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Analysis of Multilayer Coating Architecture

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Abstract- As compared to monolithic coatings, multilayer coatings with alternating hard and soft layers are finding increased applications because of the seemingly better performance in tribological and wear applications. However, the roles of overall thickness, number of layers, and individual layer thickness cannot be overlooked and need to be optimized to minimize damage in the multilayer coatings. 2-dimensional finite element models using cohesive zone elements were developed to predict damage in multilayer coatings subject to spherical indentation. Damage in coatings was characterized as through thickness coating cracks and interfacial delamination. A design of computer experiments (DACE) approach was used to build metamodels in order to predict damage variables for a design space consisting of 2, 4, 6, and 8 layers multilayer coating architecture.
Keywords- Multilayer coatings, cohesive zone finite element modeling, spherical indentation, DACE, Kriging

I. INTRODUCTION

Monolithic hard protective coatings are quite often used to increase the longevity of tools and tribological components in heavy duty service environments. However, there are limitations associated with monolithic coatings such as lack of multifunctional character, high residual stresses, problems associated with adhesion to substrate, etc. This has led to increasing use of multilayer coatings. Subramanian and Strafford [1] presented a good review of multilayer coatings for tribological applications. Multilayer coatings not only offer the combination of attractive properties from different materials, but also have observably increased tribological performance over monolithic coatings. Holleck and Schier [2] investigated the wear performance of multilayer PVD coatings. They compared single layer TiN, TiC, and multilayer TiN/TiC/B4C coatings for hardness, friction coefficients, and life of coated tools and concluded that for each category, multilayer coatings had superior performance. Bull and Jones [3] investigated the performance of two types of multilayer coatings produced in Ti-N system: Structural multilayers in which the amount of ion bombardment that the coating receives during deposition was changed in a cyclic fashion to produce alternating layers of low and high residual stresses, and compositional multilayers in which nitrogen flow was interrupted Periodically to produce alternating layers of titanium and titanium nitride. They concluded that both types of multilayers exhibited high hardness, good toughness, and improved adhesion leading to increase in wear resistance compared to single layer TiN coating. However, these properties were found to be dependent on periodic spacing of layers in multilayer TiN/Ti coatings leading to fewer cracks during indentation loads also observed coating deformation primarily being accommodated by shear sliding and plastic flow of Ti interlayers in TiN/Ti multilayer coating subject to indentation loads. They also observed that radial cracks were arrested due to multilayer structure. Enhanced toughness of TiN/TiAlN multilayer coatings is not due to increase in strain capacity (H/E) of the film, but because multilayers display additional modes of plasticity leading to permanent bending and compression of the film.

II. FINITE ELEMENT MODEL DESCRIPTION

In order to gain a better understanding of the performance of multilayer coating architecture, a benchmark finite element model consisting of monolithic coating on substrate subject to contact loading by a spherical indenter (ax symmetric conditions) was first considered. ABAQUS Standard was used for finite element simulations. Mesh containing 4-noded quadrilateral ax symmetric elements was employed. The smallest element size in the coating thickness direction was 0.25 μm. The nodes of the bottom and left boundaries of the mesh were constrained against displacement in the vertical and horizontal directions respectively. An illustration of the model is shown in Figure.2. The indenter was modeled as rigid with a radius of 250 μm. Contact was established between the indenter and the coating using contact algorithms in ABAQUS with friction coefficient equal to 0.1 between the indenter and the coating. Load control option was considered where the normal load applied to the indenter increased linearly to the maximum prescribed load. A coating thickness of 2μm (= tB) was considered and the coating was assumed to be homogeneous, isotropic, and perfectly elastic. Deformation plasticity model of ABAQUS was used for substrate. Yield strength of 2000 MPa and hardening exponent of 10 was used. The constitutive model for substrate was chosen to roughly represent 52100 steel and for coating to represent TiN. or a similar sans-serif font). Callouts should be 9-point non-boldface Helvetica. Initially capitalize only the first word of each figure caption and table title. Figures and tables must be numbered separately. The purpose of having a benchmark model was to establish baseline loading conditions for which damage just initiates in a monolithic coating-substrate system. Damage in the coating-substrate system subject to spherical indentation constitutes of through thickness circumferential cracks because of radial tensile stresses and delamination because of interfacial shear stresses. The loading conditions were chosen such that the maximum normal radial stress in the coating and maximum shear stress along the coating-substrate interface reach their respective critical fracture values (3000 MPa and 1500 MPa respectively) at end of the loading cycle. To reach the state of when damage just initiates, the maximum indentation load was 5N. Damage initiation criterion, for through thickness crack, QCB, (letter C in the subscript refers to circumferential crack and B refers to benchmark model) was defined as:

$$\boldsymbol{Q_{CB}} = \left(\frac{\boldsymbol{\sigma}}{\boldsymbol{\sigma_c}}\right)$$

where σ_C = 3000 MPa, the fracture strength of coating, and σ is the maximum normal radial stress in the coating. Obviously, for the state when the indenter was pushed to the maximum load of 5N, damage initiation criterion for through thickness crack, QCB =1.Damage initiation criterion, QIB (letter I in the subscript refers to interface and B refers to benchmark model) for interface crack was monitored via the cohesive elements at the interface.

Once the benchmark model was established and the damage criteria recorded, the model was extended for multilayer coatings keeping loading conditions the same (i.e.,peak indentation load =5N). The constitutive models were chosen to roughly represent coating layers of TiN/Ti deposited on 52100 steel. The multilayer designs to be considered had even number of layers between 2 and 8 (i.e., 2, 4, 6, and 8). In all the multilayer. designs, TiN layer was always the topmost layer and Ti layer was always the bottommost layer, just above the substrate. A schematic representation of the multilayer structure is shown in Figure

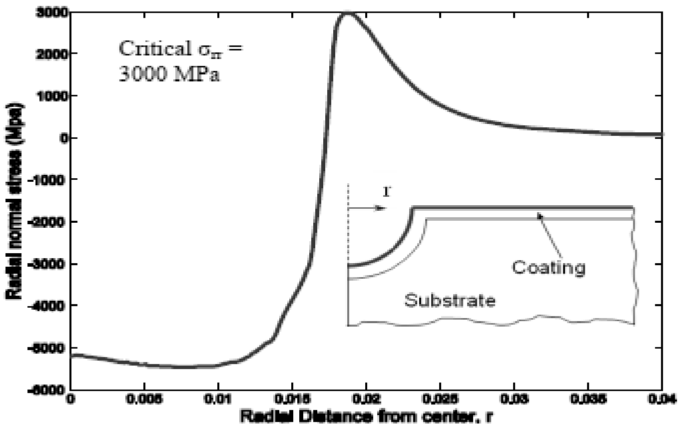

Fig. 1. Distribution of stresses during indentation in benchmark model Radial normal stress along coating surface

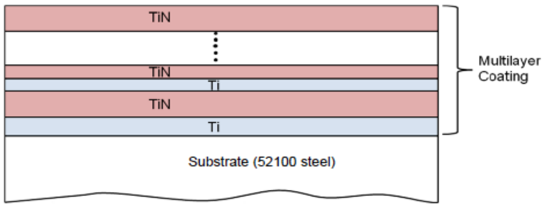

Fig. 2. Schematic of multilayer coating architecture consisting of alternating TiN and Ti Layers

The criterion for damage initiation in brittle TiN layers of multilayer architecture is

$$Q_{C\ multipliyer} = \left(\frac{\sigma N\ T_i}{\sigma_c}\right)^2$$

Where σTiN is the maximum normal radial stress in any of the TiN layers. The damage initiation criterion at the interface for multilayer coating architecture, Q *, was monitored via the cohesive elements at the interface. It has to be noted here that the maximum shear stress at the interface is limited by the plastic flow in the bottom most Ti layer. For instance, if the Ti layer would have been modeled as elastic-perfect plastic, then the maximum shear stress at the interface would be 0.577σY where σY is the yield stress of Ti. Hence, Q values will be much smaller than QIB. The initial FEM experiment consisted of fixing the total thickness to 6μm and equal layer thicknesses (e.g., all the layers in the 6 layer architecture would each be 1μm thick) and obtaining the values of QC* and Q *. It can be seen from Figure 3 that normal stresses are highest for 2 layer design and lowest for 8 layers design.

Also, normal stresses in Ti layers for all the designs are compressive. Figure 4.8 show the variation of peak normal stress and shear stress with change in number of layers. Next, the top TiN layer thickness was reduced by 0.25μm and the thickness of Ti layer above substrate was increased by the same amount for all the designs and QC* and Q * were recorded. This process of decreasing the top layer TiN thickness and increasing the bottom Ti layer was repeated again and QC* and QI were recorded. Figure 6 shows the variation of QC and QI for above mentioned FEM experiments. It can be seen that QC* and Q * are exhibiting some form of inverse trend and is common to all the multilayer designs. Decreasing the thickness of top layer decreased QC* and increase in Ti layer thickness increased Q * values. Furthermore, both QC*and values decrease with increase in number of layers for the same overall thickness. This trend points to adopting a procedure to search for such "Pareto fronts" in an exhaustive space of multilayer architecture designs where there is variation in number of layers, overall thickness and individual layer thickness.

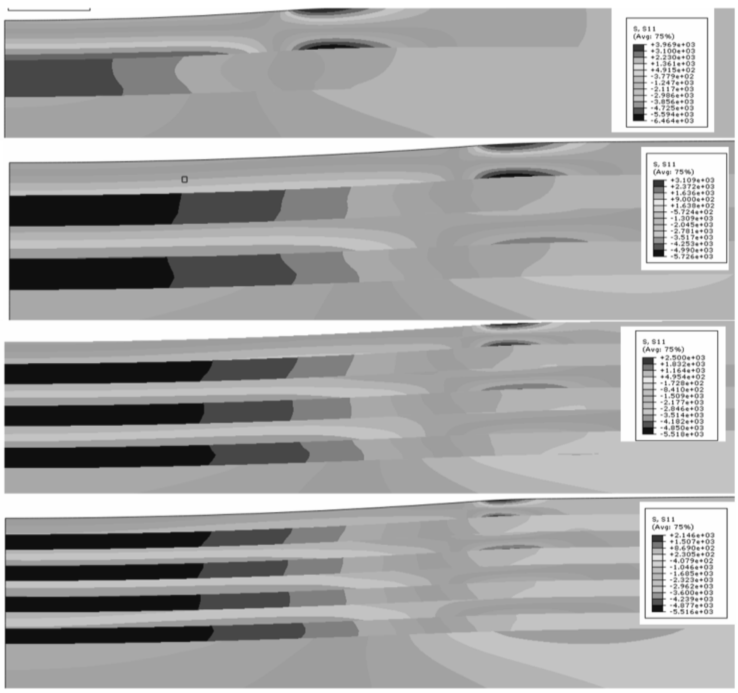

Fig. 3: Contour plots of normal radial stresses for (a) 2 layer, (b) 4 layer, (c) 6 layer and (d) 8 layers

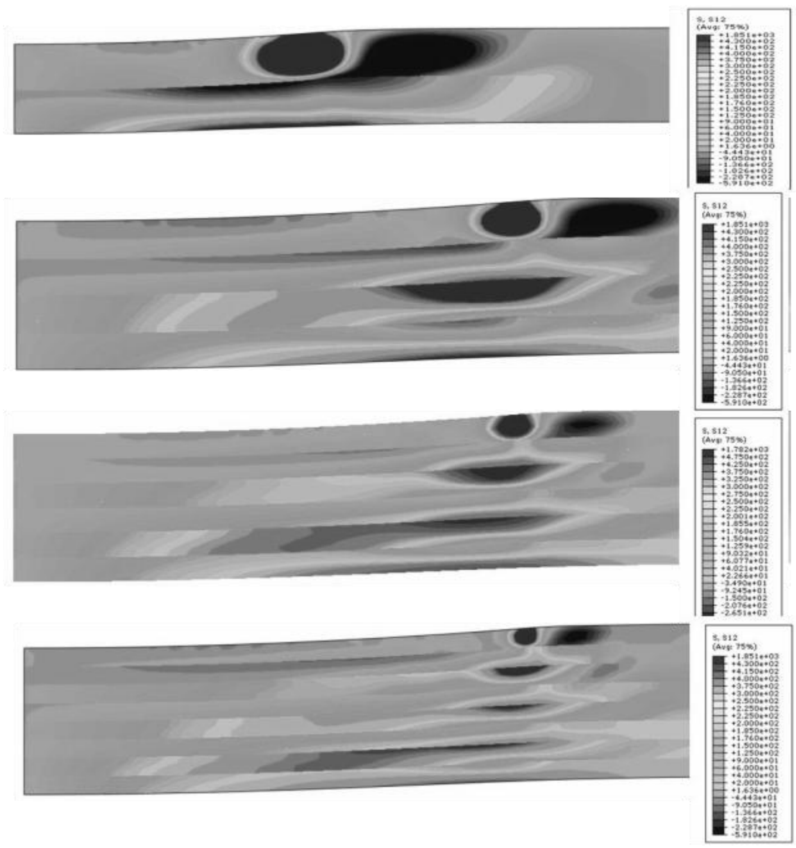

Fig. 4: Contour plots of shear stresses for (a) 2 layer, (b) 4 layer, (c) 6 layer and (d) 8 layers

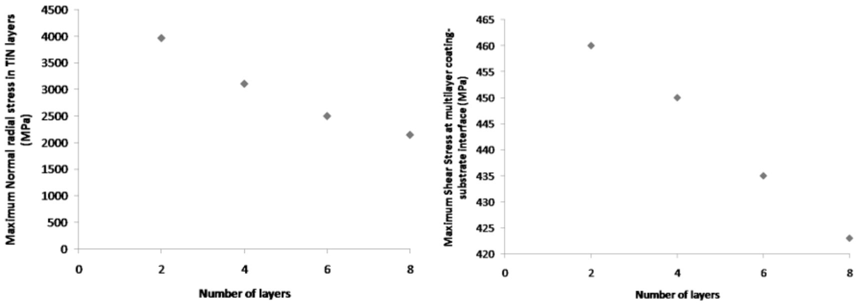

Fig. 5: Variation of maximum radial normal stresses and shear stresses with change in number of layers for the same overall thickness

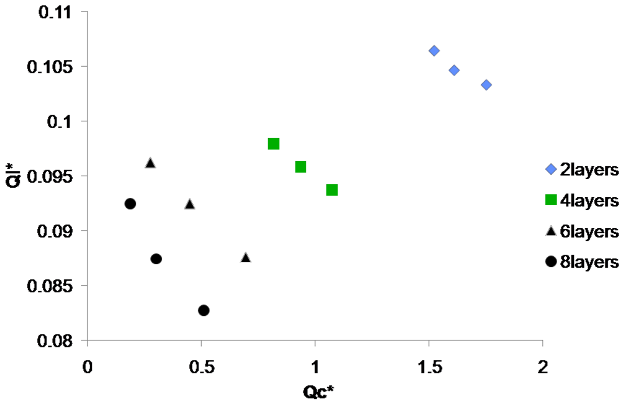

Fig. 6: Variation of damage initiation parameters for different number multilayer designs

III. FOOTNOTES

In this study, response of multilayer coating architecture to spherical indentation was considered by the use of finite element models. A benchmark model was first considered consisting of 2 µm thick monolithic coating (TiN) on ductile substrate (52100 steel). Loading condition were chosen such that it would initiate through thickness and interfacial fracture. Damage variables indicating these two fracture modes were quantified. Finite element model was extended to multilayer coating architecture consisting of 2, 4, 6, and 8 alternating hard (TiN) and soft (Ti) layers on substrate. Loading conditions were kept same as that for the benchmark case. Design of computer experiments and a metamodel can established with the objective to minimize damage in multilayer coating architecture.

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