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NUMERICAL STUDY OF STRESSES DURING THE INDENTATION TESTING IN CERAMIC FILMS

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Abstract. *Nowadays, the need for components with high wear strength and better corrosion resistance has fostered a growing interest at the surface engineering. The search for better tribological properties of materials contributes to development of processes to increase the lifetime of components and their applications in ever harsher environments. Therefore, the thin ceramic coatings have been an option used to improve the tribological properties of components that operate under these conditions. However we must conduct experimental testings to evaluate the behavior of these films, specially, in the interface between the film and substrate. In another way, with the computational progress, the use of numerical analysis to solve many technological problems has been increasingly frequent, and currently allows its implementation with low costs. In this paper, It was proposed to simulating the spherical indentation test in ceramic coatings deposited on metallic substrate with a commercial finite element code. The main goal of this study was to evaluate the influence of friction between the indenter and the sample, as well as studying the behaviour of the stress field at the interface. Finally, it was proposed a new modelled to simulate the adhesion between the film and the substrate.*

Keywords*: Friction, FEM, Indentation Test.*

1. INTRODUCTION

The search for more resistant components that meet with greater confidence in more demanding applications, has driven advances in surface engineering. This area uses the technology of preparation and surface modification to fulfill specific functions within certain applications. The surface ceramic thin films have been one of the options being used to improve tribological properties. However, it is necessary to evaluate the mechanical behaviour of these films and their interface with the substrate. Currently, the instrumented indentation testing is used to evaluate the mechanical properties of these conjugated compounds of ceramic thin film on metallic substrate. Due to its versatility, numerous works have been developed in this field, studying new methodologies and applications for these testings. Recent studies suggest the use of indentation testings as a tool to obtain mechanical proprieties like the surface hardness (H), the modulus of elasticity (E), the Poisson's ratio (ν), the fracture toughness (K_{IC}) and a power law equation to elastoplastic deformation behaviour under compression (Zeng and Chiu, 2001, Lee, *et al* 2005, Dias and Godoy, 2010).

However, implementation of this indentation technique for evaluation of mechanical properties and their results still cause doubts in the scientific community. According to the literature, these problems are more intense when it comes to evaluating the mechanical behaviour of thin films deposited on soft substrates (Fischer-Cripps, 2006). One of the difficulties in carrying out instrumented indentation testing is that it requires high-precision equipment capable of monitoring very low loads (P) and small depths of penetration (h), to assess reliably the mechanical properties using micro and nano scales (Huang e Pelegri, 2007). Because these limitations in the analysis of indentation testings the use of a numerical technique able to evaluate the stress fields and deformation during the indentation cycle could help in a more reliable interpretation of this test. This numerical methodology was first studied using finite element models to evaluate the behaviour of different materials under indentation testing (Sun *et al*, 1995; Souza *et al*, 2001; Antunes *et al*, 2006; Dias *et al*, 2006; Dias and Godoy, 2010).

The Finite Element Method (FEM) has proven a reliable methodology for numerical analysis of stresses and strains and for the simulation of various engineering problems. This method has been widely used to simulate and solve many nonlinear problems in the areas of structural instability, dynamical systems, and fluid systems, electromagnetic and metal forming. Although, the use of this numerical technique to evaluate the indentation testing in thin films also has presented problems due to computational limitations, the difficulty in implementing the damage criteria, the difficulty to characterize these films, and especially in obtaining mechanical properties for the interface between the film and substrate.

Plastic deformation is a major concern in the design and performance of engineering components. Failure of hard film deposited on soft substrate system under many tribilogical situations is seldom caused by convencional wear but by debonding of the film from the substrate (adhesive failure), or fracture of the film (cohesive failure), or even by subsurface fracture (substrate failure). Accordingly, it is imperative to determine the spatial distribution of the plastic strain and the initiation and development of the plastic zone, so as to have the better undestanding of the mechanisms of surface and subsurface wear involving localized plastic flow (Sun *et al*, 1995).

The simulation proposed in this work used discrete models based on the MEF, to reproduce the spherical indentation testing (Brinell), as represented in Fig 1. The studied systems were formed by a metallic substrate alloy steel AISI 4140 coated with ceramic film of Aluminum Nitride with Chromium (CrAlN), with different thicknesses. To better understanding the interface behaviour, this region was modeled in such a way that permitted the simulation provided from a perfect adhesion between film and substrate to a weak adhesion. In the numerical procedure, it was evaluated the influence of friction between the indenter and the sample surface and their effects in the stress and strain fields.

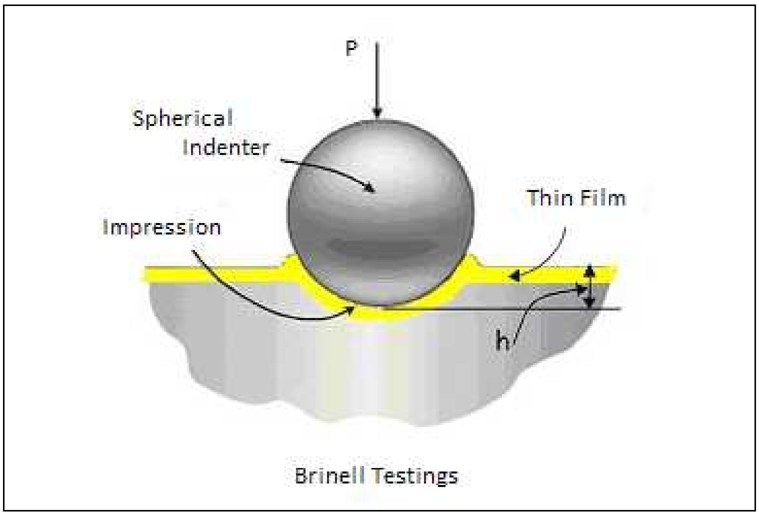

Figure 1. The Brinell Indentation Testing in Thin Film and *h* is the deep indentation.

2. MATERIALS AND METHODS

The numerical simulation performed in this work reproduced the spherical indentation testing in a system composed of ceramic thin film deposited on a metallic substrate, using commercial finite element software MARC™ (2007). The symmetry of the problem was considered and two dimensional axisymmetric elements were used in the model, which greatly reduced the complexity and computational effort need to analyze the problem. Also, the pile-up and sinking-in surface displacements, which can occur during the testing, were not taken into consideration in this work (Dias *et al*, 2010). Both the ceramic film of CrAlN as the substrate alloy steel AISI 4140 materials were modeled as homogeneous, isotropic, and represented through an elastic-plastic flow curve under compression, as Eq. 1. In this equation, σ_e, ε_e, n and σ_o are, respectively, the effective stress, effective deformation, the strain hardening coefficient and the yield stress. The other mechanical properties adopted, such as Young's modulus (E) and Poisson's ratio (ν), for the film and the substrate are shown in Table (1).

$$\sigma_e : \max\left[\left(K\varepsilon_e^n\right), \sigma_o\right] \tag{1}$$

The Fig. 2 shows the numerical behaviour of the indentation load versus depth of penetration during the indentation testing in a sample with a film 1.66 μm thick. The penetration depth during this testing was one third the thickness of film. The other results presented in this paper illustrate only the numerical behaviour of the testing using the film with 3.00 μm thick.

The interface was modeled as an elastic perfectly plastic material with 0.167 μm thick. To model the interface behaviour, it chose to vary its Young's modulus between 238 GPa to 2 GPa representing, respectively, a perfect adhesion to a weak. Also, it was adopted as the yield stress of this region the same value of the substrate, ie, 565 MPa.

In the numerical simulation of the indentation cycle, including both loading and unloading steps, a prescribed displacement scheme was used to guarantee a better control in the beginning and during all the indentation cycle. This procedure is consistent with experimental indentation testing, since the indenter displacement is applied with small penetration speed and the behaviour of the load versus displacement is obtained by the load sensor installed on the indenter table.

Table 1. Mechanical proprieties used in thin film and substrate (Dias and Godoy, 2010).

Material	E (GPa)	ν	σ_o (MPa)	K (MPa)	n
Substrate (Steel AISI4140)	238	0.29	565	2230	0.228
Thin Film (CrAlN)	350	0.22	3790	10615	0.229

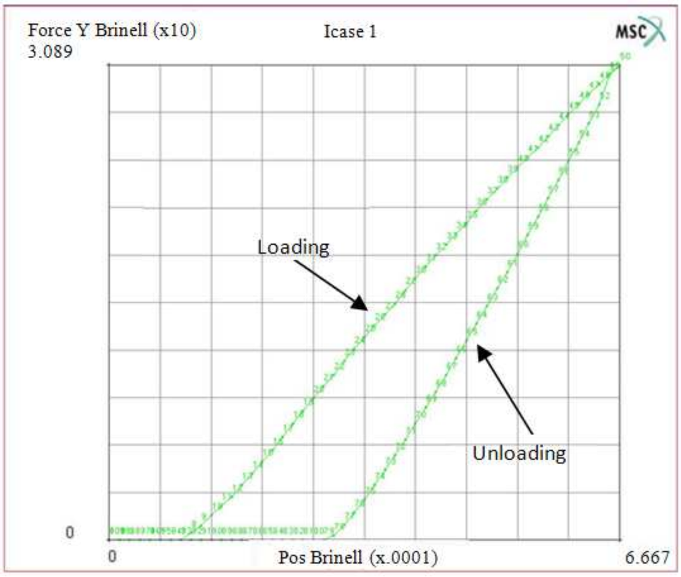

Figure 2. Load curve as a function of penetration depth of the Brinell indentation testing in a sample with film with 1.66 μm thick. The penetration depth was one third of the thickness of the film.

The spherical indenter was modeled as a rigid semicircular shell, with 400 μm diameter. The boundary conditions included a displacement restriction that was imposed to the base of sample and radial restrictions to the nodes localized in the axis of symmetry (Dias *et al*, 2010). The number of elements used in the mesh is showed in the Table (2) for the system to the film with 3.00 μm thick.

Table 2. Mesh characteristics of numerical model to the film with 3.00 μm thick.

System	Substrate (number of elements)	Film (number of elements)	Interface (number of elements)
CrAlN film – Steel AISI 4140 substrate	7920	945	105

In order to obtain a better distribution of stress and strain fields in the surface contact and in the interface between film and substrate, we used a more refined mesh in these regions, as showed in Fig. 3. Besides the numerical control, the simulation was development in two phases, one related to the indenter coming down, followed by its coming up. One hundred increments were used to represent the penetration of the indenter and one hundred to model its removal from the sample, completing the indentation cycle.

The dimensions of the sample were 0.3 mm in height and 0.5 mm in length. It was used four-node axisymmetric elements, with dimensions of 0.33 x 1.33 μm in the regions of the mesh refined. Assays were performed with three different depths of maximum penetration (h_{max}), namely 10%, 25% and 50% of the thickness of the film. It was also analyzed the influence of friction coefficient between the indenter and the surface sample. In the present work, it was used the following values for this friction coefficient: zero (no friction), 0.1; 0.2, 0.5, and 1.0.

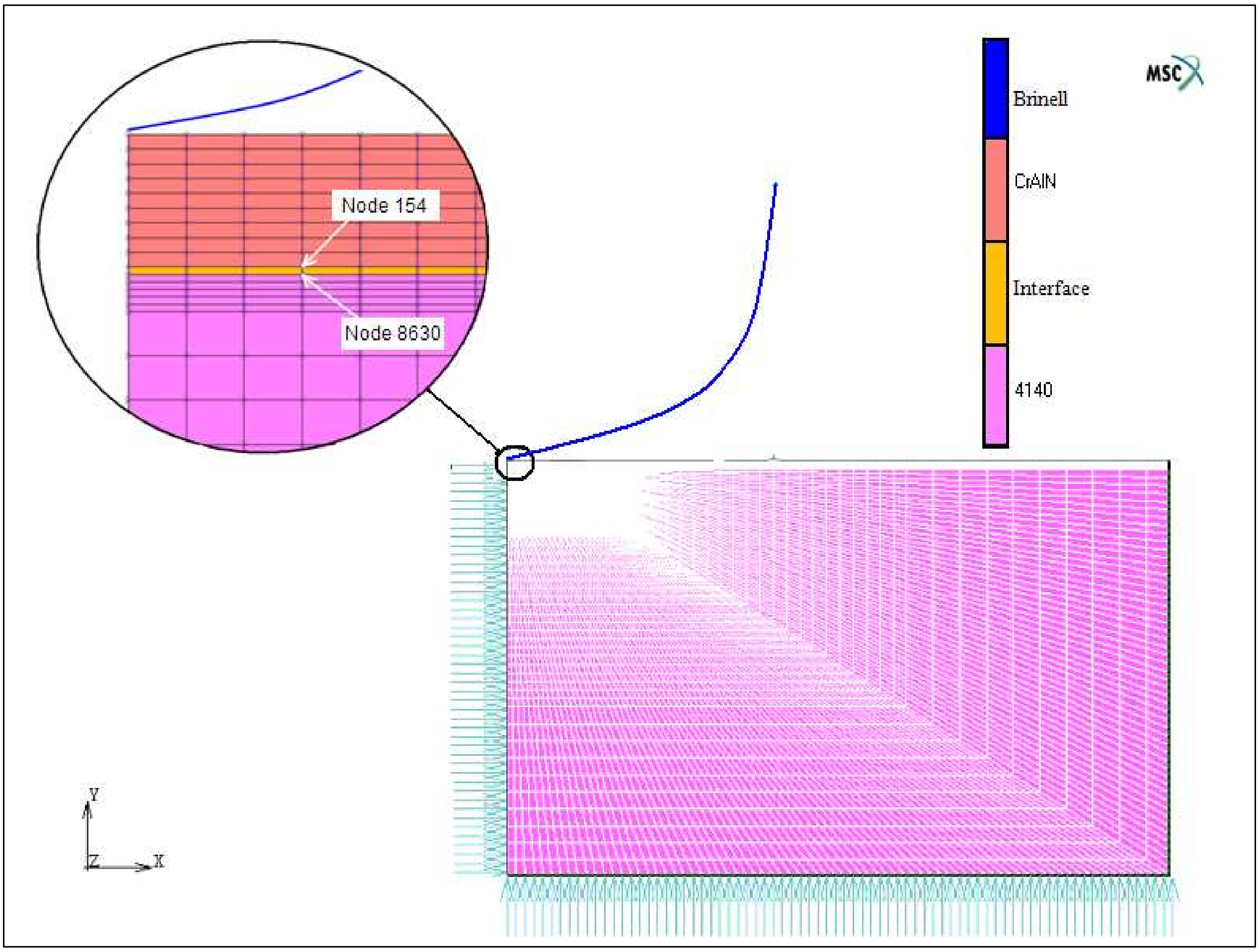

Figure 3. Numerical model of the Brinell indentation testing in a sample with thin film deposited in metallic substrate (CrAlN / AISI 4140). In the zoom picture, it was identified two nodes in the mesh at the interface between the film and the substrate.

3. RESULTS E DISCUSSIONS

Table 3 compares the numerical results for the indentation load as a function of the interface's Young modulus. It was considered perfect adhesion between film and substrate when the elastic modulus of the interface was equal to the substrate. Gradually diminishing the value of this modulus, it was expected to represent an indentation testing with a low adhesion between the film and the substrate. The numerical results for the indentation load showed little variation in its value as a function of the interface's Young modulus. Except for low values of the interface's modulus, eg, below 4 GPa, from which there is an appreciable reduction in the indentation load. It also notes that this behaviour is repeated for different depths of penetration. Figure 4 better illustrates the behaviour of indentation load as a function of the interface's modulus for different depths of penetration. The appreciable decrease in the amount of indentation load for low values of interface's Young modulus could indicate the possibility of simulating an adhesive failure or a delamination process.

Then, it was evaluated the behaviour of the maximum principal stress, Rankine theory, near the interface between film and substrate. The numerical results of the behaviour of maximum principal stress as a function of the interface's Young modulus are illustrated in Figure 5. In this figure, it was recorded the numerical behaviour of indentation testing in a sample with film 3 μm thick and the depths of penetration was 20% and 50% of film thickness. For according to the literature, indentation testings with penetration depths less than 10% of film thickness have no influence of the substrate strength and, consequently, have no influence the behaviour on interface (Ficher-Cripps, 2006; Dias and Godoy, 2010). The stress filed at the interface shows a similar trend of decrease of these results for low values of interface's Young modulus. The behaviour of this stress field repeated the behaviour of the indentation load as a function of the interface's modulus. The maximum principal stress at the interface seems to confirm the assessment that for low values of the interface's modulus could be representation indentation testing in films with their delamination. Since, in these cases, the stress field produced by the action of the indenter is distributed within the film, with little or no influence of the substrate.

Table 3. Maximum indentation load as a function of the interface's Young modulus in the film with 3 µm thick and different depths of penetration.

Interface's Young modulus (GPa)	Maximum indentation load (N)		
	h_{max}= 10% thickness film	h_{max}= 20% thickness film	h_{max}= 50% thickness film
238	20,15	36,10	70,88
200	20,10	36,01	70,73
100	20,04	35,95	70,68
50	19,94	35,84	70,60
20	19,67	35,52	70,35
10	19,25	35,04	69,97
9	19,17	34,95	69,90
8	19,06	34,84	69,80
7	18,94	34,72	69,68
6	18,78	34,54	69,53
5	18,57	34,32	69,34
4	18,27	34,04	69,06
3	17,82	33,54	68,66
2	17,06	32,71	68,02
1	15,42	31,14	66,85

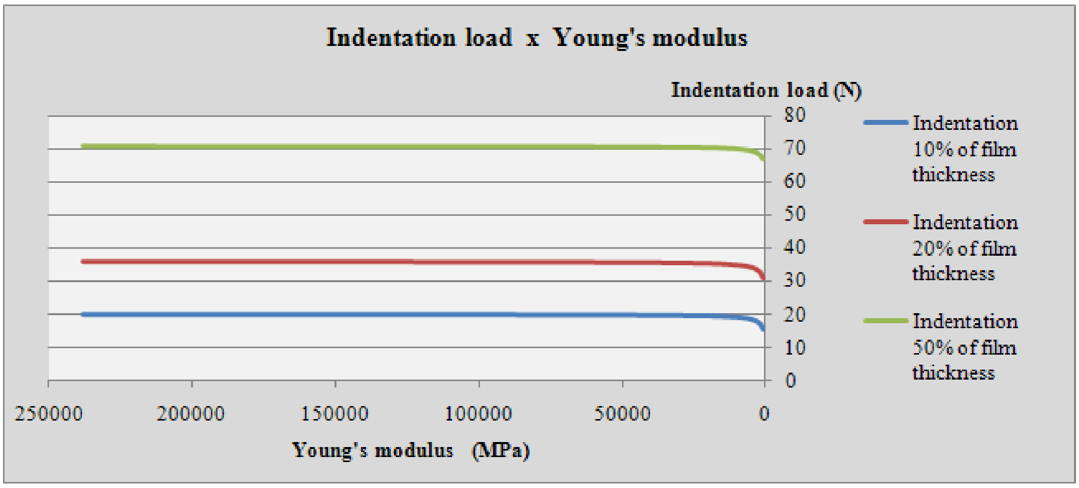

Figure 4. Indentation load (N) as a function of the interface's Young modulus (MPa) for different depths of penetration.

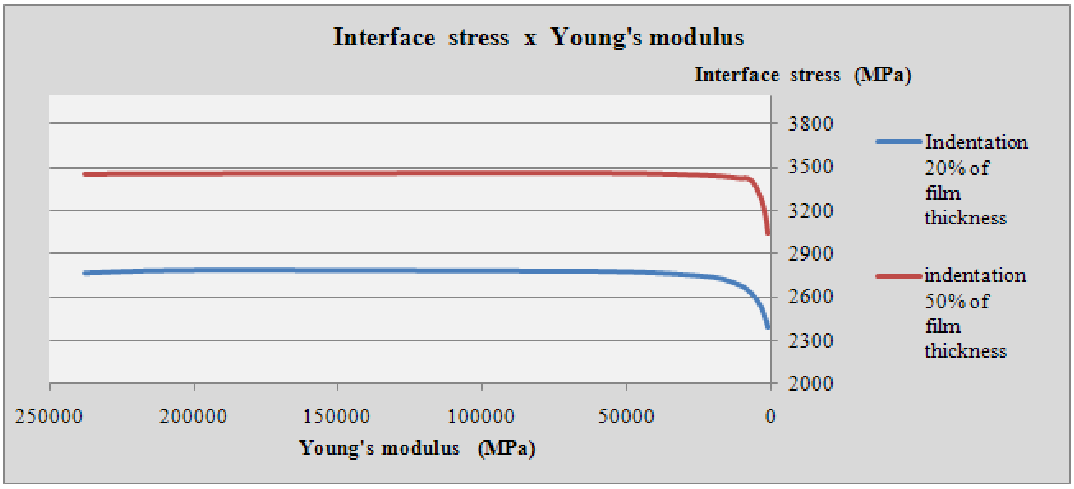

Figure 5. Maximum principal stress (MPa) in the interface region as a function of the interface's Young modulus (MPa)

The Figures 6 and 7 show the numerical results for maximum principal stress as a function of the interface's Young modulus at this region and considering different coefficients of friction between the indenter and sample. These results show that numerically the variation of coefficient of friction between the indenter and the film surface has influence on the distribution of the stress field in the film. The maximum principal stress at the interface increases with the increase of the coefficient of friction (Araújo *et al*, 2010; Huang e Pelegri, 2007; Bressan *et al*, 2004). Even with the increase of the coefficient of friction between the indenter and the sample, the the maximum principal stress behaviour at the interface decreases for low values of the interface's Young modulus. Once again, the numerical analysis showed the indentation testing cycle with a weak interface and, probably, during delamination process.

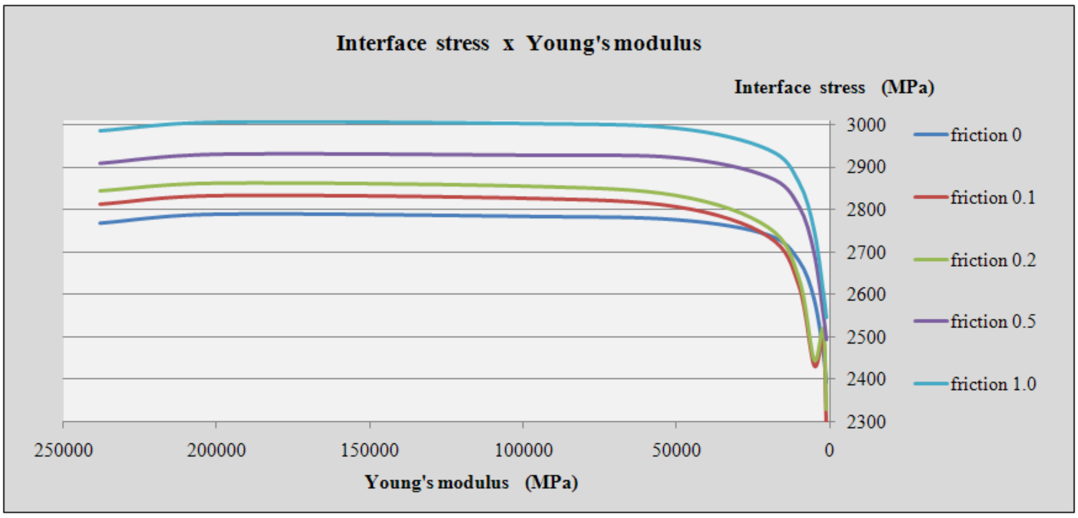

Figure 6. Maximum principal stress (MPa) as a function of the interface's Young modulus (MPa) for the penetration depth for 20% of film thickness, with friction between the indenter and the sample that ranged the zero to 1.0

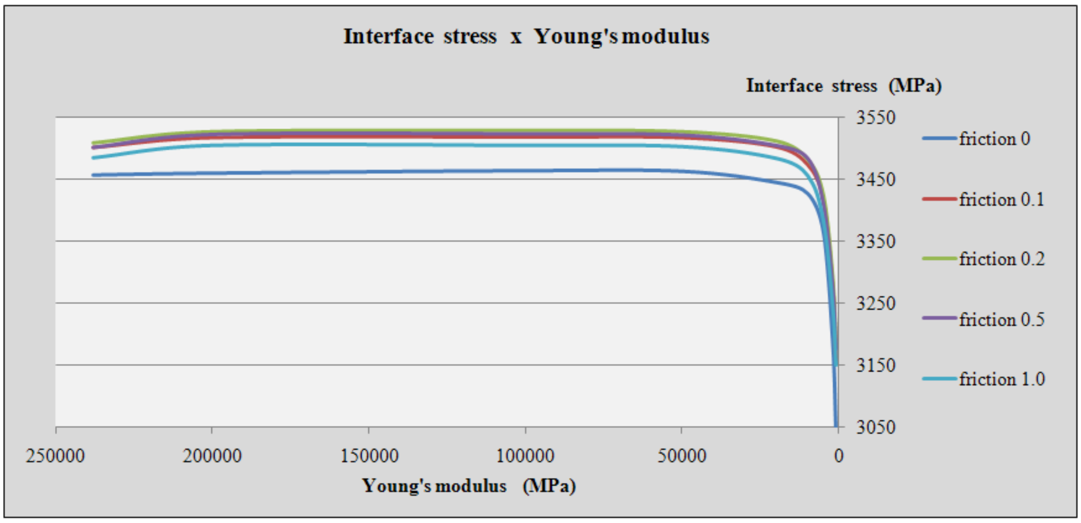

Figure 7. Maximum principal stress (MPa) as a function of the interface's Young modulus (MPa) for the penetration depth for half film thickness, with friction between the indenter and the sample that ranged the zero to 1.0.

Figure 8 illustrates different graphs for the displacement behaviour during the indentation cycle. It was used two nodes, that were located at interface, to obtain the results for radial displacement as a function of the interface's Young modulus. These results reproduced the simulation of the 3 mm thickness film and penetration depth of 20 % of its thickness. Node 153 was located at the interface near the film and node 8630 also located at the interface but near the substrate, as previously shown in Figure 3. The displacement of these nodes was evaluated in models with the interface's Young modulus between 2 GPa and 200 GPa, simulating from a stronger adhesion to a weaker one. For the higher values of the interface's Young modulus, there wasn't a significant slip between the two nodes, showing that the interface has remained the stronger adhesion between the film and the substrate. On the other hand, for lower interface's modulus, the behaviour of displacement in the radial direction during the indentation test of these two nodes took a very different way. This results seems to reinforce the indication of a delamination of the film.

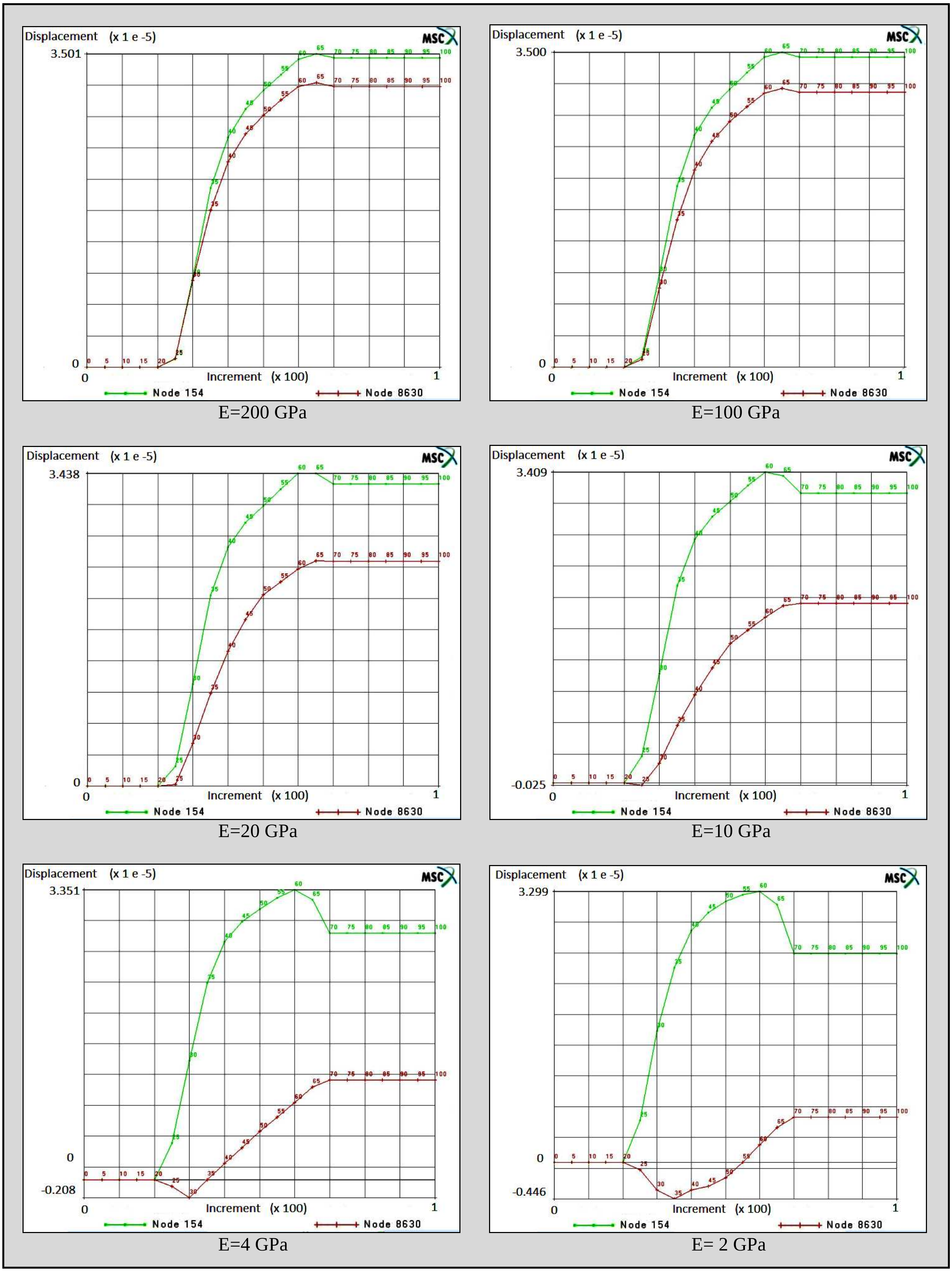

Figure 8. Different graphs representing the radial displacement of the nodes 154 and 8630 during the indentation testing for different values of the interface's Young modulus.

4. CONCLUSIONS

In this study it was simulated the Brinell indentation testing on different systems consisting of a hard film (CrAlN) deposited on a metallic substrate (AISI 4140), using the finite element method. It was used a new numerical model to represent the interface behaviour using a very fine mesh and varying its elastic modulus. The stress field was evalueted in the film for different models with the incorporation of layer capable of representing the interface behaviour that represented a perfect adhesion between film and substrate to a weak adhesion. It was also possible to evaluate different coefficient of friction between the indenter and sample, studying their influence on the stress field of the film.

In all simulations, it was found that friction coefficient has significant influence on the stress field, including the region of the interface. The simulations were also able to model the adhesion between film and substrate. The results showed the possibility of adhesive failure in the use of models with low values of the interface's Young modulus. In these systems with low adhesion between the film and the substrate there was a decrease in the tribological properties of the system, since it showed a low load indentation. Moreover, it could observed a great difficulty to numerically represent the real system film/substrate.

Finally, it is also necessary a deep analysis of these numerical procedures to improve the parameter proposed here can model more representative of the adhesion between coating and substrate.

5. ACKNOWLEDGEMENTS

This research work was supported by FAPEMIG (Foundation for the Support of Research in the State of Minas Gerais).

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