numerical models of different extents of undulation and compare the indentation response and internal deformation fields with those from the perfect (flat) layer geometry. Implications of the numerical findings to physical experimental measurements are also discussed.

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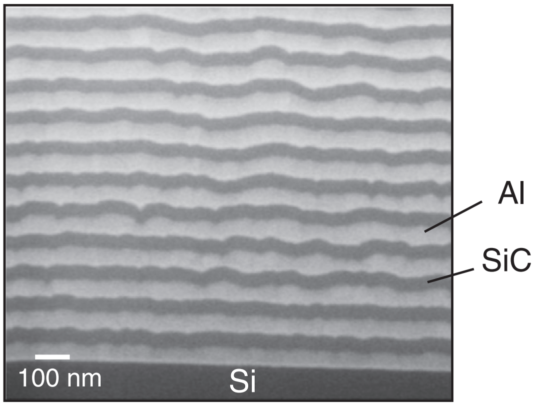

Fig. 1. SEM Cross section of Al/SiC multilayer thin films on a Si substrate [17].

2. Model description

The finite element model used in the indentation analysis consists of 41 alternating Al and SiC thin films on a substrate of Si. This corresponds to the actual nanolayered system studied previously [16]. A schematic of the baseline model, with a perfect geometry (no undulation), is shown in Fig. 2. Both the top layer (to be in contact with the indenter) and the bottom layer (adjacent to the Si substrate) are Al. A conical diamond indenter with a semi-angle of 70.3° is assumed. This indenter geometry results in the same projected contact area, for a given depth, as that of a Berkovich indenter in common nanoindentation experiments. Use of the conical indenter is a practical way to model the indentation process in a two-dimensional setting [18]. The model is axisymmetric, with the left boundary being the symmetry axis. The overall size of the entire specimen is 40 μm in lateral span (radius) and 43 μm in height. The thicknesses of the individual Al and SiC layers are 50 nm each. During deformation the left and bottom boundaries are allowed to displace only in the axial and radial directions, respectively. The right boundary is not constrained. The top Al surface, when not in contact with the indenter, is also free to move. When contact with the indenter is established, the surface portion engaged by the indenter follows the shape of the indenter. The coefficient of friction between the indenter and the top surface is 0.1, which is a typical value for the diamond/metal contact surface [19,20].

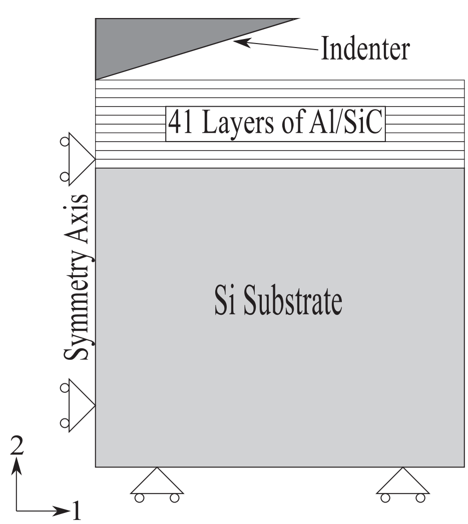

Fig. 2. Schematic showing the Al/SiC laminates above a Si substrate and the boundary conditions used in the axisymmetric model. The left boundary is the symmetry axis. The entire specimen is 40 μm in lateral span (radius) and 43 μm in height. Each individual Al and SiC layers are 50 nm thick.

To simulate the undulated layer geometry, two regular waveforms of the SiC layers are considered in the multilayer part of the model, shown in Fig. 2. The free surface of the topmost Al film and the interface with the Si substrate are kept perfectly flat. The two waveforms considered are 180° out-of-phase and are referred to as the “crest” and “trough” models. These labels refer to the point on the wave that is at the symmetry axis, i.e. the crest of the waveform of the SiC layer is at the symmetry axis in the “crest” model, and similar for the “trough” model. For each of these two models, each waveform has 60 cycles in the lateral direction, which is equivalent to a wavelength of 0.67 μm. The amplitude of each waveform varies from 10% to 50% of the thickness of a single SiC layer.

Fig. 3 shows a representation of the crest and trough waveform geometries at the indentation location. In images Fig. 3a and b, the solid black lines represent the original flat geometry, the colored lines represent the crest and trough type SiC layers, respectively, and the dotted lines represent the centerline of the SiC layer. The ordinate represents the axial coordinate of the geometry and the topmost free surface of Al is at 43 μm. The top surface of the first SiC layer is displaced at distance δ while the thickness of the layer is held constant at 50 nm. This profile is then propagated through the rest of the layers. An example of the mesh near the free surface of the nanolaminate, for both a crest and trough model, is shown in Fig. 4.

A total of 125,340 fully integrated linear axisymmetric elements are used in the nanolaminate model, with a finer mesh size near the upper-left corner of the test material. The element size near the indenter is 5 nm and increases in size far from the indenter. The indenter consists of 7,454 elements with an element size of 10 nm near the tip. The mesh was created using CUBIT (Sandia National Laboratories, Albuquerque, NM). The finite element program ABAQUS (Version 6.12, Dassault Systemes Simulia Corp., Providence, RI) was used to carry out the analysis.

The Young's moduli for Al and SiC are assumed to be 59 GPa and 277 GPa, respectively. Nanoindentation of single-layer Al and SiC films provided the moduli for these materials. The somewhat lower modulus of SiC, relatively to crystalline SiC (which is around 410 GPa), is due to the fact that the physical vapor deposited SiC layers in the present

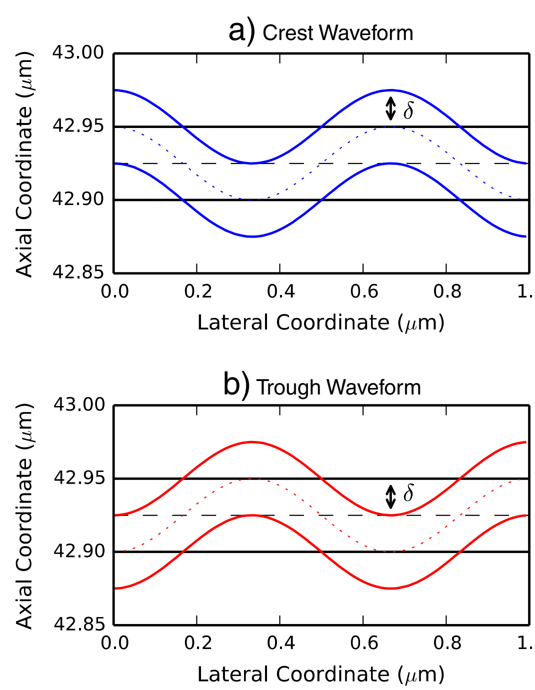

Fig. 3. Representative waveform images for the (a) crest model and (b) trough model. The amplitude is represented by δ.