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Finite Element Analysis of the Critical Ratio of Coating Thickness to Indentation Depth of Soft Coating on a Harder Substrate by Nanoindentation

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ABSTRACT: This study presents the critical ratio of coating thickness to indentation depth (CRTD) of a soft coating on a harder substrate by nanoindentation. The indentation processes were simulated with the finite element (FE) software programme. In the FE model, the influence of the yield strength ratio (Yc/Ys) and the indenter tip radius (r) have been investigated. In addition, the critical ratio of coating thickness to depth at which the substrate effect is less than 5% has been presented. It was found that increasing Yc/Ys and tip radius increases the CRTD. Furthermore, the CRTD is strongly dependent on the allowable degree of substrate effect. For example, when the substrate effect is increased from 5% to 10%, the CRTD is considerably reduced. Based on the FE calculations, an empirical equation has been derived in terms of the effect of substrate to determine the critical indentation depth when yield strength ratio is between 0.1 and 0.8 and the indenter tip radius is between 0 and 2 mm.

KEYWORDS: Nanoindentation, Finite element analysis, Coatings, Hardness.

INTRODUCTION

The rapid development of surface engineering technologies and their successful applications in various areas of industry has led to the increase in demand for assessing the mechanical properties of their coatings for controlling and improving the coating quality. Nanoindentation is one of the simplest ways to measure the mechanical properties of very thin films, particularly, the two important properties, hardness and elastic modulus[1]. Other reasons for the popularity of the nanoindentation method are that the mechanical properties can be measured without removing the film from its substrate and its ability to probe a surface at numerous points and to spatially map its mechanical properties[2].

Recently, finite element techniques have been developed and used in many fields of science and engineering, including indentation problems. They have been applied to study very complex stress–strain field of thin films or bulk materials in a nanoindentation process[3-4]. Some investigators have studied the indentation process using the numerical approach of finite element method[5-7].

In order to obtain intrinsic film properties from indentations, it is necessary to understand how the mechanical properties of the substrate affect measurements of coating properties. Many models have been proposed to account for this substrate effect[8-11]. Most of these models, however, are empirical or semi-empirical in nature. Tsui et al.[11] developed an FE model to simulate the indentation of soft films on hard substrates using Knoop indenter. The effort studied an effect of the substrate on the measurement of the hardness of a soft film. However, the main question still exists as to how deep the indentation on coating material should be, in order to eliminate the substrate effects to ensure credibility of the obtained results. Therefore determination of the critical ratio of the coating thickness to indentation depth (CRTD) is crucial for a given coating-substrate system.

This study aims to elucidate the effect of substrate deformation on hardness measurement of a soft coating. Attempts have been made in the present work to simulate the nanoindentation process of various soft coatings on harder substrate systems using the finite element method (FEM). A conical indenter was chosen in the model in order to make the same projected area as a standard Berkovich indenter. This paper focuses on determining CRTD in terms of the yield strength ratio and the indenter tip radius.

Finite Element Modeling

In this study, a 2-D axisymmetric model was developed to simulate the elastic-plastic indentation process by capabilities of the *ABAQUS* finite element (FE) code[12]. The conical rigid indenter was used in the model in order to define the axisymmetric model (semi-angle = 70.3°). The axisymmetric indenter is constrained to have the same project area of the Berkovich indenter, as a function of the indentation depth. The film and substrate were modelled with 1,892 four-node axisymmetric reduced integration elements (CAX4R element type[12]), as shown in Fig. 1. A fine mesh was used near the contact area. The mesh was continuously coarser further away from the tip (Fig. 2). The indentation process was simulated both during the loading and the unloading step. During loading the simulation was performed to a depth of 500 nm; during unloading the indenter tip returned to the initial position.

The contact constraint was defined by the master and the slave surfaces. Due to the fact that only the master surface can penetrate into the slave surface, the contact direction was then determined to the master surface. The model chose the indenter as the master surface and the sample surface as the slave surface. The boundary conditions were applied along the original point, centerline and bottom of the specimen. Friction between the indenter tip and the specimen surface was assumed to be zero. The rigid indenter was simulated by assuming various tip radii, including a perfect sharp tip, r = 0 (Fig. 1), round tips of radii 0.2, 0.5, 1 and 2 mm. Fig. 2 illustrates schematically a typical round tip when tip radius is 0.5 mm.

The present work has simulated the indentation processes of various soft coating/hard substrate systems. The coating and substrate materials were assumed to be elastic perfectly plastic. Table 1 shows all material properties used in the FE model. All of the coating/substrate systems have the same substrate material, i.e. the Young's modulus, E = 200 GPa, Poisson's ratio, n = 0.25, and yield strength, Y_S = 5 GPa. The thickness of all coatings was assumed to be 1 mm. The coatings have the same Young's modulus, E = 200 GPa and Poisson's ratio, n = 0.25, but the yield strengths of

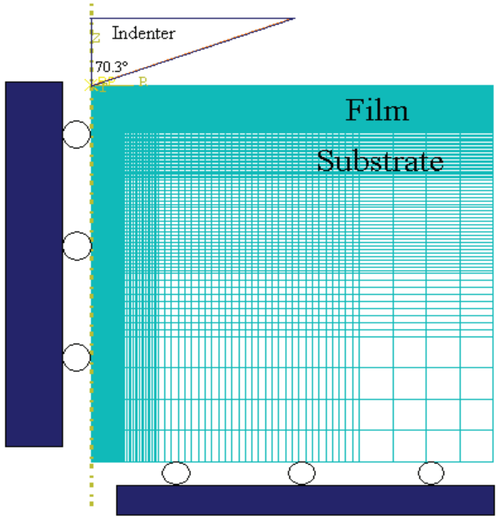

Fig 1. The boundary conditions and finite element meshes of the indentation model.

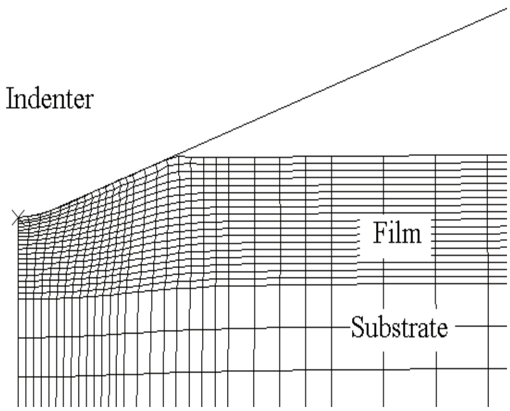

Fig 2. Details of the mesh of thin film and substrate in the region near the tip of the indenter during loading stage.

Table 1. Properties of substrate and coating materials used in FE calculation.

Material	Elastic Modulus, E (GPa)	Poisson's ratio, ν	Yield strength, Y (GPa)	Yc/Ys	Thickness (μm)
Substrate	200	0.25	5	-	-
Coating 1	200	0.25	4	0.8	1
Coating 2	200	0.25	3	0.6	1
Coating 3	200	0.25	2	0.4	1
Coating 4	200	0.25	1	0.2	1
Coating 5	200	0.25	0.5	0.1	1

0.5, 1, 2, 3 and 4 GPa were used in the calculation.

Results and Discussion

From the FE calculation, the loading-unloading curves of nanoindentation process were produced. However, only the loading curves are required to derive the substrate effect. Figures 3 (a) and 3 (b) show the simulated loading curves of selected systems illustrating the influence of coating/substrate yield strength ratios for a perfect tip and a round tip radius of 2 mm, respectively.

As expected, with increase in the yield strength of the coating i.e. increasing the yield strength ratio, increases the mean contact pressure: the load required to produce a fix indentation increases. It is obvious that, at the relatively shallow depths, the difference in the loading behaviour of various systems is not so significant as at larger depths where plastic deformation has more influential (Fig. 3 (a)). In addition to increase depths the difference in indentation response of various systems with different Yc/Ys ratios becomes greater (Figs. 3 (a) and (b)). In fact, the indenter tip cannot be made to be perfectly sharp. The variance of the round tip geometry affects both the area function of indentation and the deformation behaviour during indentation process. Increasing the tip radius increases the load rapidly, as confirmed in Fig. 4 (a). As shown in Fig. 4 (b), it is noted that a slight deviation of indenter tip radius results in a strong deviation of load in the indentation as well as in the higher Yc/Ys (Fig. 4 (a)). There is no doubt that the load of indentation process of soft coating/hard substrate depends on the genuine indenter tip radius. This result suggests that the calibration of tip radius for any specific indenter in the nanoindentation processes is of great importance.

The indentation process of the halfspace with

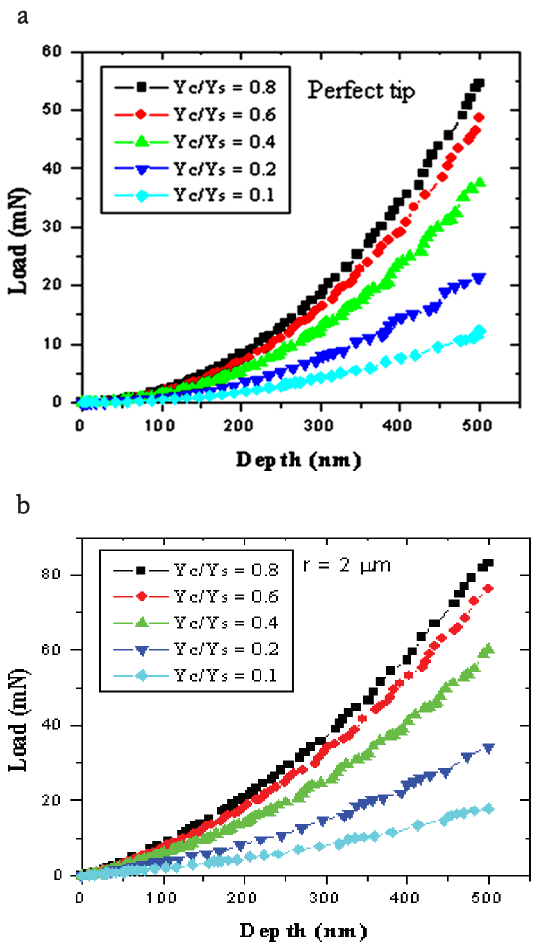

Fig 3. Typical loading curves of selected coating/substrate systems illustrating the influence of yield strength ratio at the tip radius of (a) perfect tip (r = 0 mm) and (b) r = 2 mm.

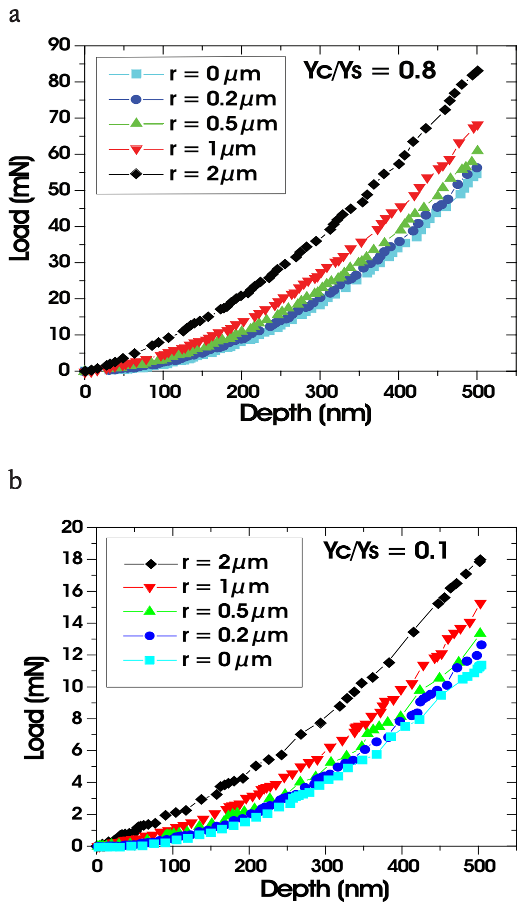

Fig 4. Typical loading curves of selected coating/substrate systems illustrating the influence of indenter tip radius in the loading behaviour of layered systems at the yield strength ratio of (a) Yc/Ys = 0.8 and (b) Yc/Ys = 0.1.

properties of the coating materials has been modelled. The loading curves of selected coating/substrate systems and the corresponding coating halfspaces illustrating the effect of yield strength ratio are plotted together, as shown in Fig. 5. Clearly, at shallow indentation depths, the loading behaviour of the coating/substrate systems is almost similar to that of the corresponding coating halfspaces, particularly, in the very soft coating systems, Yc/Ys = 0.1. As the indentation depth is increased, the loading curves of the coating/substrate systems gradually deviate from those corresponding to the coating halfspaces, suggesting that the effect of substrate increases gradually. It is noted that with increasing Yc/Ys, the effect of substrate increases, on the other hand, the very soft coating (Yc/Ys = 0.1) is affected by the substrate at the deeper indentation, as shown in Fig. 6.

In Fig. 7, the loading curves of selected coating/substrate systems and the corresponding coating halfspaces illustrating the effect of tip radius on the critical indentation depth are plotted together. As shown in Figs 5, 6 and 7, it can be seen that in the soft coating/harder substrate systems the load of the corresponding coating halfspace is always lower than the load from the coating/substrate system because of the substrate effect. Consequently, it is noted that the degree of substrate effect and the critical indentation depths at which the substrate has various degrees of effect on the load can be determined.

In the next section, the determination of the critical ratio of the coating thickness to indentation depth (CRTD) at which the substrate effect is less than 5% is focused on. Figures 8 and 9 are produced from Figs 4, 5 and 7 in terms of substrate effect less than 5%. Fig. 8 shows the critical ratios of coating thickness to indentation depth, CRTD$_{5\%}$[1], as a function of yield strength ratios for indenter tips with radii 0, 0.2, 0.5, 1 and 2 μm. It can be seen that the CRTD$_{5\%}$ increases with increasing coating/substrate yield strength ratio and tip radius. For all tip radii, the increase in the yield

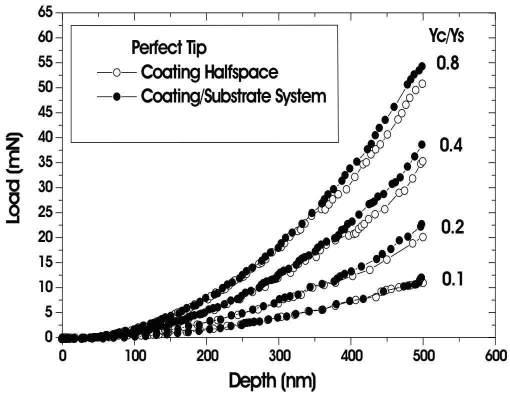

Fig 5. Loading curves of selected coating/substrate systems and the corresponding coating halfspaces illustrating the effect of yield strength ratio.

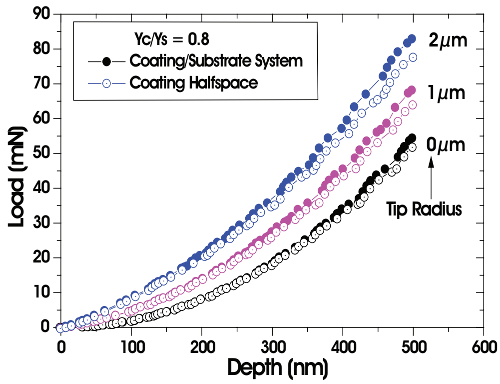

Fig 7. Loading curves of selected coating/substrate systems and the corresponding coating halfspaces illustrating the effect of tip radius on the critical indentation depth.

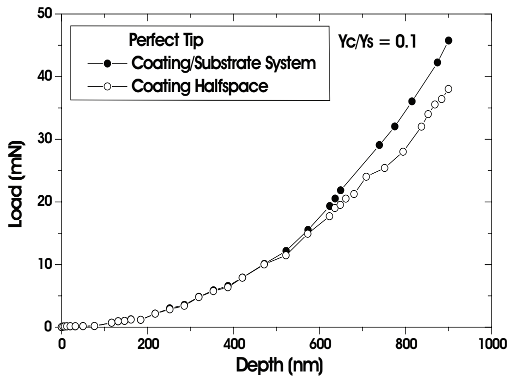

Fig 6. Loading curves of a selected coating/substrate system and the corresponding coating halfspace illustrating the effect of yield strength ratio when Yc/Ys = 0.1.

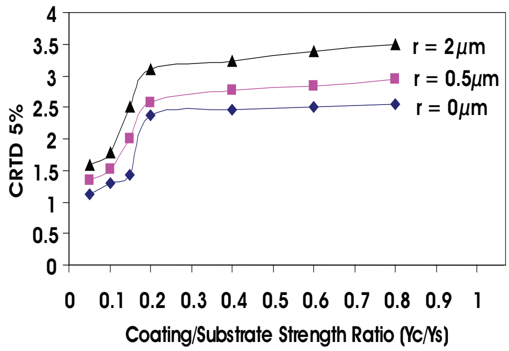

Fig 8. Critical ratios of thickness to depth, CRTD$_{5\%}$, as a function of yield strength ratios for indenter tip with radius 0, 0.5 and 2 μm.

strength ratio is sharp at the beginning when Yc/Ys is low (from Yc/Ys = 0.1 to 0.2). However, when Yc/Ys > 0.2, $CRTD_{5\%}$ increases gradually. For the perfect and small radii tip, the values of $CRTD_{5\%}$ increase continuously with increasing Yc/Ys, however the critical ratio is almost constant at high yield strength ratio (from Yc/Ys = 0.2 to 0.8).

The effect of indenter tip radius on the $CRTD_{5\%}$ can be more clearly observed in Fig. 9, which shows the $CRTD_{5\%}$, as a function of indenter tip radius for the systems with Yc/Ys = 0.1, 0.2, 0.4 and 0.8. It can be demonstrated that the $CRTD_{5\%}$ increases approximately linearly with increasing tip radius and the $CRTD_{5\%}$ increases significantly for larger tip radius (Fig. 9). For example, for the Yc/Ys = 0.2, the $CRTD_{5\%}$ is increased from 2.32 to 2.41, 2.56, 2.75 and 3.03 when the tip radius is changed from 0 mm to 0.2 mm, 0.5 mm, 1 mm and 2 mm respectively. Furthermore, the more useful results of this work are those for the round tips. As can be seen from Fig. 8, the entire tip radius results in $CRTD5_{\%}$ values well under 10 for various yield strength ratios. According to the UK National Physical Laboratory's Recommendation[8], during microindentation Vickers hardness testing the indentation depth should not exceed one-tenth of the thickness. Obviously, the one-tenth rule overestimates the critical ratio of thickness to depth for round indentor tips in this soft coating system. From Fig. 10, it is noted that the critical ratio is strongly dependent on the allowable degree of substrate effect. When the substrate effect is increased from 5% to 10%, the CRTD is considerably reduced: i.e. a deeper indentation depth is allowed.

Based on the FE results, an equation has been derived in terms of the effect of substrate 5% presented in a polynomial form to determine the critical indentation depth, as follow:

$$R_{5\%} = a_0 + a_1\left(\frac{Yc}{Ys}\right) + a_2\left(\frac{Yc}{Ys}\right)^2 \qquad (1)$$

[1] $CRTD_{5\%}$ is the critical ratio of coating thickness to indentation depth in which the substrate effect is less than 5% in coating/substrate system. The $CRTD_{5\%}$ was calculated when the ratio $(P_{C/S}-P_H)/P_H$ isequal to 0.05 or 5% where $P_{C/S}$ is the load of coating/substrate system and P_H is the load of coating halfspace.

where the constants a_0, a_1 and a_2 are functions of the indenter tip radius r, i.e.

$$a_0 = -0.4955\,r^2 + 1.5647\,r + 1.4899$$

$$a_1 = 2.6485\,r^2 - 6.5744\,r + 3.7516$$

$$a_2 = -3.1138\,r^2 + 7.7845\,r - 3.1138$$

Equation (1) is derived by fitting the $CRTD_{5\%}$ curves

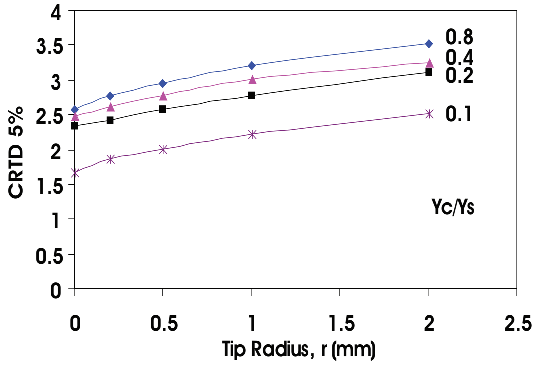

Fig 9. Critical ratios of thickness to depth, $CRTD_{5\%}$, as a function of indenter tip ratios for the systems Yc/Ys = 0.1, 0.2, 0.4, and 0.8.

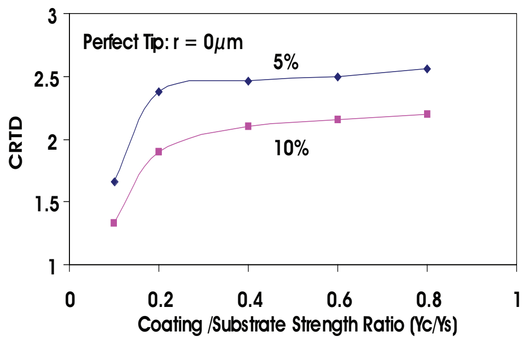

Fig 10. Critical ratios of thickness to depth, $CRTD_{5\%}$ and $CRTD_{10\%}$ as a function of yield strength ratios for a perfect tip (r = 0 mm).

when yield strength ratio is between 0.1 and 0.8 and when the indenter tip radius is between 0 and 2 mm. Accordingly, Equation (1) can be used to determine the critical indentation depth for soft coating on the harder substrate system when yield strength ratio and indenter tip radius are in the range of this study.

Conclusions

Based on the finite element analysis results, several points could be summarized as following;

1. All the simulated loading curves of the coating/substrate systems are similar to the corresponding coating halfspaces curves, particularly in the very soft coating systems (Yc/Ys = 0.1).
2. The model reveals that the CRTD is a function of the yield strength ratio of the coating to substrate and the tip radius.
3. The $CRTD_{5\%}$ increases linearly with increasing tip radius and the $CRTD_{5\%}$ increases significantly for larger tip radius

An empirical equation has been derived in terms of the effect of substrate 5% to determine the critical indentation depth.

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