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Molecular dynamics simulation of nanoindentation in Cr, Al layers and Al/Cr bilayers, using a hard spherical nanoindenter

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Abstract

Three-dimensional molecular dynamics (MD) simulations of a nanoindentation technique using the hard sphere method for Cr (bcc) and Al (fcc) thin films and (Cr/Al)_n (n=1,2) systems were carried out. For the model implementation, Morse interatomic potential was used for describing the single crystal interaction and the contact between Cr and Al structures. On the other hand, fixed boundary conditions were used and the repulsive radial potential was employed for modeling the spherical tip, and ideal mechanical properties at 0 K were obtained by simulating load-unload curves. Bilayers presented higher hardness and Young's modulus than Cr and Al layers. Moreover, the region of atoms movement after the unload process shows a continuous parabolic boundary for Al and Cr layers and a discontinuous boundary for the bilayers caused by the interfaces.

Keywords: Hardness; Interface; Morse potential; Nanoindentation; Young's modulus.

Simulación del proceso de nanoindentación con dinámica molecular en capas de Cr y Al y bicapas de Al/Cr, empleando un nanoindentador esférico

Resumen

En este trabajo se realizaron simulaciones empleando dinámica molecular tridimensional aplicada a la técnica de nanoindentación, usando el método de la esfera dura en películas de Cr (bcc), Al (fcc) y sistemas (Cr/Al)_n (n=1,2). Se empleó un potencial interatómico de Morse con el fin de describir la interacción en cada cristal y el contacto entre las estructuras de Cr y Al. Se emplearon condiciones de frontera fijas y un potencial radial repulsivo para modelar la punta esférica del indentador. Con estas condiciones se obtuvieron las propiedades mecánicas ideales a 0 K, simulando curvas de carga-descarga. Las bicapas presentaron dureza y módulo de Young altos, comparados con valores obtenidos en capas de Cr y Al. Además, la región de los átomos en movimiento después del proceso de descarga muestra un límite parabólico continuo en las capas de Al y Cr, y límites discontinuos en las bicapas, causados por las interfaces.

Palabras clave: Dureza; Interfase; Modulo de Young; Nanoindentación; Potencial de Morse

1. Introduction

Thin films have been widely used for improving contact surfaces' performance for applications such as magnetic storage devices, hard coatings, microelectromagnetics mechanisms among others [1-4]. Nevertheless, there is a remarkable difference between mechanical properties of materials in bulk and thin films. This difference is higher when

films are produced as single thin films and multilayers, the latter presenting better mechanical behavior because of the interface presence. On the other hand, the most useful technique for measuring mechanical properties in systems with low dimensions such as thin films is nanoindentation, as it uses very small loads, in the order of nanonewtons (nN) [5]. This method uses an indenter with a known geometry that comes into contact in a specific place of the surface applying a load.

For this type of tests on the nanometer scale, complex and expensive equipment and a long time for analysis are needed. One alternative for studying mechanical properties at a nanometer scale is the use of modeling and simulation techniques that allow understanding the materials behavior in a deeper way. For example, molecular dynamics (MD) is one of the most used methods for this kind of studies [6]. MD simulations are a powerful tool for studying material properties in different fields such as bioscience, chemistry and material science among others [7]. Because of the computational technological developments, now simulations including a hundred million atoms can be developed.

Recently, several works employing MD for simulating the nanoindentation process for studying mechanical properties of thin films and multilayers using different interatomic potentials have been reported. For example A. Ritcher et al. [8] compared experimental and theoretical results of mechanical properties for a nanoindentation method applied to several forms of carbon materials with different mechanical properties, namely diamond, graphite and fullerite films. Molecular dynamics simulations of the indentation process have been performed. Although results were not in the same magnitude because of computing power limitations, the simulations capture the main experimental features of the nanoindentation process showing the elastic deformation that takes place in both materials. In the case of thin films, P. Peng et al. [9] investigated the nanoindentation of aluminum thin film on a silicon substrate by three-dimensional MD simulation, combined with the Lennard-Jones (LJ) potential for describing the interaction at the film-substrate interface. Results showed that the hardness of the film increased with the loading rate. A. K. Nair et al [10] studied the indentation response of Ni thin films of nanoscale thicknesses using molecular dynamics simulations with the embedded atom method (EAM) interatomic potentials. The simulation results for single crystal films show that the contact stress necessary to emit the first dislocation under the indenter is nearly independent of film thickness. In the literature, there are other works showing similar studies to those presented before [11-13]. Regarding multilayers simulation, the literature reports several works that include the influence of the interface presence. T-H Fang et al. [14] applied MD simulations combined with the tight-binding second-moment approximation and Morse potentials for studying the effects of indention deformation, contact, and adhesion on Al, Ni, and Al/Ni multilayered films. Results show that when the indention depth of the sample increased, the maximum load, plastic energy, and adhesion increased. L. Ming-Liang et al. [15] carried out molecular dynamics simulation to investigate the nanoindentation behavior of a Cu(100)/Cu(110) bilayered thin film. It was found that at the indenting stage, the maximum indentation load of the bilayered thin film is lower than that of its constituents; however, they have nearly the same maximum indentation load. Similar studies were carried out by Y. Cao et al. [16]. In these works the indenter was assumed to be a rigid probe with a great number of carbon atoms; nevertheless, considering that the indenter does not present any deformation, it could be considered as a perfect rigid and

structureless sphere capable of repulsion of all atoms in contact with it. The spherical shape is not far from the real case, because although in experimental measurements the most used shape of indenter is a pyramid, the indenter vertex has always a finite curvature radius of several tens of nanometers; therefore, it would be reasonable to consider it a spherical indenter, taking into account the scale of MD simulations. This type of indenter has been used by A. V. Bolesta and V.M. Fomin [17] for Cu thin films using the DM code LAMMPS. Nevertheless, this method has not been used for multilayer coatings. In this work we present similarities between mechanical properties in a study of Al, Cr and Al/Cr coatings obtained by MD simulations, combined with Morse potential, and a simple indenter with a spherical shape, and experimental results.

2. Model Description

Molecular dynamics simulations for carrying out nanoindentation tests were carried out for Cr, Al, Al/Cr and (Al/Cr)₂ coatings. The indenter was assumed to be a totally rigid and structureless sphere of diamond with diameter of 12 nm [14]. The sample was considered to be films with well-defined atoms in thermal equilibrium at 0 K, orientation in the plane (100) and of equal thickness. The samples size was $L \times L \times d = 20 \times 20 \times 8 \text{ nm}^3$ (where L is the dimension in the x - y plane and d is the thickness of each layer). The system construction for the case of two Al/Cr bilayers is present in Fig. 1.

Fixed boundary conditions were considered, but the x - y dimensions were large enough in order to avoid the edges influence on the results obtained. Movement equations combined with the Verlet algorithm with a time interval of 0.92 fs [18] were used. The maximum penetration depth of the tip is 2 nm at a speed of 4.3 m/s, in order to guarantee a The nanoindentation was carried out controlling the spherical indenter position, simulated by means of a repulsive potential with the atoms of the sample surface. The repulsive potential for the indenter is described by: time relaxation between two consecutive simulation steps.

$$F = A(R - r_i)^2 \quad (1)$$

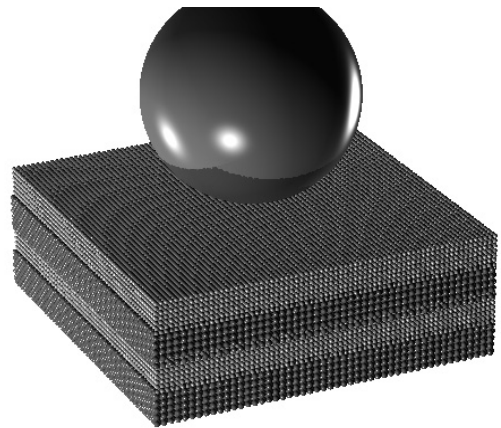


Figure 1. 3D scheme for the (Al/Cr)₂ sample and spherical nanoindenter employed for molecular dynamics simulations
Source: The authors

Where A is a constant related to the indenter effective stiffness, R is the indenter radius and r_i is the distance between the center of the indenter and the i -th atom belonging to the sample. Values used in this simulation for A and R are 44.14 eV/Å³ and 6 nm respectively. These values were taken evaluated from the work carried out by Lilleodden et al. [19].

The load acting on each individual atom was obtaining by adding two contributions: the first part considers the interaction between the atom and its neighbors; the second part represents the repulsive potential between the atom and the indenter. The Morse potential (Eq. 2) was selected for this simulation because it is computationally simpler and according to several author including Ziegenhain et al. [20] its results are similar to those obtained by using a EAM potential

$$U(r_{ij}) = D \left(e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)} \right) \quad (2)$$

Where D is the dimmer energy, r_0 is the equilibrium distance and α is the fit of the bulk material modulus and r_{ij} is the distance between two atoms in the sample. The interatomic energies for Cr-Cr, Al-Al and Cr-Al were obtained from the Lorentz-Berthelot mixing rule [21]:

$$D_{A-B} = (D_A D_B)^{1/2} \quad (3)$$

$$\alpha_{A-B} = \frac{1}{2}(\alpha_A + \alpha_B) \quad (4)$$

$$r_{oA-B} = (\sigma_A \sigma_B)^{1/2} + \ln \left(\frac{2}{\alpha_{A-B}} \right) \quad (5)$$

$$\sigma_A \sigma_B = r_{oA-B} + \ln \left(\frac{2}{\alpha_{A-B}} \right) \quad (6)$$

Where D_{A-B} , α_{A-B} , and r_{oA-B} are the fit energy, lattice constant and equilibrium distance for A-B compound and D_A , D_B , α_A , α_B , r_{oA} and r_{oB} are the same parameters for A and B elements respectively. The Morse potential parameters for Cr and Al are listed in table 1.

The reduced Young's modulus (E^*) is obtained from Eq. (7) which takes into account the combination of the tip and film elastic effects [23].

$$E^* = S \frac{\sqrt{\pi}}{2\beta\sqrt{A_c}} \quad (7)$$

Where $\beta = 1$ for a spherical indenter, S is the slope of the unload curve initial part and A_c is the projected contact area at a maximum load. The Young's modulus of the sample E_s is obtained from the expression:

$$\frac{1}{E^*} = \frac{1-\nu_s^2}{E_s} + \frac{1-\nu_i^2}{E_i} \quad (8)$$

Where E_i and E_s are the indenter and sample Young's moduli, ν_i and ν_s are Poisson coefficients of the indenter and sample respectively. The contact area, A_c , depends on the indenter radius R and the contact depth h_c , and is given by

$$A_c = \pi R h_c \quad (9)$$

Where h_c can be expressed as:

$$h_c = h_{\max} - 0.72 \frac{P_{\max}}{S_{\max}} \quad (10)$$

h_{\max} being the maximum penetration depth, P_{\max} the maximum load and S_{\max} the maximum slope of the unload curve. The material hardness H is defined as the local resistance to the plastic deformation; then, it is determined from the indentation maximum load divided by the contact project area, according to:

$$H = \frac{P_{\max}}{A_c} \quad (11)$$

3. Results and Discussion

Fig. 3 shows the load-unload curve obtained from indentation simulations for Cr, Al Al/Cr and (Al/Cr)₂ at a temperature of 0 K. the maximum load reached by the indentation depth at approximately 2 nm is 144 nN and 202 nN for Al and Cr respectively. For samples with one and two bilayers, the load was increased being 272 nN and 302 nN, respectively.

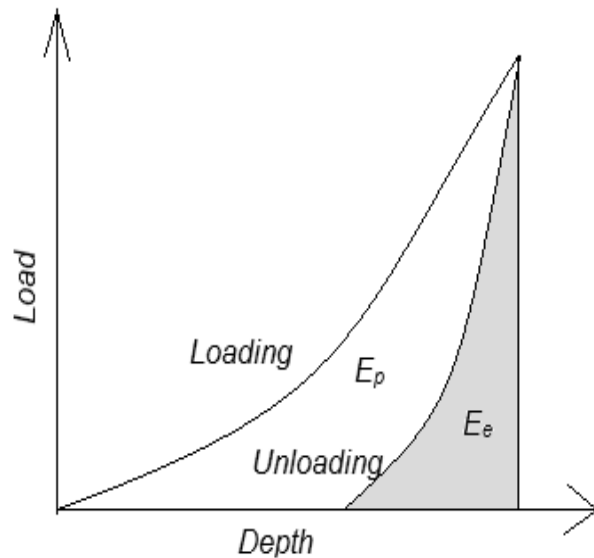


Figure 2. Scheme of a typical load-unload curve for a nanoindentation process showing elastic and plastic deformation energies.

Source: The authors

Table 1.
Morse Potential parameters for Cr and Al.

Material	D (eV)	α (Å ⁻¹)	r_0 (Å)
Cr-Cr	0.4414	1.5721	2.754
Al-Al	0.2703	1.1650	3.253
Al-Cr	0.3454	1.3686	2.990

Source: Adapted from [22]

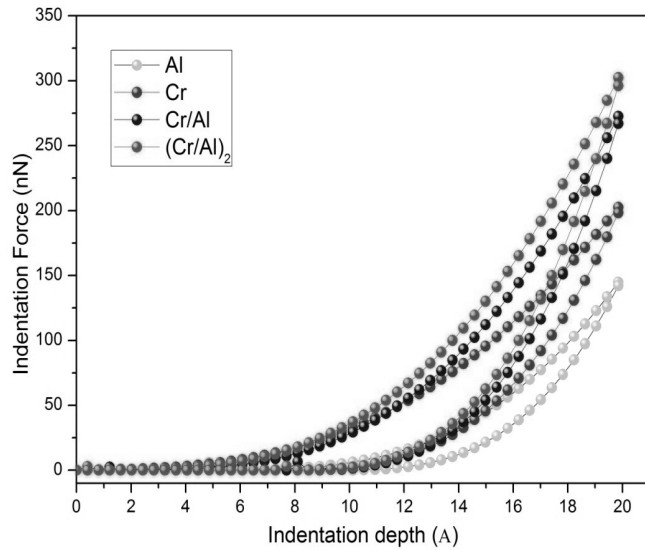


Figure 3. Load-unload curves for Cr, Al, (Al/Cr) and (Al/Cr)₂ obtained by MD simulations.

Source: The authors

From the load-unload curves of Fig. 3, values of hardness (H), effective Young's modulus ($E^* = E_s / (1 - \nu_s^2)$), plastic deformation energy (E_p) and elastic deformation energy (E_e) were obtained. The coefficient of energy dispersion (η), is calculated from the expression $\eta = E_p / (E_e + E_p)$. These values are listed in Table 2. Similar results were shown by Saraev and Miller [25].

The hardness value for Al is similar to that reported by Peng et al. [9] using MD. Experimental studies report hardness for Cr of 7 GPa [26], similar to that obtained in this work. Results show higher hardness for Cr than for Al in the case of one and two bilayers, the hardness is increased above the values obtained for single thin films, even greater than the value obtained from the mixing rule (5.41 GPa). This hardness evolution is in agreement with that reported in the literature by using nanoindentation experimental tests for Ag/Ni [27] and Cu/Ni [28] systems. There is a semi-coherent interface generated between the Al substrate and the Cr thin film due to the large mismatch of lattice parameters (fcc-bcc), and misfit dislocation networks formed at the interface accommodating this mismatch. The interface, caused by mismatch of lattice parameters, applies a repulsive force to prevent continuous dislocation slip. With successive emission of dislocations from the indented free surface, more dislocations are propagated toward the interface. It causes a pile up of dislocations on the interface, leading to significant work-hardening of Al/Cr coatings [16].

Table 2.
Mechanical properties obtained for the films during the load-unload test.

Material	H (GPa)	E* (GPa)	E _p (nN-m)	E _e (nN-nm)	η
Al	4.42	65.7	54.5	37.1	0.59
Cr	6.41	77.5	46.8	62.3	0.43
Al/Cr	8.53	114.5	49.4	78.8	0.38
(Al/Cr) ₂	9.51	125.6	59.3	89.1	0.40

Source: The authors

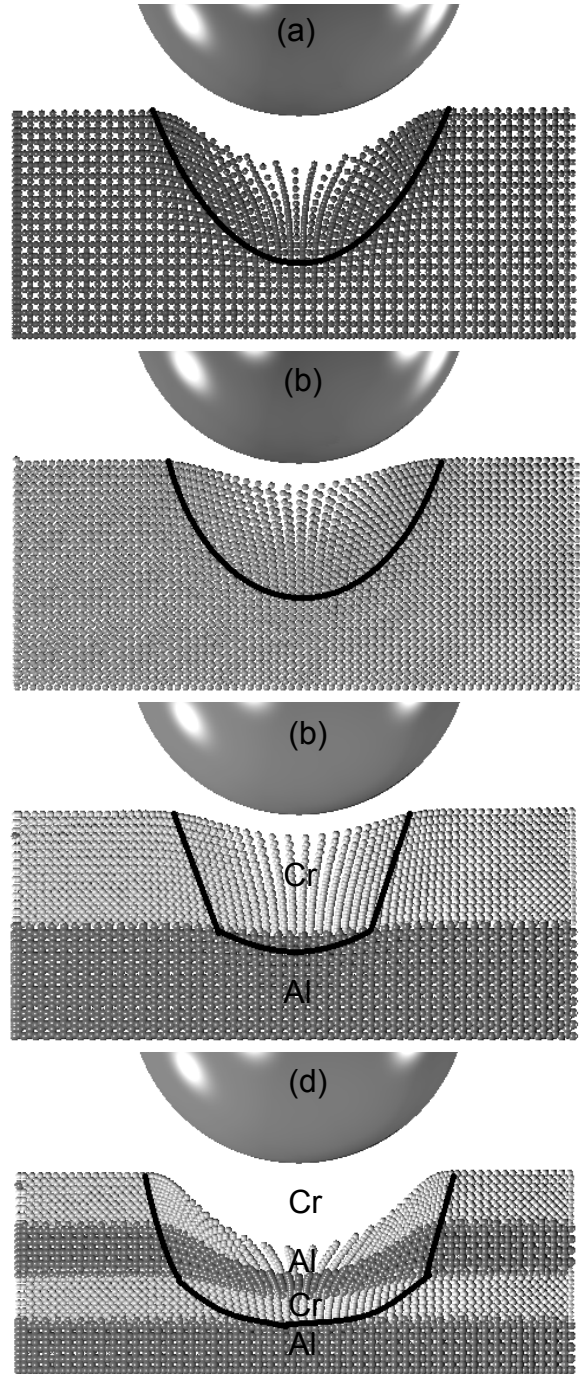


Figure 4. Cross section of the simple and nanoindenter system presenting the movement of atoms (a) Al, (b) Cr, (c) Al/Cr and (d) (Al/Cr)₂

Source: The authors

The Young's modulus of Al obtained was 70 GPa, similar to that reported by Fang et al. [6]. In the case of Cr, no reports for Young's modulus obtained by simulation were found. In experimental tests, a value of 300 GPa was determined, different to the value obtained in our simulations, possibly because in the experimental studies the sample is polycrystalline. The value of η that is associated to the tendency for plastic deformation of the films [29], shows a greater value for Al compared to the

other films. The response to the plastic deformation is greater in single layers than in multilayers. The interface creation generates a reduction in the coefficient of energy dissipation; then, multilayer interfaces act as a barrier for the plastic deformation. In other words, interfaces are considered as zones of dissipation energy [30]. In the case of two bilayers, η is also higher than it for one bilayer, possibly because the shear modulus between the materials in contact is similar.

Fig. 4 shows the movement of the atoms driven by dislocations and gliding mechanisms for different samples. The line in the images describes the boundaries of this movement. In Fig. 4 (a) and (b), the movements for Al and Cr layers are presented respectively, describing a parabolic boundary without any discontinuity. On the contrary, For Al/Cr and (Al/Cr)₂ (Fig. 4 (c) and (d) respectively) the continuity of the parabola is interrupted by the presence of interfaces, indicating that the atoms' movement decreases as the interfaces appear.

The Cr atoms try to recover their positions after the unload process; nevertheless, the plastic behavior of Al produces dislocations as is shown in Fig. 4 (d).

4. Conclusions

A nanoindentation study for films in single layers, (Al and Cr) and (Al/Cr and (Al/Cr)₂), was carried out using molecular dynamics simulations, combined with Morse potential, and using a totally rigid and structureless spherical tip as an indenter. Mechanical properties were evaluated from the load-unload curves, determining the hardness and Young's modulus. The influence of the interface between two different materials on mechanical properties was evaluated. The coefficient of energy dissipation is greater for Al than for other films. The region of atom movement after the unload process describes a parabolic volume for single thin films. In the case of bilayers this zone presents discontinuities caused by the interfaces.

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