

Modelling of Nanoindentation of TiAlN and TiN Thin Film Coatings for Automotive Bearing



Wan Fathul Hakim W Zamri, Ng Jie Suang, Intan Fadhlina Mohamed, Ahmad Kamal Ariffin, Muhammad Faiz Md Din

Abstract: Bearings are critical components for the transmission of motion in machines. Automotive components, especially bearings, will wear out over a certain period of time because they are constantly subjected to high levels of stress and friction. Studies have proven that coatings can extend the lifespan of bearings. Hence, it is necessary to conduct studies on coatings for bearings, particularly the mechanical and wear properties of the coating material. This detailed study focused on the mechanical properties of single-coatings of TiN and TiAlN using the finite element method (FEM). The mechanical properties that can be obtained from nano-indentation experiments are confined to just the Young's modulus and hardness. Therefore, nanoindentation simulations were conducted together with the finite element method to obtain more comprehensive mechanical properties such as the yield strength and Poisson's ratio. In addition, various coating materials could be examined by means of these nanoindentation simulations, as well the effects of those parameters that could not be controlled experimentally, such as the geometry of the indenter and the bonding between the coating and the substrate. The simulations were carried out using the ANSYS Mechanical APDL software. The mechanical properties such as the Young's modulus, yield strength, Poisson's ratio and tangent modulus were 370 GPa, 19 GPa, 0.21 and 10 GPa, respectively for the TiAlN coating and 460 GPa, 14 GPa, 0.25 and 8 GPa, respectively for the TiN coating. The difference between the mechanical properties obtained from the simulations and experiments was less than 5 %.

Keywords : Automotive bearings, wear, Nanoindentation and Finite element method.

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I. INTRODUCTION

Bearings are critical components for the transmission of motion in machines. Automotive components, especially bearings, will wear out over a certain period of time because they are constantly subjected to high levels of stress and friction. Therefore, automotive components need to be resistant to wear and friction in critical situations. As such, various types of coating materials have been introduced to overcome the problem of friction, which was causing the bearings to wear out. In tribology applications, coatings can harden and protect the surfaces of automotive components that are constantly shifting in critical situations.

Nanoindentation experiments were carried out to determine the mechanical properties of thin film coatings. However, the mechanical properties that were obtained through the nanoindentation experiments were confined to just the hardness and Young's modulus [21]. Therefore, for those mechanical properties that are difficult to determine experimentally, such as the yield strength and Poisson's ratio, nanoindentation simulations with the finite element method (FEM) were conducted. In addition, the nano-indentation simulations could be used to study various parameters without incurring any costs, which otherwise could not be controlled in experiments, such as the effects of the substrate, the geometry of the indenter, the friction between the indenter tip and the surface of the coated specimens [3], [8], [11].

This study was aimed at investigating the mechanical properties of monolithic (single) coatings using nanoindentation simulations by the finite element method. The simulation results were validated by comparing them with the experimental results obtained by [11] and [18].

II. MATERIAL & MODELLING PROCEDURES

Figure 1 shows the workflow for the entire study. The ANSYS Mechanical APDL R16.0 software was used for the nano-indentation simulations. The validation of the precision of the model by the finite element method was done by comparing the modelling results with the data from the nano-indentation experiments performed by [18] and [11]. The data from the nanoindentation experiments that were used as the basis for the comparison were the load-displacement curves.

At the start, the type of element was modelled using PLANE 182, which had four nodes with two degrees of freedom at each node. The PLANE 182 is suitable for models with solid structures.

The convex tip of the indenter, which had the same properties as a Berkovich indenter with an included angle of 70.3°, was used in the FEM simulation. As the indenter was made of diamond, which does not undergo any plastic deformation, it was modelled as a rigid or perfectly inelastic material. The coating materials were modelled as elastic with linear strain hardening (bi-linear material models). The HSS (High speed steel) substrate was modelled as a perfectly plastic material since no plastic deformation occurred at the substrate. It was assumed that the coating and substrate were homogeneous and isotropic materials.

The contact between the 2-D (TARGE 169) target surfaces was modelled using the CONTA 171. In this case, the coating surface represented a deformable contact surface, while the target surface represented the surface of the indenter tip. For the boundary conditions, all the nodes on the Y-axis could only move towards Y and all the nodes on the X-axis were fixed and immovable. The base of the indenter had a fixed and restricted boundary. When the base of the substrate was displaced, the coating moved together with the substrate to be finally penetrated by the indenter tip. Furthermore, it was assumed that there was no residual stress in the coating and the substrate following the deposition process. The contact was perfect and it was assumed that there was no friction between the indenter tip and the coating. A high degree of meshing was applied to the point of contact between the indenter tip and the coating. Figure 2 shows the boundary conditions of the model.

Next, iterative inputs for the Young’s modulus (E), Poisson’s ratio (ν), yield strength σ_y , and tangent modulus (E_T) were carried out to obtain the equivalent load-displacement curves to those that had been obtained experimentally. The mechanical properties of the coatings could be determined if the gradient of the unloading curve

$$S = \frac{dP}{dh}$$

were less than 10% compared to the experimental load-displacement curves. The nano-indentation simulations were divided into two parts, the loading and unloading. The nano-indentation loading was simulated with a lower displacement towards Y until the coated specimen came into contact with and was penetrated by the indenter tip to achieve the maximum depth of indentation. Meanwhile, the unloading process occurred with the coated specimen returning to its original position. The maximum depth of indentation had to be less than 10% of the thickness of the coating to avoid any impact on the substrate [7].

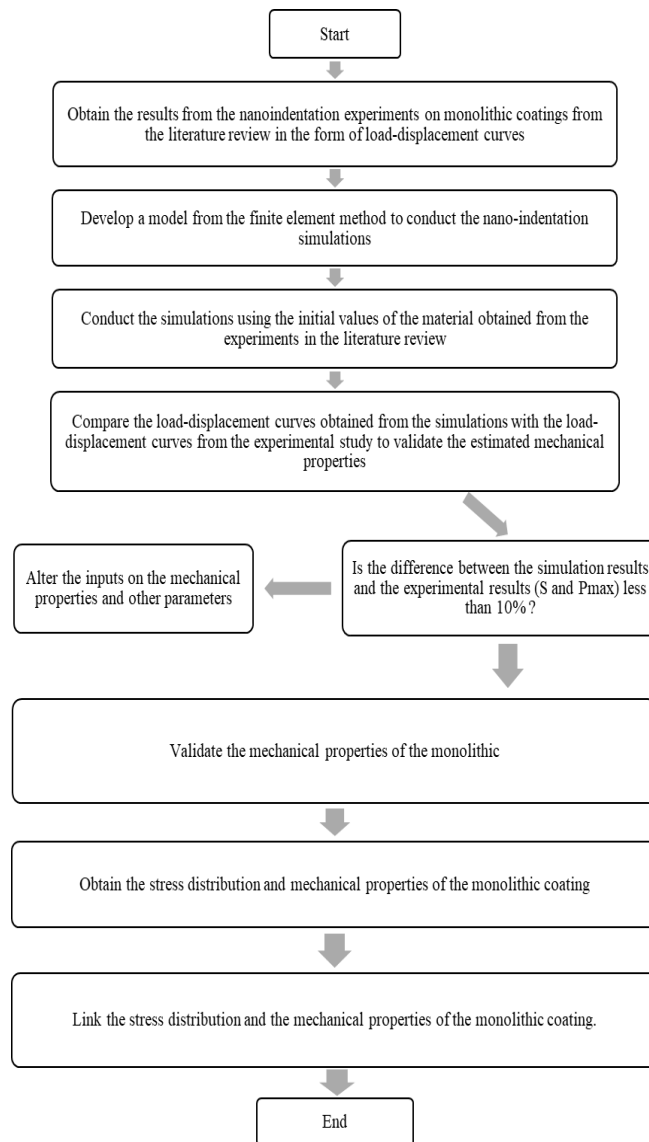


Fig. 1. Workflow of the entire study.

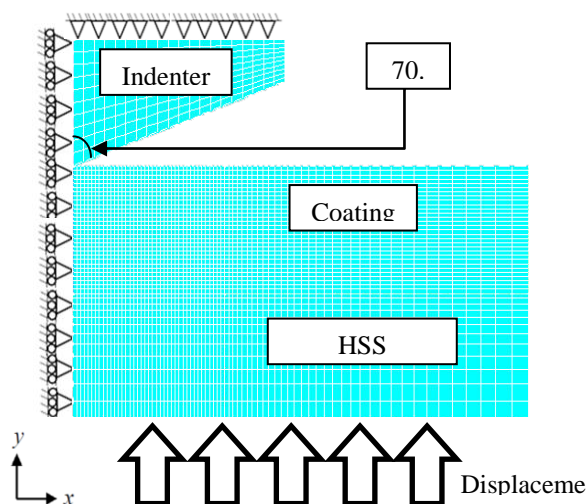


Fig. 2. Model of boundary conditions.

A. Formula for the calculation of the nanoindentation load-displacement curve

Figure 3 shows an example of the load-displacement curve with maximum load, P_{max} , maximum depth of indentation, h_{max} , and empty load indentation depth, h_f .

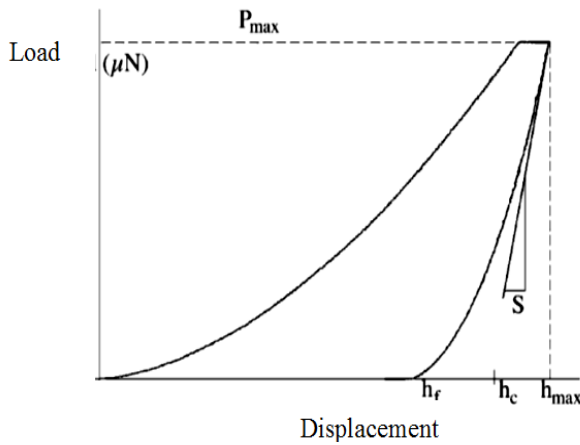


Fig. 3. Load-displacement curve.

The hardness, H was calculated using equations (1), (2) and (3).

$$H = \frac{P_{max}}{A_c} \tag{1}$$

$$A_c = 24.5h_c^2 \tag{2}$$

$$h_c = h_{max} - \epsilon(h_{max} - h_f) \tag{3}$$

where A_c is the area of contact between the indenter tip and the material being tested, and h_c is the depth of the point of contact. The intercept factor, ϵ of the convex indenter was 0.72 for the indenter and 0.75 for the Berkovich indenter [16].

In this study, the formula that was used to calculate the hardness, H improved the speed of the calculation and the accuracy of the answer, as reported by [20] and [8] compared to the method of drawing lines at the unloading curve.

III. RESULT AND DISCUSSION

The load-displacement curves for the TiAlN and TiN coating experiment and simulation are shown in Figure 4 and Figure 5, respectively. The results for the TiAlN nano-indentation experiment were taken from the latest nanoindentation study by Swain et al. (2017), while the results for the TiN nanoindentation experiment were taken from [11]. Both simulations gave good results which were almost similar to the experimental results. The differences in the unloading

gradient (unloading curve) $S = \frac{dP}{dh}$ and the maximum load

P_{max} for the experiments and the simulations were less than 10%.

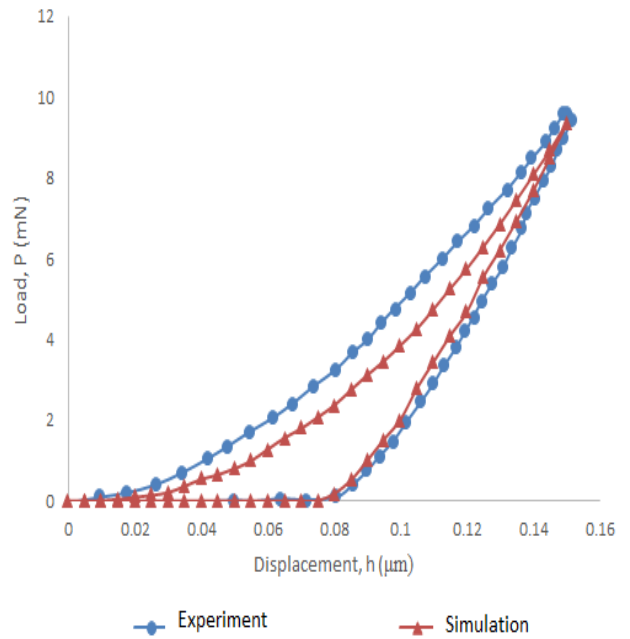


Fig. 4. Load-displacement curves for monolithic TiAlN coating experiment and simulation.

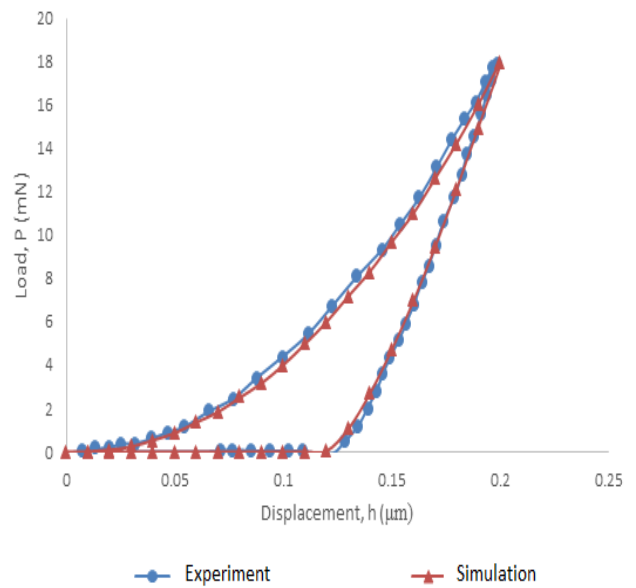


Fig. 5. Load-displacement curves for monolithic TiN coating experiment and simulation.

Table I and Table II show the comparison of the mechanical properties of TiAlN and TiN, respectively that were obtained through nanoindentation simulations with the mechanical properties cited from a literature review of such experiments.

Based on Table I, the Young's modulus for the TiAlN coating was in the range of 30 GPa to 38 GPa. The hardness for the TiAlN coating, according to the current simulation results, was 38.39 GPa, which was 12.81 % higher than the average of all the hardness values in the literature review.

For the Young’s modulus, the current simulation result was 7 % lower than the average of the Young’s modulus taken from the literature review. On the other hand, the hardness of the TiN coating was in the range of 21 GPa to 37 GPa. The hardness of the TiN coating according to the current simulation result was 36.07 GPa, which was 21.65 % higher than the average result of the literature review so far. The relatively high difference for the TiN coating was because all the studies in the literature review to date did not have very

consistent values for the TiN coating. For the Young’s modulus, the current simulation result was 7.05 % higher than the average result from the literature review. All these differences in values can be attributed to the residual stress, roughness of the coating surface and the geometry of the indenter (Fischer-Cripps, 2002). In addition, more comprehensive mechanical properties could be obtained by using the finite element method of simulation compared to the nanoindentation experiment.

Table- I: Comparison of mechanical properties from a literature review of experiments with the current simulation of a TiAlN monolithic coating

Hardness, H (GPa)	Young’s Modulus, E (GPa)	Poisson’s Ratio, ν	Yield Strength, σ_y (GPa)	Tangent Modulus, E_T (GPa)	Reference
38.39	370	0.21	19	10	Current simulation results
36.2	-	-	-	-	[10]
37.4	460	-	-	-	[24]
32.02	350	-	-	-	[4]
30	-	-	-	-	[17]
36.1	459	-	-	-	[25]
35	388	-	-	-	[13]
38	-	-	-	-	[18]
30.7	-	-	-	-	[5]
30	-	-	-	-	[12]
31.4	322.2	-	-	-	[15]
33.8	-	-	-	-	[14]

Table- II: Comparison of mechanical properties from literature review of experiments with the current simulation of a TiN monolithic coating

Hardness, H (GPa)	Young’s Modulus, E (GPa)	Poisson’s Ratio, ν	Yield Strength, σ_y (GPa)	Tangent Modulus, E_T (GPa)	Reference
36.07	460	0.25	14	8	Current simulation results
37	450	0.25	14.5	-	[11]
35	-	-	-	-	[2]
21	300	0.25	-	-	[9]
-	300	0.25	-	-	[26]
24	-	-	-	-	[12]
-	400	0.25	-	-	[19]
33.6	447	0.21	-	-	[6]
27.3	351.3	-	13.83	-	[1]

Figure 6 shows the von Mises stress distribution for the TiAlN and TiN coatings during maximum loading. The maximum stress occurred at the point of contact between the coating surface and the indenter tip. The maximum depth of indentation for the TiAlN and TiN coatings was less than 10% of the thickness of the coating. This was so in order to reduce any impact on the substrate. According to Figure 6, no von Mises stress contours were applied to the HSS substrate. The stress contours for the TiAlN and TiN coatings were circular in shape and spread out smoothly from the point of contact between the surface and the indenter tip. The TiAlN coating experienced a higher von Mises stress of 39.348 GPa

compared to the TiN coating, which was 31.48 GPa. In other words, TiAlN has a higher hardness because the TiAlN coating required a greater stress to be indented to a specified depth during the loading process.

Figure 7 shows the equivalent plastic strain distribution for the TiAlN and TiN coatings during the full unloading. The plastic strain, which is also known as the plastic deformation, occurred at the point of contact between the coating surface and the indenter tip.



Furthermore, a few plastic strain contours spread smoothly from the point of contact between the surface and the indenter tip, and these had no effect on the equivalent plastic strain contours to the HSS substrate. This was important to prevent any impact on the substrate and to accurately obtain the mechanical properties of the coatings. The maximum equivalent plastic strain for the TiAlN coating was 0.472701,

while the maximum equivalent plastic strain for the TiN coating was 0.679421. The TiAlN and TiN coatings experienced plastic strain because the von Mises stress experienced by the coatings exceeded their yield strength and indirectly contributed to the plastic deformation of the coatings, whereby the coatings would never fully return to their original shape (Silicon As 1982) [22], [23].

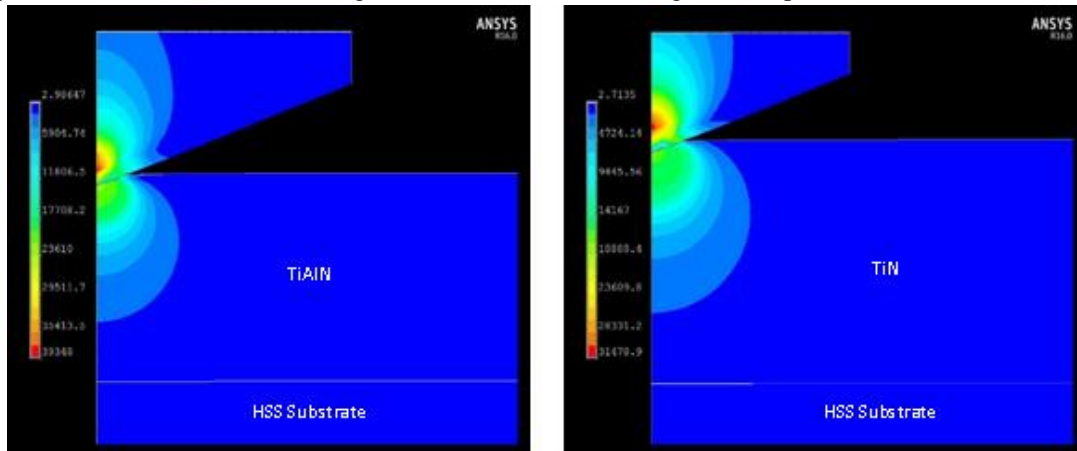


Fig. 6. Von Mises stress distribution for TiAlN and TiN coatings during maximum loading (stress unit in MPa)

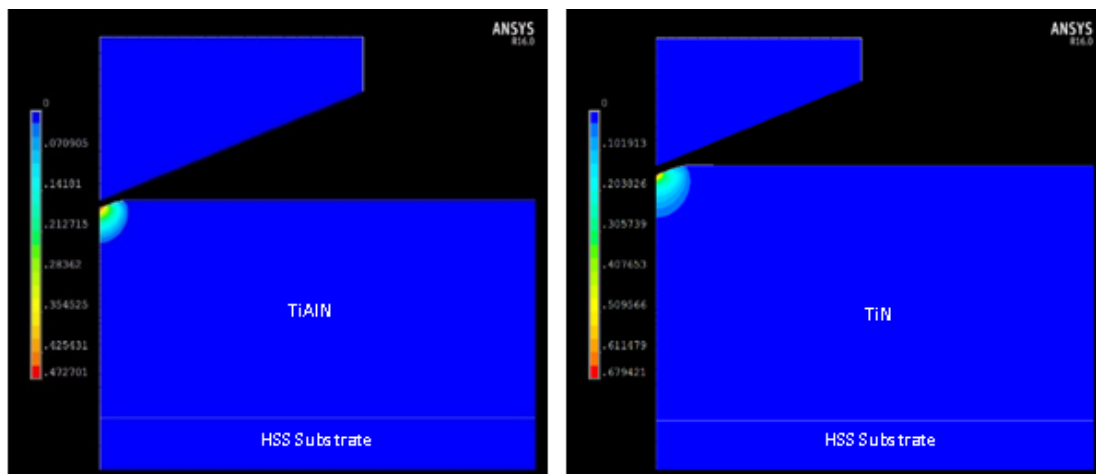


Fig. 7. Equivalent plastic strain distribution for TiAlN and TiN coatings during full unloading.

IV. CONCLUSION

The advantage of using the nanoindentation simulation was that it was able to provide those mechanical properties that are difficult to obtain through experiments such as the yield strength and Poisson's ratio. The mechanical properties of the TiAlN coating, such as the Young's modulus, yield strength, Poisson's ratio and tangent modulus were 370 GPa, 19 GPa, 0.21 and 10 GPa, respectively, while for the TiN coating they were 460 GPa, 14 GPa, 0.25, 8 GPa, respectively. The difference in the mechanical properties between the simulation and experimental results was less than 5 %. In addition, the nanoindentation simulations were able to provide the stress contours and the stress that was experienced by the coatings. Apart from not incurring high costs, the nano-indentation simulations were able to alter the experimental perimeters such as the geometry of the indenter, the depth of the indentation, the thickness of the coating and so on.

V. ACKNOWLEDGEMENT

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