The Significant Application of FEM to Evaluate the Mechanical Properties of Thin Films

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Abstract:
Currently all the automobile, mechanical, electronics and other industries are looking to improve the performance of the materials in their application point of view. But it is very difficult to find the materials to fulfill the requirement and to assess their reliability and to predict failures. To overcome this problem all the industries are utilizing applications of thin films and coatings. The extraction of mechanical properties of these by using FEM is relatively new. In this work Nylon coatings are deposited on the Soda-lime glass substrates and finally find the mechanical properties of the film materials.

1. Introduction:

   The indentation technique was introduced for the first time in the 19th century. It was primarily used to measure hardness \( H \) of the material. Historically, the indentation was done by indenters of various shapes, thus leading to a variety of tests and analytical definitions of hardness. The indentation technique, called nanoindentation (A. Bolshakov, W.C. Oliver and G.M. Pharr), was introduced in 1992 to examine mechanical properties such as elastic moduli \( E \) of investigated materials. Currently, the nanoindentation technique is used to find the mechanical properties of common applications in the biological field (teeth and bone), the semiconductor industry, ceramics, thin films, polymers, and most recently microelectronics and MEMs testing, etc.

2. Introduction to indentation:

   A popular application of contact mechanics is found in depth-sensing or instrumented indentation; this type of indentation testing is usually applied to depths of penetration in the sub-micron range and is termed “nanoindentation”. In this type of test, the applied load and the depth of penetration of an indenter into the specimen are recorded and used to indirectly determine the area of contact and hence the hardness of the test specimen.
The Berkovich indenter [Ch. Srinivasa Rao and C. Eswara Reddy], [M.V.Ramesh Kumar and R.Narasimhan] is generally used in small-scale indentation studies and has the advantage that the edges of the pyramid are more easily constructed to meet at a single point, rather than the inevitable line that occurs in the four-sided Vickers pyramid. The face angle of the Berkovich indenter normally used for nanoindentation testing is 65.27°, which gives the same projected area-to-depth ratio as the Vickers indenter. Originally, the Berkovich indenter was constructed with a face angle of 65.03°, the tip radius for a typical new Berkovich indenter is on the order of 50–100 nm.

The three-sided Berkovich indenter is the most popular geometry for nanoindentation testing since the tip of the indenter can be made very sharp and avoids the line of conjunction usually found in a Vickers indenter. The contact area can be calculated from geometry for a Berkovich indenter of face angle “θ”, and then the area is given by:

\[ A = 3\sqrt{3}h_c^2 \tan^2 \theta \]  

Where \( h_c \) is the distance measured vertically from the indenter tip.

If \( d \) is the length of one side of the triangular impression, then the projected area of contact is given by:

\[ A = \frac{1}{2} \sqrt{3}d^2 \]
Treating that the contact is an axis-symmetric cone, the contact between a rigid conical indenter and an elastic half space is found from

\[ P = \frac{\pi a}{2} E^* a \cot \alpha \]  \hspace{1cm} (3)

Where \( \alpha \) is the effective cone semi-angle (65.27º Machining equipment) for a Berkovich indenter [Ch. Srinivasa Rao and C.Eswara Reddy]. The quantity \( a \cot \alpha \) is the depth of penetration \( h_c \) measured at the circle of contact.

Historically, it was noted that the initial unloading response for many materials was linear. This implied that the contact conditions were those of a cylindrical punch instead of a cone where:

\[ P = 2aE' h \]  \hspace{1cm} (4)

Where \( a \) is the radius of the indenter equal to the radius of the circle of contact and where it should be noted that the depth of penetration is linearly dependent on the load.

The derivative of the load \( P \) with respect to the displacement \( h \) (the contact stiffness) is given by:

\[ \frac{dp}{dh} = \frac{2E \tan \alpha}{\pi} \]  \hspace{1cm} (5)

Substituting into equation 6, then we get

\[ P = \frac{1}{2} \frac{dp}{dh} h \]  \hspace{1cm} (6)

If the total depth of penetration is \( h_{max} \), at load \( P_{max} \) then as the load is removed, the indenter moves through a distance \( h_c \) as shown in Fig.1.

\[ h_c = h_{max} \left\{ \frac{2(\pi - 2)}{\pi} \right\} \frac{dP}{dh} \]  \hspace{1cm} (7)

Where \( P_{max} \) and \( dP/\text{dh} \) are measured during an experiment. The square-bracketed term in Eq.7 is often given the symbol \( \epsilon \) and evaluates to 0.72 but it is common practice to use a value of 0.75 since this has been shown to account for non-uniformities in the material response as the load is withdrawn.

Once a value for \( h_c \) has been determined, the area of contact is found from Eq.1 where, for a Berkovich indenter (\( \alpha = 65.27^\circ \))

\[ A = 24.5 h_c^2 \]  \hspace{1cm} (8)

From the above equations the reduced elastic modulus is found that

\[ E^* = \frac{dp}{dh} \frac{1}{2} \frac{\sqrt{\pi}}{\sqrt{A}} \]  \hspace{1cm} (9)

Experiments and finite element analysis shows that a correction factor \( \beta \) is needed for Eq. 10. The correction factor is applied as the factor \( 1/\beta \) to the measured value of \( dP/dh \). Accordingly we have:
\[ E^* = \frac{1}{\beta} \frac{dp}{dh} \frac{\sqrt{\pi}}{2\sqrt{A}} \]  

(10)

and so Eq. 9 becomes

\[ h_c = h_t - \epsilon \beta \frac{F_{\text{max}}}{dp/dh} \]  

(11)

Where \( dp/dh \) is the actual experimental quantity. There are various estimates and explanations of the value of \( \beta \) in the literature, the most popular being that of King at 1.034\(^3\). From this test the hardness of a thin film is obtained by the well known relation:

\[ H = \frac{P_{\text{max}}}{A} \]  

(12)

3. Finite element analysis:

Finite Element Method (FEM) is one of the most widely used technique, for analyzing mechanical loading characteristics in modern engineering components. Traditional analysis techniques can only be satisfactorily applied to a range of conventional component shapes and specific loading conditions.

A number of problems in contemporary engineering can be solved by numerical modelling. There are a number of modelling techniques but the analysis presented here exploits the FEM method, using ANSYS 11. In fact, FEM models and data analysis of nanoindentation experiments can accurately describe the loading and unloading stages.

One of the benefits of FEM models is they can exploit different mathematical models of materials. For example, they are suitable for investigating elasticity, elastoplasticity, or even viscoelasticity, with or without the hardening effect. In addition, it can be used to simulate nanoindentation, either using 2D or 3D models. Based on several numerical experiments, it was found that 2D ax-symmetric numerical models are precise enough to simulate nanoindentation. Figure 3a shows an example of a 2D FEM model, and in Fig. 3b corresponding experimental data are shown and the data fit curve provided by numerical analysis.

3.1. Material properties:

Table 1: Input to the model

| S.NO | Material          | Young’s modulus E (GPa) | Poisson’s ratio (\( \nu \)) |
|------|------------------|-------------------------|-----------------------------|
| 1    | Soda lime glass | 72                      | 0.23                        |
| 2    | Nylon            | 105                     | 0.38                        |
| 3    | Diamond indenter| 1140                    | 0.07                        |

Specimen size 700,000×700,000 nm  
Film thickness 2\( \mu \)m  
Indenter radius 1.5mm and 2mm  
Load 10mN-50mN.
3.2. Boundary Conditions:

Along the axis of symmetry, roller boundary conditions are applied [Ch. Srinivasa Rao and C.Eswara Reddy], all the nodes on the y axis can only have the displacement in y direction. The x direction displacement is set to zero. The bulk material or substrate base is constrained by fixed boundary conditions. All the nodes on the base cannot move in any directions, and the nodes on the upper surface of the indenter are coupled together. In this way, those nodes have the same y displacement. The load applied to the indenter is the displacement load. This kind of load can help avoid the convergence problems caused by initial contact gap.

![2D FEM model](image1)

![load-displacement curve](image2)

3. Results and Discussions:

The Finite Element Analysis was performed on the nylon 6, (6/6) thin layers. The test is performed by considering the applied load on the indenter is from 10mN-50mN for every time by changing the indenter radius as 1.5mm and 2mm, for this test the film thickness is taken as 2μm. The Nanoindentation tests for experimental validation are planned to carrying on a Nano-indenter XP (MTS) tester. All the experiments are conducting by the Berkovich indenter, which was made of diamond. The system is equipped with a continuous stiffness measurement (CSM) module and is capable of giving the mechanical properties as a function of depth. The thin films are processed by PVD, CVD and sol-gel methods [Ch. Srinivasa Rao and C.Eswara Reddy]. The figures [4] & [5] explain the simulation details with possible curves compared with theoretical curves.

![Simulation details](image3)

Figures 3(a) - 3(c) shows the different indenter size.
5. Conclusions:

With the performance of finite element (FE) analysis, the nanoindentation loading-unloading process of nylon was simulated. Figures (4) & (5) show the curves that resulted from the experimental and the simulation values. From the results of the elastic analysis, the Nanoindentation test is size dependent. The hardness and elastic modulus of the material is extracted from experimentally is compared with the simulation data, which are have a good agreement between the simulation and experimental results.

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