Surface & Coatings Technology 303 (2016) 3–11

Contents lists available at ScienceDirect

Surface & Coatings Technology

journal homepage: www.elsevier.com/locate/surfcoat

Delamination analysis of metal–ceramic multilayer coatings subject to nanoindentation

Ryan D. Jamison [a,b], Yu-Lin Shen [a,*]

[a] Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM 87131, USA
[b] Component Science & Mechanics, Sandia National Laboratories, Albuquerque, NM 87185-0346, USA

ARTICLE INFO

Article history:
Received 26 October 2015
Revised 15 January 2016
Accepted in revised form 21 January 2016
Available online 22 January 2016

Keywords:
Nanoindentation
Multilayer coating
Delamination
Finite element analysis

ABSTRACT

Internal damage has been experimentally observed in aluminum (Al)/silicon carbide (SiC) multilayer coatings subject to nanoindentation loading. Post-indentation characterization has identified that delamination at the coating/substrate interface is the most prominent form of damage. In this study the finite element method is employed to study the effect of delamination on indentation-derived hardness and Young's modulus. The model features alternating Al/SiC nanolayers above a silicon (Si) substrate, in consistence with the actual material system used in earlier experiments. Cohesive elements with a traction–separation relationship are used to facilitate delamination along the coating/substrate interface. Delamination is observed numerically to be sensitive to the critical normal and shear stresses that define the cohesive traction–separation behavior. Axial tensile stress below the edge of indentation contact is found to be the largest contributor to damage initiation and evolution. Delamination results in a decrease in both indentation-derived hardness and Young's modulus. A unique finding is that delamination can occur during the unloading process of indentation, depending on the loading condition and critical tractions.

1. Introduction

Coatings involving hybrid materials can offer intriguing properties or functionalities. One form of hybrid materials commonly encountered in natural and engineered structures is multilayers. With a total thickness of up to tens of microns and individual layer thicknesses of a few to hundreds of nanometers, these coatings see a wide range of applications including ultrahigh-strength materials, optical devices, high-performance capacitors, thermo-electric materials, high wear resistance and low friction coatings for gears, bearings, cutting tools, and thermal protective layers in aircraft and automobile engines [1–8]. In particular, thin films consisting of alternating layers of metal and ceramic can offer higher strength-to-weight ratios, less friction and wear, higher operation temperatures, corrosion resistance, and fracture toughness compared to homogenous metallic or ceramic coatings. Therefore, designing and manufacturing metal–ceramic multilayers at the micro- and nanoscales are attractive strategies for developing a new generation of protective and infrastructure coatings, and thus have been subjects of intensive research [9–15].

Mechanical characterization of thin film and coating materials relies primarily on the nanoindentation technique. However, the scale and complexity of multilayer coatings often make it difficult to interpret nanoindentation data. 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 differ from that of a homogeneous material on which the indentation theory is based. Further, internal damage may also be induced by the indentation loading itself [16–22]. An example is shown in Fig. 1, which is a cross-section transmission electron microscopy (TEM) image of multilayer aluminum (Al) and silicon carbide (SiC) films above a silicon (Si) substrate, directly below the indentation site after nanoindentation testing [17]. The individual Al and SiC layers were nominally 50 nm thick, and loading was carried out by a Berkovich indenter to a maximum indentation depth of 1000 nm. It can be seen that a symmetric pattern of damage exists. Two mid-level cracks appeared below the edge of the indentation. Further below, prominent delamination of the multilayer/substrate interface has also occurred. It is worth mentioning that, aside from serving as a model system to study metal–ceramic multilayers, the Al/SiC multilayer system is also being considered as reflective coatings in ultraviolet applications [23,24].

One immediate question is how the internal damage would influence the indentation-measured properties, such as hardness and elastic modulus. It is also unclear at what stage of the nanoindentation testing did cracking occur. It is virtually impossible to answer these questions by common experimental observations. In the same material system, any experimentally measured quantities will have been affected by the damage already (without a "clean" set of results to compare with). Therefore, in this study we employ numerical finite element modeling to study the

* Corresponding author.
E-mail address: shenyl@unm.edu (Y.-L. Shen).

http://dx.doi.org/10.1016/j.surfcoat.2016.01.038
0257-8972/

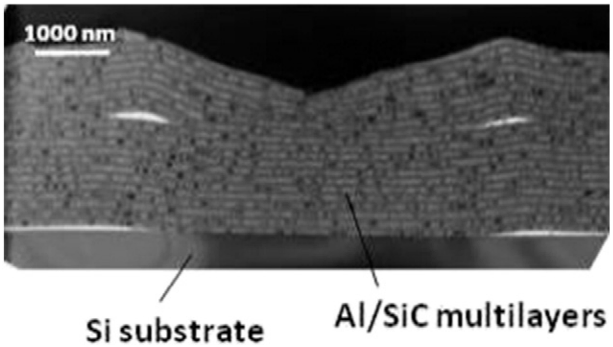

Fig. 1. TEM image of post-indented Al/SiC multilayers, revealing indentation-induced internal cracks and permanent deformation [17].

evolution of delamination and its effect on indentation response. Cohesive zone elements were built into the model at the coating/substrate interface, to allow for crack development during indentation loading. Comparisons of results with and without the cohesive zone will then provide quantitative insight to the effect of cracking. The effects of cohesive zone model parameters were also investigated.

2. Model description

The finite element model consists of 41 alternating Al and SiC thin films on a substrate of Si. This geometry corresponds to the actual multilayer system shown in Fig. 1 studied previously [16,17]. A schematic of the model 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 [25]. 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. In addition to the multilayer model, a separate reference model is also used. The reference model consists of a 1 μm-thick single-layer Al film on the same Si substrate. The reference model is used to determine if the indentation model is sensitive to cohesive elements at the Si interface.

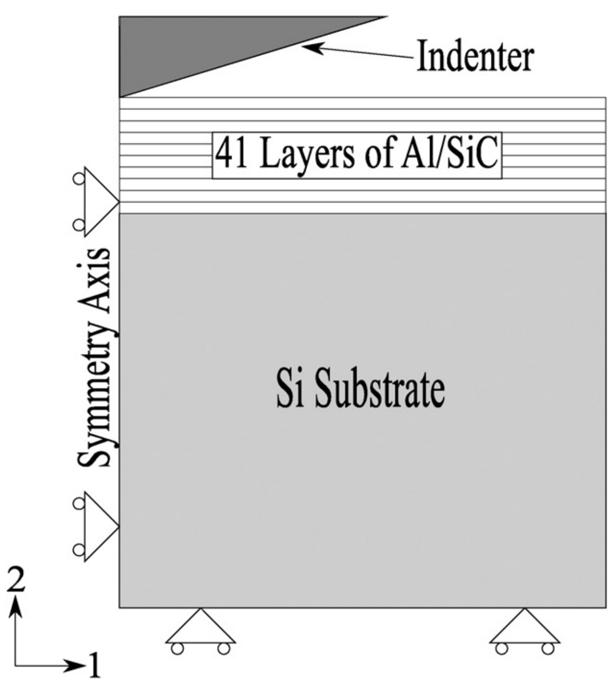

Fig. 2. Schematic showing the Al/SiC multilayers above a Si substrate and the boundary conditions used in the axisymmetric model.

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 directly interacts with 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.

Approximately 100,000 fully integrated linear axisymmetric elements are used in the finite element model with a finer mesh size near the upper-left corner of the test material. The element size near the indenter tip is approximately 8 nm and increases in size far from the indenter. The indenter consists of approximately 8000 elements with an element size of approximately 15 nm near the tip. The mesh was created using CUBIT (Sandia National Laboratories; Albuquerque, NM, U.S.A.). The finite element program ABAQUS (Version 6.13, Dassault Systemes Simulia Corp.; Providence, RI, U.S.A.) was used to carry out the analysis.

2.1. Material parameters

The Young's modulus for Al is assumed to be 59 GPa. Nanoindentation measurement of single-layer Al provided the modulus for this material. The Poisson's ratio for Al is 0.33. The plastic response of Al was based on the tensile loading data of single-layer Al with initial yield strength of 200 MPa. Rate-independent isotropic elastic–plastic response was assumed, with plastic yielding following the von Mises criterion with isotropic hardening and the incremental flow theory. The piecewise linear strain hardening response features hardening slopes of 199.33 MPa from initial yielding up to the strain of 50.51% and then 39.97 MPa up to the strain of 300.68%, beyond which perfect plasticity ensues.

The Young's modulus for SiC is assumed to be 277 GPa. Nanoindentation measurement of single-layer SiC films provided the modulus. The somewhat lower modulus of SiC relative to crystalline SiC is due to the fact that the physical vapor deposited SiC layers in the present case were amorphous [26]. The Poisson's ratio for SiC is taken as 0.17. SiC is a very brittle material; nevertheless, a very high yield point of 8770 MPa (estimated from the indentation hardness of a single-layer SiC film) was used followed by perfect plasticity. The plasticity assumption is necessitated by the fact that a purely elastic SiC in the model will generate unrealistically high loads during the indentation simulation, and it is validated by the fact that in the experiment the SiC layers exhibited a glassy/plastic-type response due to the amorphous nature of the film.

Both the Si substrate and diamond indenter are assumed to remain elastic. The Young's modulus and Poisson's ratio of the Si substrate are 187 GPa and 0.28, respectively. The Young's modulus and Poisson's ratio of the diamond indenter are 1141 GPa and 0.07, respectively. All the interfaces between different materials in the composite structure are modeled as perfectly bonded, unless otherwise noted in Section 2.2 (the cohesive zone allowing for delamination). The same set of material parameters were used previously to numerically study basic nanoindentation response [16], cyclic indentation behavior [27], the effect of layer undulation [28] and the effect of unloading induced plasticity [29] in the Al/SiC multilayer coatings. In the present work the effect of delamination is investigated.