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Mechanical Properties Simulation of Ti-based Hard Multilayers by Using the Finite Elements Method[1]

Simulación de Propiedades Mecánicas de las Multicapas Duras Basadas en Ti mediante el Método de Elementos Finitos

Elisabeth Restrepo Parra
Ingeniera Eléctrica
Maestría en ciencias – Física
Doctorado en Ingeniería – línea Automática
Grupos de investigación PCM Computational Applications - Laboratorio de Física del Plasma
Docente Investigadora Universidad Nacional de Colombia – Sede Manizales
erestrepopa@unal.edu.co

Claudia Milena Bedoya Hincapié
Ingeniera Física
Grupos de investigación PCM Computational Applications
Universidad Nacional de Colombia – Sede Manizales
cmbedoyahi@unal.edu.co

Juan Carlos Hernández Parra
Ingeniero Físico
Grupos de investigación PCM Computational Applications
Universidad Nacional de Colombia – Sede Manizales
juhancpco@gmail.com

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ABSTRACT

In this paper, mechanical behavior of TiAlV/TiAlVN bilayers was studied by means of nanoindentation experiment simulated using ANSYS software.

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In the simulations, a Vickers type diamond tip, a steel substrate and TiAlV/TiAlVN bilayers distributed in a constant thickness of 2 μm by an axisymmetric geometry were considered. The parameters used in the simulation as Young's modulus E, Poisson ratio ν *and yield stress* σ_e *for TiAlV and TiAlVN were 113.6 GPa and 350 GPa, 0.342 and 0.2, and 830 MPa and 870 MPa respectively. Results showed the radial stress distribution seems to be tooth -like and the maximum shear stress decreased as the number of bilayers increased.*

Key Words: mechanical properties, stress, nanoindentation, bilayers.

RESUMEN

En este trabajo, se estudio el comportamiento mecánico de bicapas TiAlV/TiAlVN mediante experimentos de nanoindentación simulados con el uso del software ANSYS. En las simulaciones se consideró un indentador de diamante tipo Vickes, un sustrato de acero y bicapas TiAlV/ TiAlVN distribuidas en un espesor constante de 2 μm, en una geometría de eje simétrico. Los parámetros usados en la simulación como modulo de Young E, relación de Poisson ν *y punto de fluencia* σ_e *para el TiAlV y TiAlVN fueron de 113.6 GPa ay 350 GPa, 0.342 y 0.2, y 830 MPa y 870 MPa respectivamente. Los resultados mostraron que la distribución de estrés radial presenta un comportamiento en forma de sierra y el máximo en el estrés de corte disminuye en la medida que el número de bicapas se incrementa.*

Palabras Clave: propiedades mecánicas, estrés, nanoindentación, bicapas.

1. INTRODUCTION

Ceramic films have been widely used in mechanical and tribological applications to solve surface problems i.e. for increasing the lifetime and decreasing the cost of cutting tools (Randhawa, 1988). Because of the higher hardness, wear resistance, fatigue and corrosion resistance of the ceramic films than other materials, these systems are widely used as a method of surface modification in engineering materials (Knotek, 1987).

Particularly, titanium-based thin hard coatings such as TiN, Ti–Si–N and Ti–Al–N exhibit excellent mechanical and tribological properties; Moreover, they provide superior wear resistance compared with materials used as substrates (Chawla, 2008). Thereby, in order to improve materials features such as TiN-based films, for instance (TiAl)N, (TiZr)N, (TiAlV)N and (TiAlZr) N have found many applications in recent years. Specifically, (TiAl)N and (TiAlV)N films have better mechanical and tribological properties than TiN films (Hermann, 1987) and (Efeoglu, 1993). Regarding to mechanical applications advances, nanoindentation processes have been extensively employed because it is the simplest approach for measuring mechanical properties of small material structures including thin films (Doerner, 1986), (Oliver, 1992), (Tsui, 1999), (Chen, 2006) and (Cheng, 2004). Existing theories for extracting material properties from indentation response are based on the assumption that the material being indented is a homogeneous body with a unique set of properties (Fischer, 2002), (Oliver, 1992), (Cheng, 1999), (Dao, 2001).

On the other hand, finite element method (FEM) is a successful technique of numerical analysis for understanding the materials behavior under small indentation loads (Knapp, 1999). Therefore, nanoindentation has been frequently studied using FEM (Sun, 1995), (Cheng, 1998), (Cheng, 1999) and (Knapp, 1997). Many works have been found focused in elastic and plastic mechanical response by using specialized software e.g. ANSYS, COMSOL, ABAQUS, etc. For example, X. Zhao et al. (2010) studied the stress distribution in TiSiN-based multilayer coatings during the loading nanoindentation process by COMSOL software. Their results were compared to a monolithic system, showing a reduction in the maximum shear and the radial tensile stress with the introduction of multilayers. Likewise, M Lichinchi et al. (1998) simulated the load-unload behavior of titanium nitride thin films employing the ABAUQUS software. The work carried out by S. Amaya-Roncancio et al. (2008) presents the mechanical behavior of Cr/CrN multilayers coatings by using ANSYS software. This work showed an increase of Young's modulus depending on the number of layers and thickness, which means an increase in hardness.

In this work, finite element modeling (FEM) is used for obtaining the radial, axial and shear stress distribution in TiAlV/TiAlVN bilayers. The model performed with a Vickers indenter, was simulated by axisymmetic geometry analysis that has been widely used in different contributions (Lichinchi, 1998), (Amaya-Roncancio, 2008) and (He, 2003). For this study, the total layer thickness was fixed as constant and the number of bilayers was varied.

2. FINITE ELEMENT MODELING

FEM was carried out with the commercial software ANSYS. The system performed for the simulation consists of TiAlVN/TiAlV bilayers with constant total thickness of 2 µm, a substrate of stainless steel and a Vickers diamond tip with an angle of 136°. In the simulations, a 2D axial symmetry model (figure 1.a) was used in order to decrease the computational time without compromising the accuracy, allowing the system mesh with a restricted number of degrees of freedom (He, 2003). The scheme of a substrate-bilayer system and the indenter size used in these simulations is illustrated in figure 1(b), in the axisymmetric geometry.

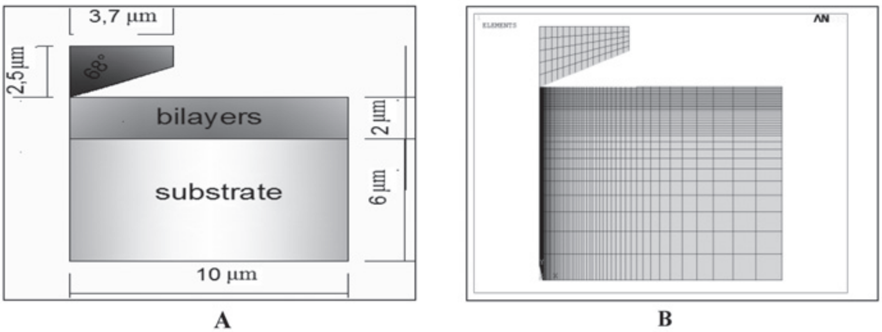

Figure 1 (a) Substrate-bilayer system and indenter size and
(b) Axisymmetric model employed in the simulation

The coating is assumed to be perfectly adhered to the substrate and the contact between the coating and the indenter is considered frictionless. According to figure 1(b), the system was meshed with a higher concentration of elements near to the symmetric axis (where the indententation is applied) and in the bilayer (more than in the substrate), in order to have greater accuracy. In the simulations, geometrical boundary conditions were considered in the x axis allowing the nodes to move along y axis. The sample was displaced up and down towards the indenter for reproducing the indentation process. For ensuring the indenter and sample contact, a contact surface between them was used. For carrying out static analysis, the loading process was slow. The parameter values used in the simulations are listed in Table I.

Table I. Materials and mechanical properties

Material	Young´s modulus E (GPa)	Poisson's coefficient (v)	Yield stress (MPa)	Reference
Diamond	1141	0.07	-	(He, 2003).
Structural steel	180	0.23	-	[http://www.engineeringtoolbox.com]
TiAlV	113.8	0.342	~830	(Bauer, 2012)
TiAlVN	350	0.2	~850	(Poláková, 2003)

3. RESULTS AND DISCUSSION

Results of nanoindentation in the loading and unloading process are shown in fig. 2. The displacement as a function of the load varying the number of bilayers from 1 to 10, within a constant thickness of 2 μm is observed. The maximum indentation depth was 200 nm. The curves shape is in agreement with the experimental loading and unloading tests reported in the literature (Doerner, 1986) , (Lichinchi, (1998) and others simulated (Tang, 2010).

The difference between loading and unloading curves is caused by the inelastic material behavior (Oliver, 1992). Although, it has been reported that as the number of bilayers is increased the Young´s Modulus and the hardness are higher (Claude, 1992), results obtained in our simulations present the opposite behavior. It could be due to TiAlV (metallic layer) presents lower hardness and Young´s Modulus than TiAlVN (ceramic layer) as the number of bilayers increases, the effect of the softer TiAlV layer is more appreciable, because the indenter reaches this layer at lower indentation depth. This effect is normally referred in the literature as the size indentation effect (SIE) (Gong, 1999).

This property could be favorable for the material behavior. The low toughness of hard ceramic coatings could be improved by bonding them with a ductile layer. Moreover, is possible to introduce ductile layers useful in the deflection of cracks that may be generated during the performance of the coated components (Vieira, 1999).

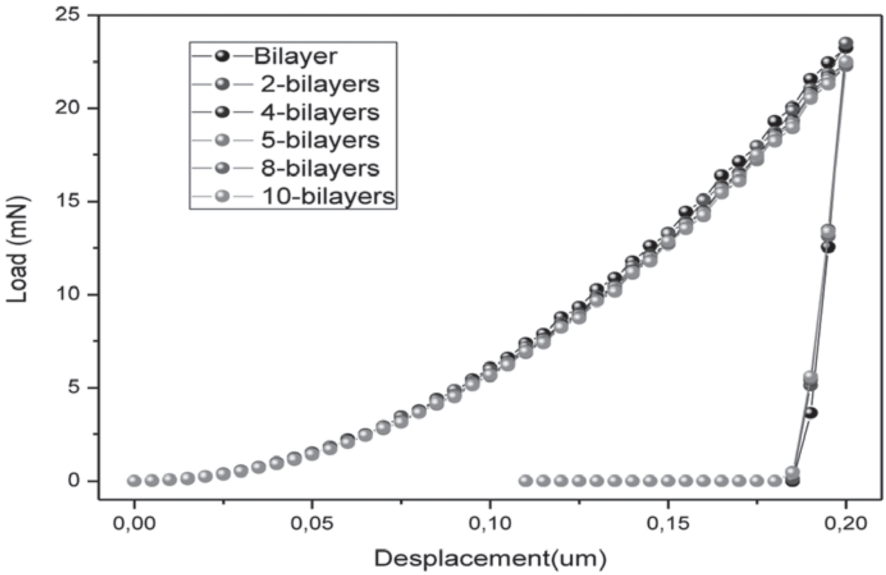

Figure 2 Load-displacement curve during indentation loading and unloading as a function of the number of bilayers

Figures 3 and 4 present an analysis of the radial stress distribution varying the number of bilayers. In figure 3 the maximum radial stress is placed below the indenter and the stress distribution tends to be discontinuous as the number of bilayers increases. This behavior is caused by the concentration of stress in the harder regions (Zhao, 2010).

According to figure 3, notably the stress value is high within the first TiAlVN layer above the substrate, indicating that radial crack is likely to occur in this layer. It is possible to minimize such risk by increasing the number of layers; then, there is a slight reduction in the area surrounding the radial stress, which helps to reduce the likelihood of ring cracks.

Figure 4 presents simulations of the radial stress distribution in the coating depending on the number of bilayers. Results show radial stress curves as a function of the length for different number of bilayers. In the case of one bilayer, the maximum radial stress emerges above the interface along the symmetry axis. Nevertheless, in multilayer systems, as a consequence of relaxation system in TiAlVN and TiAlV layers, the stress distribution is sawtooth-like being more ripple as the number of bilayers is increased.

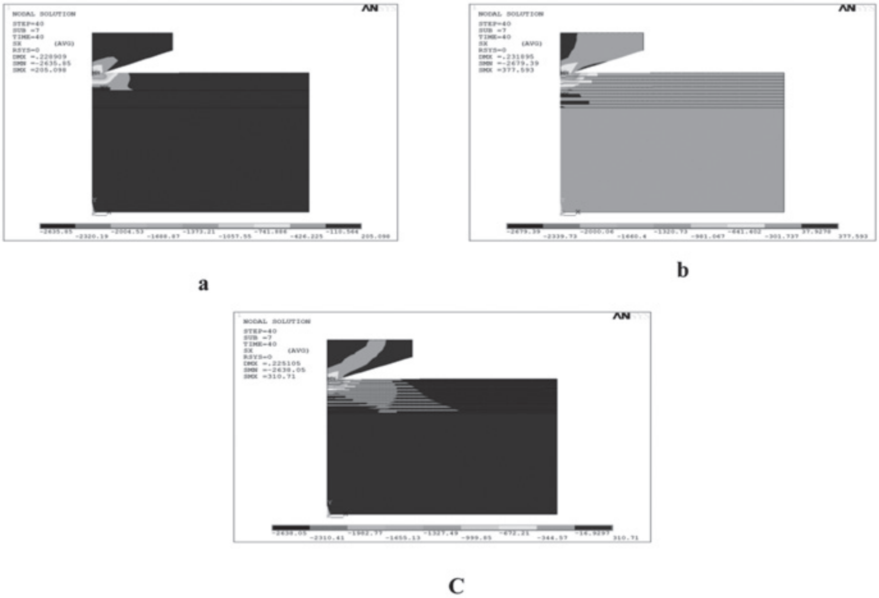

Figure 3 Strain radial distributions during the nanoindentation process determined by developing FEM simulation of the nanoindentation test. (a) 1 bilayer, (b) 5 bilayers, c) 10 bilaters

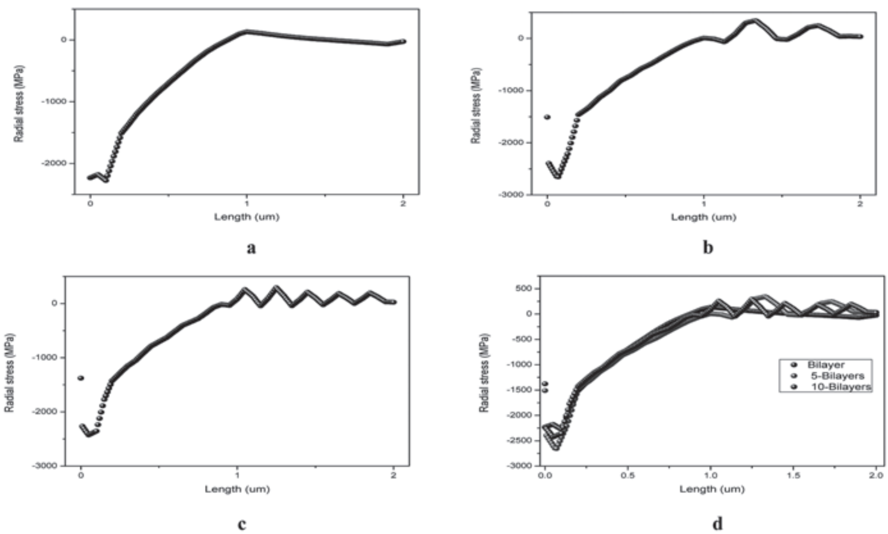

Figure 4 Curves of radial stress (a)1 bilayer, (b) 5 bilayers, (c) 10 bilayers, (d) overall

Similarly, figure 5 illustrates the axial stress for different number of bilayers, being observed the reduction in the minimum axial stress as a consequence of the increase of bilayers.

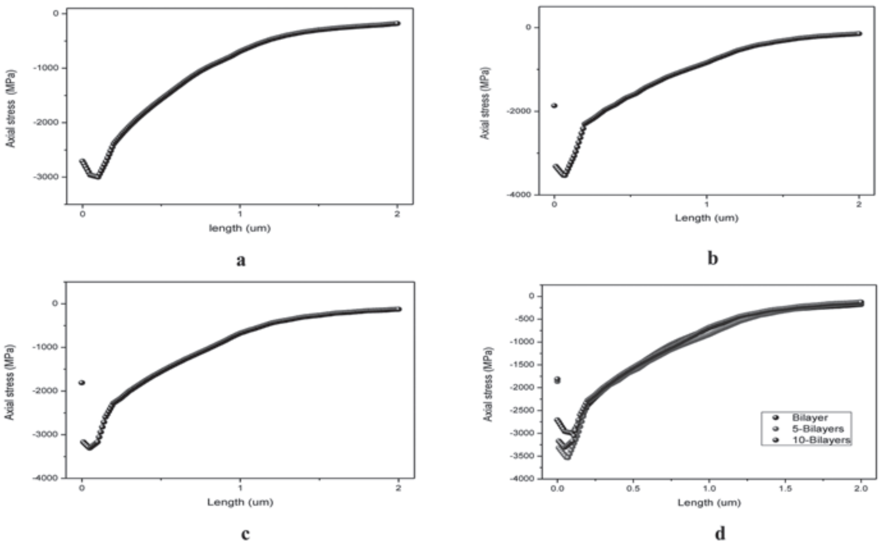

Figure 5 Axial stress results in the final of the process (a)1 bilayer, (b) 5 bilayers, (c)10 bilayers and (d) overall

One of the most important aspects in stress analysis is to identify the relationship between stress concentration and the initiation of cracks. There are three common types of indentation cracks occurring in hard coatings; i.e., radial, ring and lateral cracks (also known as delamination) (Xie, 2007). Radial cracks usually initiate at the coating/substrate interface directly below the indenter at excessive radial or hoop stresses. Lateral cracks during the loading process normally result from large shear stress (Abdul-Baqui, 2001). By introducing multilayers into these thin films, the maximum shear stress is reduced, diminishing the probability of lateral cracks (Zhao, 2010).

This influence in the surface shear stress distribution is observed in figure 6, where it is found below the indenter in a radial way (figure 6(a)). During the loading process, the shear stress yields the move of dislocations lines in an elastic deformation manner and the consume of certain amount of energy. This behavior can be modified by consider the coating formed by TiAlV/TiAlVN multilayers more than a bilayer, in which case the maximum shear stress can be diminish, as it is shown in figure 6(b).

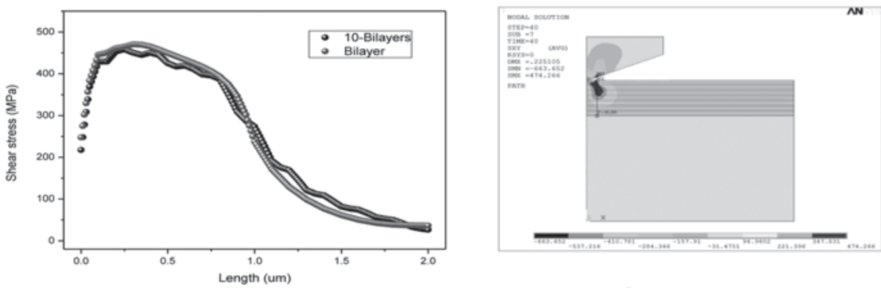

Figure 6 Shear stress (a) curve behavior and (b) surface distribution

4. CONCLUSIONS

A stress mechanical simulation in TiAlV/TiAlVN bilayers was carried out by employing the finite element method. The simulations of the hardness match experimental results obtained for other materials such as in the loading –unloading curves. Moreover, the radial stress distribution showed a sawtooth-like behavior and the minimum axial stress decrease as a result of the increase in the number of bilayers. This effect could be favorable for the material behavior, because it produces a decrease in the system toughness. On the other hand, a decrease in the maximum shear stress can be obtained by increasing the number of bilayers.

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