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SIMULATION OF THE INTERFACE BEHAVIOR OF THIN FILMS DURING INDENTATION TESTING

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ABSTRACT

The search for improved tribology properties in materials contributes to the development of processes that extend the useful life of components and their applications in increasingly severe environments. In this respect, thin ceramic films have been used to enhance the properties of components that operate under these conditions. However, expensive experimental assays are needed to assess the behaviour of these films and system compounds by films and substrates. These experimental analyses are also destructive, requiring the use of sophisticated equipment and specialized hand tools. On the other hand, with advances in computational mechanics, the application of numerical analysis to solve numerous technological problems has become increasingly common, owing to its low operational costs. This study aims to simulate indentation testing with a spherical penetrator in systems composed of thin ceramic film deposited on metallic substrate using a Finite Element commercial code. The main objective of this study was to evaluate the field behaviour of stresses in the contact region of the indenter with the sample and on the film-substrate interface.

Keywords: Finite elements, indentation test, thin films, interface behaviour.

INTRODUCTION

The need to improve mechanical properties, such as resistance to oxidation and wear, has led to advances in surface engineering. This field of engineering involves the preparation and modification of surfaces to fulfill specific functions within certain applications. One of the options employed to improve these surface properties is the use of ceramic coatings obtained by deposition processes such as PVD. However, the mechanical properties of these films and their interface as substrate must be assessed.

Indentation tests have been applied during the last hundred years to determine surface hardness in different classes of materials (Souza, 2000). In recent years, instrumented indentation testing has been used to characterise these tribology systems (Araújo, 2014). The instrumented indentation technique is conducted using precision instruments equipped with sensors that monitor variations in penetration depth (h) of a penetrator as a function of the applied load (P) when it penetrates the study material, reaches maximum displacement, and then returns to the initial position, completing a loading and unloading cycle (Fischer-Cripps, 2006). Due to their versatility, a large number of studies have been carried out to investigate new methodology and applications for these assays. Recent proposals used indentation tests as a tool to assess the mechanical characteristics of materials such as surface hardness (H), modulus of elasticity (E), Poisson's ratio (ν), fracture toughness (K_{IC}), film thickness and a stress curve as a function of elastic/plastic strain behaviour (Sun, 1995; Begley, 1999; Zeng, 2001; Lee, 2005; Dias, 2010; Pulécio, 2010; Mousse, 2012). However, implementation of this experimental methodology to assess mechanical properties and the results obtained still raise doubts in the scientific community. According to the literature, these problems are more serious when assessing the mechanical behaviour of thin films deposited on soft substrates (Fischer-Cripps, 2006; Dias 2010).

Due to these limitations in analysing indentation tests, the use of a numerical technique capable of evaluating stresses and strains during the indentation cycle may contribute to a better interpretation of this test. Recently, this numerical methodology has been studied using the Finite Element Method (FEM) to assess the behaviour of different materials in indentation testing (Lichinchi, 1998; Souza, 2001; Bressan, 2005; Dias, 2006; Mousse, 2012; Fukumasu, 2015, Libório, 2016).

The FEM has proved to be a reliable numerical technique for analysing stresses and strains and simulating different engineering problems. This method has widely been used to simulate and resolve numerous nonlinear problems related to structural instability and dynamic, electromagnetic, and mechanical conformation systems. However, the use of this numerical technique to assess the indentation test in thin surface coatings has also posed problems due to computational limitations, difficulty in implementing damage criteria and, chiefly, in characterizing these coatings (Huang, 2005; Dias, 2010; Fukumasu, 2015).

The simulation proposed in this study will use finite element models to reproduce the indentation test with a spherical indenter, as illustrated in Fig. 1. The system under study was composed of a metallic substrate coated with different thicknesses of ceramic film. A simulation was also used to assess the mechanical behavior of the interface in these systems that combine high-hardness coatings with a middle-hardness substrate. This interface was modeled by introducing a thin layer of elements with mechanical properties capable of simulations ranging from perfect adhesion to possible delaminating of the film.

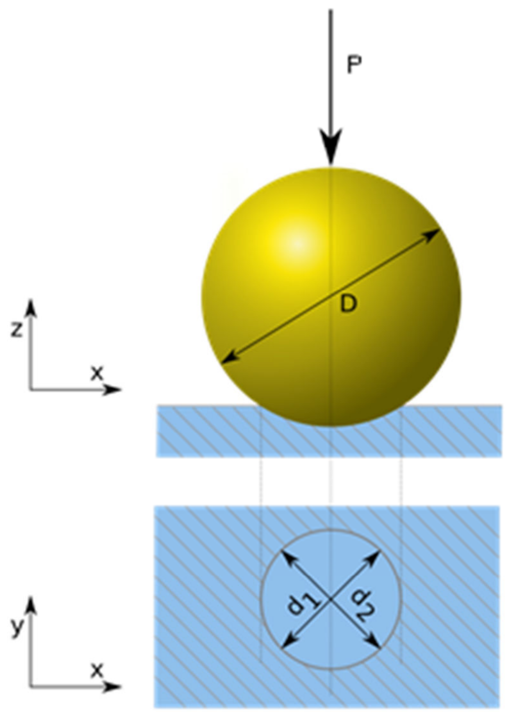

Fig. 1 - Spherical model of indentation testing and the impression itself (Dias, 2010)

METHODOLOGY

The numerical simulation performed in the present study used the finite element commercial code to model the indentation test with a spherical penetrator in a thin ceramic film deposited on a metallic substrate (MARC™, 2015). Due to the symmetry of the problem, axis symmetric elements were used in the numerical model, significantly decreasing computational efforts (Araújo, 2014). The studied system was composed of an AISI 4140 alloy steel substrate coated with a chromium aluminium nitride (CrAlN) film with four different thicknesses (1.67 µm, 3.00 µm, 6.00 µm and 9.00 µm). The studied materials, of both the film and the substrate, were considered isotropic and homogeneous. The elastic-plastic behaviour of these materials was illustrated by means of a curve depicting the linear elastic regime and plastic yield (Equation 1), primarily as described by Hosford and Caddell (1993) In this expression, σ, σ_o, ε, E are effective stress, yield limit, effective strain and Young's Modulus, respectively. K and n are constants that describe the strain hardening characteristics of the material, n known as the strain-hardening coefficient (Hosford, 1993).

$$\sigma = \max\left[\left(K\varepsilon^n\right), \sigma_o\right] \quad (1)$$

Table 1 shows the mechanical properties of the film and the substrate adopted in the present study. The experimental values of yield strength (σ_o) and Poisson's ratio (ν), as well as Equation (1) data, were obtained from the literature (Dias, 2010; Matweb, 2015).

Table 1 - Mechanical properties adopted for the film and substrate (Dias, 2010; Matweb, 2015)

Material	E (GPa)	ν	σ_o (MPa)	K (MPa)	N
Substrate (AISI 4140 steel)	238	0.29	565	2,230	0.228
Film (*CrAlN*)	350	0.22	3,790	10,615	0.229

The indentation cycle (loading and unloading phases) was simulated using the prescribed displacement of the penetrator, allowing better numerical control at the outset and during simulation of the test (Dias, 2006; Libório, 2016). The incremental analysis of the problem used one hundred increments for both the loading and the unloading phases. The numerical model used four-node isoparametric axis-symmetric elements. In order to obtain better distribution of the field of stresses and strains in the contact region of the indenter and at the interface with the substrate, a more refined grid was utilized in these regions, Fig. 2. The decrease in element size increases the rising computational costs, but reduces instability in the numerical result of the loading curve as a function of displacement in these simulations (Araújo, 2014).

In an attempt to simulate interface behaviour during the simulations, a layer with the lowest thickness possible was introduced between the film and substrate (Fig. 2). This layer was modelled with a thickness of 0.0834 µm using one ply of elements or with a thickness of 0.167 µm using two plies. The perfectly plastic mechanical behaviour was used in order to allow slip between the film and substrate. The yield strength (σ_o) adopted for this layer is the same as the substrate, that is, 565 MPa. To assess its behaviour, its modulus of elasticity (E) was varied between 238 GPa and 1.0 GPa. The former value is equal to the modulus of elasticity of the substrate, representing perfect adhesion. The latter value represented weak adhesion of the film to the substrate. The characteristics of the meshes used in the different numerical models are listed in Table 2.

Indenter penetration depths of 10%, 20%, and 50% of film thickness were adopted. According to the literature, a penetration depth of up to 10% of film thickness is used when studying film without the influence of the substrate (Lichinchi, 1998; Huang 2005). Other authors recommend that this thickness be up to 20% when the substrate exhibits high mechanical strength (Dias, 2010). To assess the behaviour between the film and substrate system, the present study adopted a depth of half the film thickness. A friction coefficient between the indenter and surface of the film was not considered, because this friction has no significant influence on indentation load (Araújo, 2014). Also, the pile-up and sinking-in surface displacements, which could occur during the indentation testing, were not taken into account in the present analysis (Dias, 2010; Araújo, 2014).

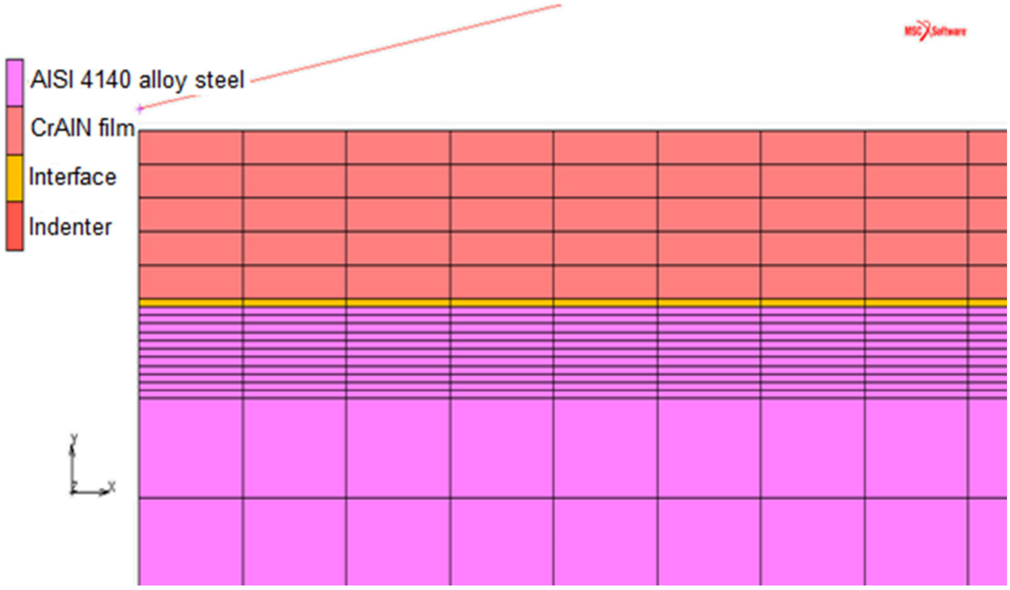

Fig. 2 - Numerical mesh at the contact region of spherical indentation testing in a system with film, interface and substrate

Table 2 - Characteristics of the meshes of numerical models simulated with a system composed of a film, interface and substrate.

System	Substrate	Interface (one ply)	Interface (two plies)	Thin Film	Film's thickness
Film CrAlN Substrate AISI 4140 alloy steel	8,550 elements	105 elements	210 elements	525 elem.	1.67
				945 elem.	3.00
				1,890 elem.	6.00
				2,835 elem.	9.00

RESULTS AND DISCUSSIONS

Figure 3 illustrates the behaviour of the load curve as a function of indenter displacement (*Pxh*) in the simulation of a test conducted in a sample of 3.00 μm thick film, considering an indentation depth of 50%, that is, 1.50 μm. In this simulation, the interface layer was modelled with a modulus of elasticity of 200 GPa and the interface layer had one ply of elements and a thickness of 0.0834 μm. This curve shows that the results demonstrate a qualitative representation of experimental testing behaviour compared to other literature studies (Araújo, 2014).

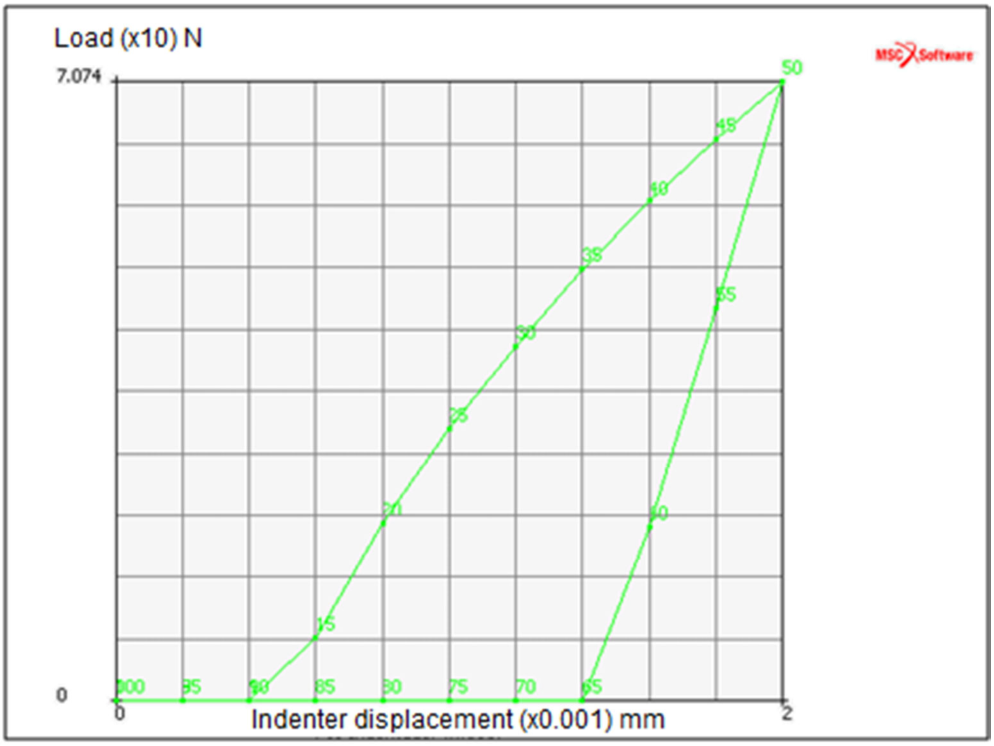

Fig. 3 - Load curve as a function of indenter displacement in the system with 3.0 µm-thick film.

At the beginning of these simulations, the indenter was positioned at a distance of 0.50 µm (gap) above the sample. Thus, the total displacement of the indenter in the simulation of the system showed in Fig. 3 was of 2.00 µm, i.e., the total depth of penetration was 50% of the film thickness (1.50 µm). The behavior exhibited by the *Pxh* curve of Fig. 3 showed a similar response to a matching curve, found in the literature, obtained experimentally in instrumented indentation tests with spherical indenters (Zeng, 2001; Martínez, 2003; Huang, 2005).

Then, all models whose interface was considered as one ply of elements between the film and the substrate were simulated. Finally, the models whose interface elements have two plies and a thickness of 0.167 micrometers were also simulated (Table 2). All *Pxh* curves of these simulations showed a similar qualitative behavior, as illustrated in Figure 3.

Table 3 illustrates numerical results of the maximum indentation load in function of Young´s modulus in the interface for a model with a 3.00 µm thick film and a penetration depth of 50% of this thickness. It was considered to be optimal adhesion between film and substrate when the interface modulus was equal with the substrate, i.e., 238 GPa. The value of Young´s modulus was reduced gradually, where indentation testing with low adherence between the film and the substrate was simulated. The numerical results for indentation load show little change in its value in the function of the variation of the interface modulus and the number of plies of the interface. However, for low values of the modulus of elasticity, for example, less than 10.0 GPa, there is a significant reduction of indenter load, in both of the different models used to represent the interface.

The reduction in indentation load value shown in Fig. 4 illustrates the possibility of simulation of delamination of the film during the indentation testing, when reducing the value of Young´s modulus at interface. Another important result in these analyses was that the decrease in the indentation load was more pronounced when using two plies of elements in the interface.

Table 3 - Maximum indentation load as a function of Young's modulus of the interface for a system with a 3.00 μm thick film.

Young's modulus at interface (*GPa*)	Indenter load (*N*)	
	One ply of elements	Two plies of elements
238	70,75	70,72
200	70,74	70,71
100	70,72	70,66
20	70,54	70,31
10	70,31	69,88
7,0	70,13	69,53
5,0	69,89	69,06
4,0	69,68	68,67
3,0	69,33	68,03
2,0	68,67	66,96
1,0	66,90	63,60

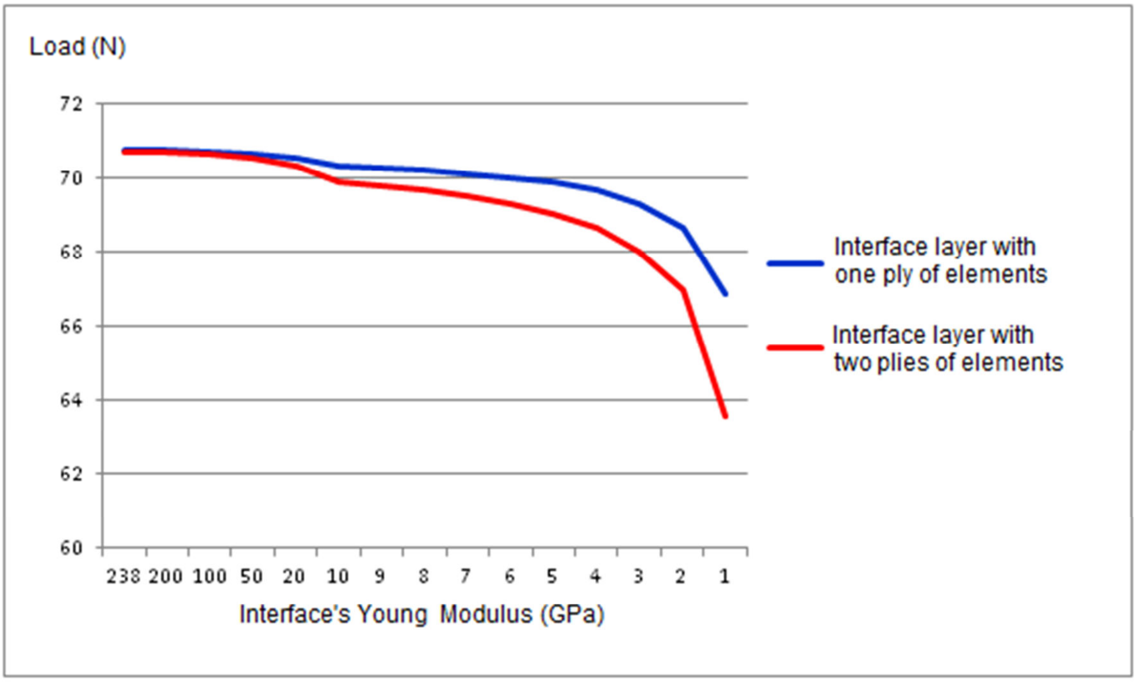

Fig. 4 - Behavior of the maximum indentation load as a function of Young's modulus of the interface for the analysed system.

At the end of this work, a comparison was made between the relative radial displacement of two neighbouring nodes positioned at the interface and at the same distance from the axis of symmetry. Figure 5a shows the behaviour of the radial displacement of these two nodes (nodes 103 and 8,633) for the model on which the interface was modelled with a layer of 0.0835 μm and with Young's modulus of 200 GPa. Figure 5b shows the same simulation, but with the interface Young´s modulus of 2.0 GPa. It could verify that for the lower Young's Modulus of interface there is a higher relative displacement for the previously mentioned neighbouring nodes. This slip indicates the occurrence of an interface delamination. These results are consistent with the one shown by Araújo and Dias (2014).

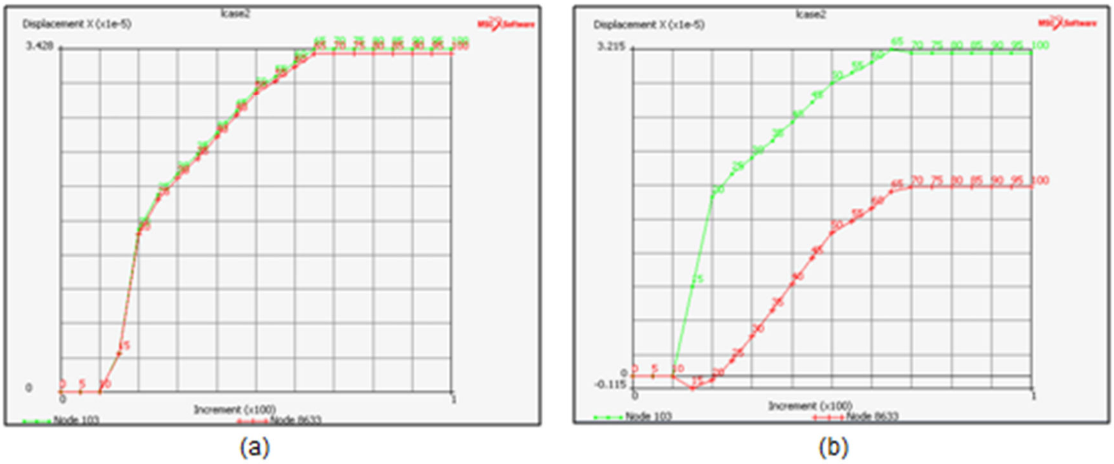

Fig. 5 - Graph of radial displacement between nodes 103 and 8,633 during indentation testing for a system with a 3.00 μm thick film and one ply of elements at interface. (a) Interface with Young's modulus of 200 GPa; (b) Interface with Young's modulus of 2.0 GPa.

Figure 6 shows the radial displacement of the behaviour of neighbouring nodes 103 and 8,634, depending on the variation of the elastic modulus of the interface. However, in these simulations, the interface was modelled with two plies of elements with a total thickness of 0.167 mm. The slip of the displacement in Figure 6 was greater when compared with the slip showed in Figure 5. That is, the delaminating process becomes evident in Figure 6 when the lower Young´s modulus at interface is used.

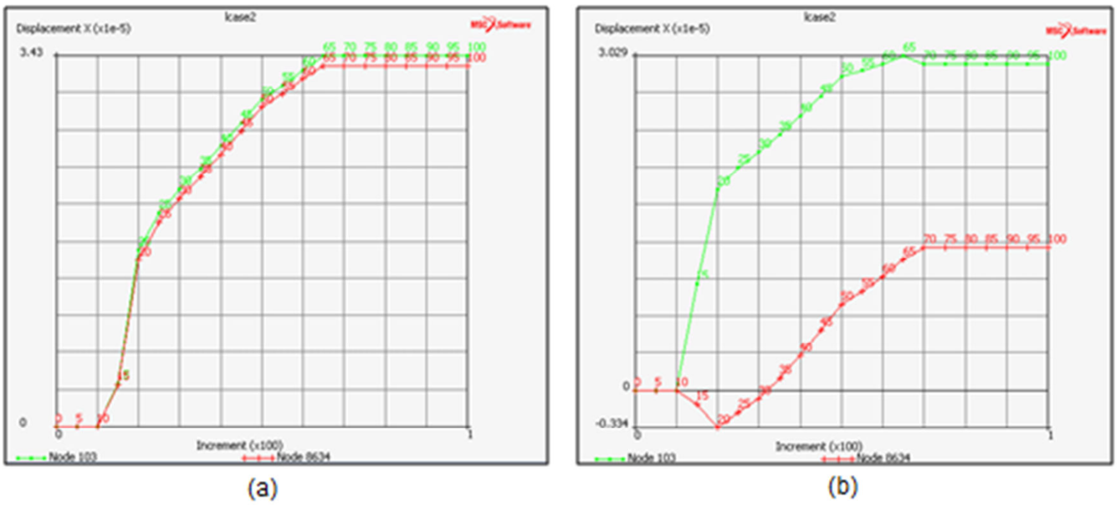

Fig. 6 - Graph of radial displacement between nodes 103 and 8,634 during indentation testing for a system with a 3.00 μm thick film and two plies of elements at interface. (a) Interface with Young's modulus of 200 GPa; (b) Young's modulus of 2.0 GPa.

In summary, for all simulations models, there was a decrease of the maximum indentation load by reducing the value of Young´s modulus at interface. There was also higher interface slip behaviour due to the decrease of Young´s modulus. On the contrary, for the simulated models with higher values of Young´s for the interface modulus, it was shown that the radial displacement behaviour of the nodes in question is similar in all indentation cycles. This result indicates that the interface model ensured adhesion between the film and the substrate, i.e., no delamination occurred.

Other studies found in the literature showed how to model the interface through decohesive elements (Pulécio, 2010, Fukumasu, 2015). However, to better simulate the behaviour of the interface, these models require knowledge of the fracture toughness of the film or interface (Fukumasu, 2015). These mechanical properties require destructive experimental testing and higher expenditures of time and money. The proposed numerical model has the advantage of avoiding further mechanical property simulations than those described in Table 1.

CONCLUSIONS

Based on the numerical results of the indentation test with spherical indenters using the finite element method, it was concluded that, from the global behavioural viewpoint, the models represented the indentation test in different systems composed of hard film (CrAlN) with different thicknesses deposited in a metallic substrate with high mechanical strength (AISI 4140 steel).

In this study, there was an attempt to represent the behaviour of the interface region during indentation testing by varying the refinement of the mesh, the value of its Young´s modulus and the number of ply elements. The results interestingly showed that the models could represent perfect adhesion between the film with the substrate and the weakest one. By evaluating these results through analysis of the maximum load indentation, it was possible to identify delamination of the interface region for the lowest values of its Young´s modulus.

However, there is still need for a more thorough numerical and experimental analysis in order to introduce a parameter capable of more representative modeling of film-substrate adhesion.

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