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Optimization 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

1.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.

2.INDENTATION TO CHARACTERIZE FRACTURE IN COATINGS

Your task is to approach the usual quality of papers typeset in technical journals. Please pay most attention to the layout and overall appearance of your paper. The manuscripts will be subjected to editorial modifications. Use an automatic spell-checker. You have to send black- and-white texts and figures, preferably. Coating systems are prone to failure due to fracture in coatings and/or substrate deformation. Fracture in coating systems primarily consist of cohesive and interfacial failure (delamination). Cohesive failure in the coating occurs when the energy release rate for flaws in the coating exceeds the fracture toughness of the coating. Similarly, fracture in the interface (of coating and substrate) occurs when the energy release rate for flaws in the interface exceeds the interfacial fracture toughness. Fracture in thin hard film coated systems is complex and controlled by the coating material, substrate and the interface which bonds the system together. There have been many investigations of failure properties of coatings using indentation Investigations have measured the adhesion of brittle films on a ductile substrate and have observed preferred pathways for local cracking and separation in thermal spray coatings. Used indentation techniques to measure the fracture toughness of thin, amorphous carbon films.

The spherical indentation technique involves pushing a hard sphere into the surface of the coating-substrate system while the load and the depth of indentation are continuously measured. After the removal of the sphere, the impression is examined under an optical or scanning electron microscope. The impression usually reveals patterns of cracks in the film caused by tensile stretching of the film. The cracks are typically circumferential in nature, located near the periphery of the impression. High radial normal stresses at the surface of the coating near the edge of indenter are responsible for circumferential cracks at the surface of coating. Cracks in the coating can also occur directly under the center of indenter near the interface because of high radial normal stresses. Figure 1 illustrates the formation of cracks in the coating during indentation. In addition, interfacial failure can also occur because of high shear stresses.

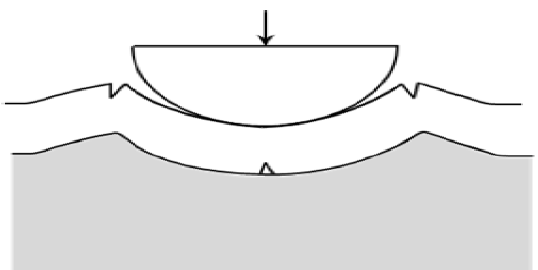

Figure 1. Formation of coating cohesive cracks during indentation

Cohesive zone modeling is a popular method of characterizing damage in Coatings. Indentation induced delamination of the film from the substrate by employing cohesive elements along the coating-substrate interface. In another study both circumferential cracking in the coating and delamination were investigated by employing through thickness and interfacial cohesive elements. The influence of material and cohesive parameters on the spacing of circumferential cracks was discussed. The current research paper aims to bridge the gap further in the area of optimization of coating architecture while addressing some of the limitations mentioned earlier.

3. 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 establishedbetween 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.

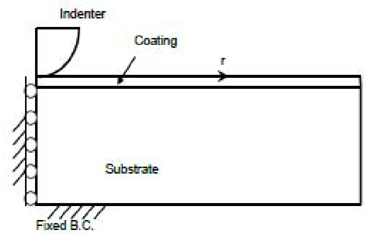

Figure 2. An illustration of the benchmark finite element model to simulate spherical indentation.

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:

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where σC = 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.

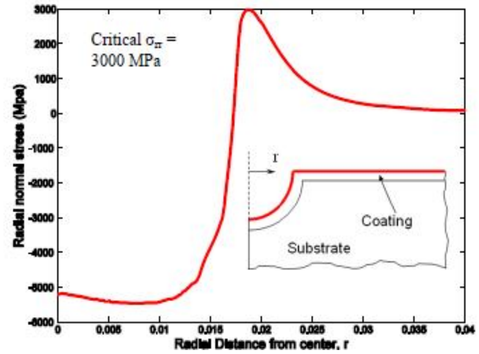

Figure 3. Distribution of stresses during indentation in benchmark model Radial normal stress along coating surface

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 4

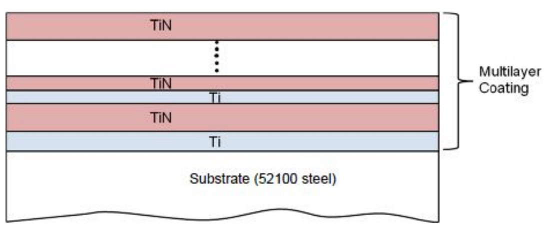

Figure 4. Schematic of multilayer coating architecture consisting of alternating TiN and Ti Layers

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

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4.OPTIMIZATION FORMULATION

A formal statement can be written

as: Minimize QI* and QC*

with $t_1^*, t_2^*, t_3^*, ……..t_n^*$; n ϵ [2,4,6,8] as design variables,

subject to $\sum_1^n t_i^* = \beta$; β ϵ [1,3],

where,

=————,

=————

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$$\beta = \frac{\sum_1^n t_i}{t_B}$$

Simply put, the above formulation is to minimize the damage in the multilayer coating architecture where the total number of layers can be 2, 4, 6, and 8 and the overall thickness can be in the range 2-6µm.

5 DESIGN AND ANALYSIS OF COMPUTER EXPERIMENTS (DACE) APPROACH

Computer models such as FEM are being increasingly used to model actual physical processes. However, even with modern computational resources, computer modeling can be time consuming. Also, lack of explicit information of the models with respect

to design variables can limit the predictive nature of the computer models with regards to optimization. Hence, meta modeling (which is essentially modeling of computer models) techniques are gaining popularity. Approaches based on fitting response surfaces to data collected by evaluating objective functions at a few data points are discussed extensively.

The response surfaces models (RSM) are then used to visualize input-output relationships and then estimate the location of the optimum. RSM based on modeling of objective functions with stochastic processes is usually termed "Kriging" To employ Kriging models, an experimental design matrix needed to be developed. For efficient Kriging models, the experimental design space needs to be (a) space-filling, and (b) non-collapsive Initial computer experimental designs for 2, 4, 6, and 8 layers multilayer coating architecture were created as follows:

Random assignment of total thickness for a design point.

Given the total thickness, a set of "L" randomly selected layer thicknesses

adding to total thickness are selected, i.e., coordinates of a design point are

(x1, x2,…xL).

Repeat steps a and b to give NL design points.

Repeat a, b, and c 10,000 times and select the "best design" based on the

criteria to minimize Euclidean distance in the "L" dimension space, and minimize geometric average Euclidean distance in all the projected 2- dimensional space

The layer thickness values were not continuous but based on a grid of 0.25 µm, i.e., minimum thickness of layers was 0.25 µm and thickness values were a multiple of 0.25. This is because the smallest element size for the mesh of the finite element model was 0.25 µm.

The above methodology of creating experimental designs roughly follows the maxi min criteria. Figure 4.10 shows the experimental designs for a 2 layer coating architecture. A total of 10, 14, 27, and 40 initial experimental designs were created. QI* and σTiN, were evaluated for the multilayer experimental designs using the finite element model. The evaluated QI* and σTiN values were used as input values to the kriging model.

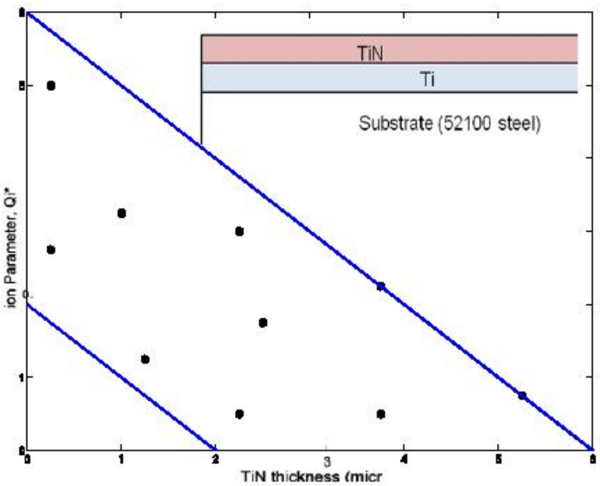

Figure 5: Design coordinates for 2 layers

6 RESULTS & DISCUSSION

The parametric kriging model using a cubic correlation function, as described above, was used to predict damage initiation parameter for the coating-substrate interface, QI* and maximum radial stress in TiN layers, σTiN, for 2, 4, 6, and 8 layers multilayer coating architecture. This section discusses uses how the kriging model was used, validated by additional experiments and then updated based on the results from additional experiments.

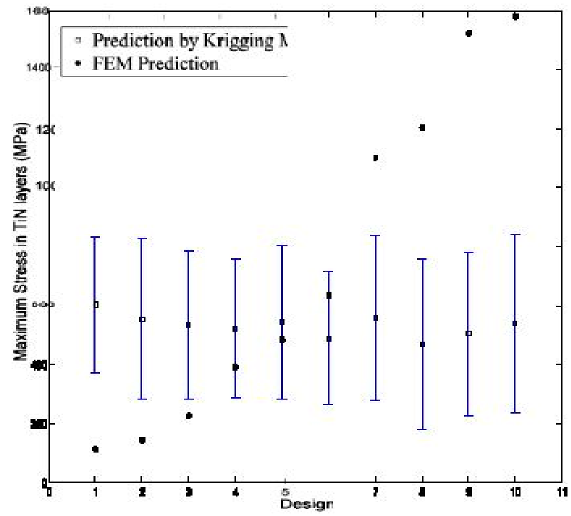

Figure 6.Comparison of FEM and Kriging model prediction stress in TiN layers, for 4 layers designs

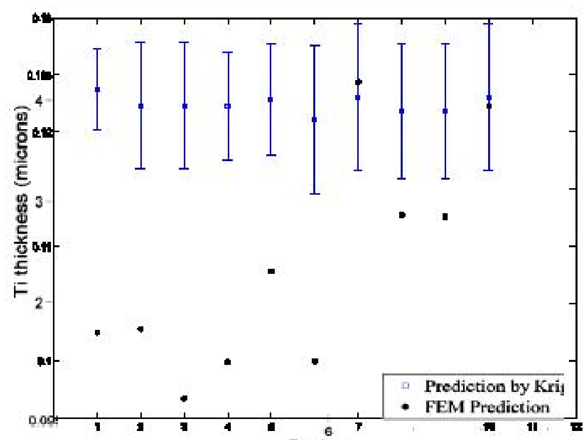

Figure 7.Comparison of FEM and Kriging model prediction Damage initiation parameter at interface for 4 layers designs

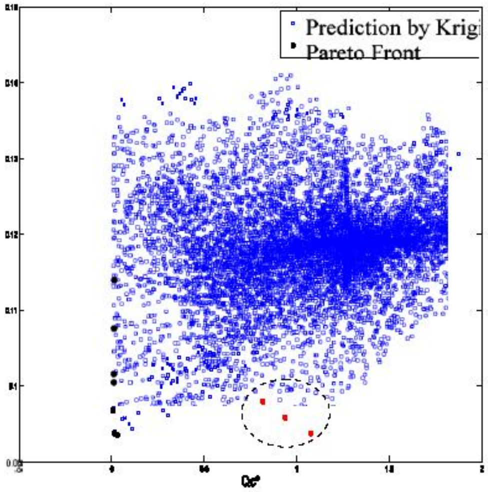

Figure7: Predicted damage initiation variables and pareto frontier for 4 layers.

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