

The effect of TiAlN-based and AlCrN-based coatings towards mechanical properties on punch tools using finite element method

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ABSTRACT

Wear problem in the application of punching tools is not something new due to the process that involved shear and friction. In order to improve the performance of the tool and the quality of the product, another alternative aside from lubrication, known as coating is widely used and it acts as a wear protection and extends the life of a punch tool. Multi layered coating has better hardness and elasticity than single coatings. However, the variety in layered coating is less studied especially in terms of thickness and structure. In this study, nanoindentation simulation using finite element method was carried out by constructing coating and substrate model with different thickness and structure. TiAlN contributes in increasing the value of elasticity while AlCrN contributes more to the value of hardness and is more suitable to be used as a surface layer. In this test result, the AlCrN / TiAlN double-coated coating with a thickness of 2.5 μm for individual layers is the most suitable coating used for punching tool applications. This is because it has the highest H / E ratio of 0.0975 and has optimum hardness and elasticity compared to other structures which are 37.45 GPa and 384.09 GPa respectively.

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1.0 INTRODUCTION

Punching tool is one of the important processes in the formation of a product. Punching tools are used in the process of evacuation, penetration and trimming. Criteria required for punching tools to produce quality cuts are convex double shear angles, puncture speeds and less shear forces. This not only enhances the quality of product results but also extends the life span of the punch tool. Punch or evacuation operation occurs when the piercing shunt through a piece of material usually has three stages: (1) plastic deformation, (2) shear, and (3) cracks. In this process, punch tools are exposed to failure in terms of weariness and will affect in determining the lifetime of the punch tool and its performance. Aside from lubricating, coatings can improve the performance of the punch tool by applying the coating to the surface of the punch tool. There are various types and structures that can be combined in producing good coatings for puncture tools. Like lubricants, coating not only enhances the precision of the punch tool, but also protects the wear and tear that happens during the punching process. For coating materials, the coating that is often used for puncture tools is TiAlN and AlCrN. The multi-layer structure will produce better mechanical properties and tribology than single coating, especially from the point of strength and wear resistance.

In ensuring that wear failures can be reduced, the coating mechanical properties are important parameters that need to be improved in the application of the punch tool. For TiAlN coating, it was shown to be effective in improving coating performance especially oxidation and wear resistance and increased hardness (PalDey and Deevi, 2003). The AlCrN coating also shows significant increase in hardness when compared to TiN's single coating (Wang et al., 2008). The combination of these two materials that are arranged in multi-layered structure can promote mechanical properties and coating tribology. This is proven when the mechanical properties of multi-layer coating such as hardness are higher than single coating (Hassan et al., 2017). Hence, this study leads to the layered-coating effects on TiAlN and AlCrN for punch tool applications.

For TiAlN and AlCrN multi-layered coating, nanoindentation modelling using finite element techniques is still lacking. Studies that have been done in nanoindentation modelling did not emphasize the difference in mesh size, coating thickness, number of layers and indenter (Hassan et al., 2017; Wang et al., 2008). The research that has been done only used the test techniques instead of simulations. Modelling of finite element methods is used to study the field of complex strained layers (Lichinchi et al., 1998). In this study, the ANSYS Mechanical APDL 15.0 software is used to develop nanoindentation simulation. Modelling using the finite element method for nanoindentation simulation will characterize TiAlN and AlCrN multiple layers of coating. The coating model will be constructed according to different types of designs with different thickness and variety of coating structures to observe the coating structure effect towards mechanical properties of the firmness distribution.

2.0 RESEARCH METHOD

Nanoindentation simulation is carried out on thin layers of TiAlN and AlCrN in layered way with various configurations. The indenter model should be developed first by using ANSYS Mechanical APDL 15.0. Therefore, the type of indenter should be identified as well as the features and parameters of the indenter. As stated by Zamri et al., (2012), initially a set of mechanical properties was used in nanoindentation simulation i.e. modulus of elasticity E , Poisson ν ratio, E_T tangential modulus and yield strength, σ_y . This includes for indenter, layers and substrate that needs to develop in the nanoindentation model. The sequence of this study is shown in Figure 1

where, in general, a simulation result is compared with previous studies, for the purpose of showing the effectiveness of simulation for nanoindentation. Then the initial tests using the simulation on the TiAlN layer and the layered AlCrN are carried out with different layers and configurations.

Figure 2 shows the nanoindentation model developed using ANSYS. A recommendation by Cai et al., (1995) are taken into account in the case of hard coating on the soft substrate, the plastic deformation is elongated easily into the substrate and the hardness measured has been improved to $d / t_x 100 = 10\%$ where the depth of the bending penetration does not exceed 10% depth of layer thickness. This is to avoid the influence of the substrate on the mechanical properties that will be obtained. Room temperature is 26°C and is considered the same at all times. The indenters are designed like coaxial symmetry cones and have a 70° angle. The diamond elasticity constant is referred to by Oliver and Pharr, (1992) where elastic modulus is $E_i = 1141$ GPa and Poisson ratio, $\nu = 0.07$. Hardness and stresses of the indenter are referred to Lichinchi et al., (1998) i.e. $H = 98$ GPa and $Y = 35.7$ GPa. In order to reduce the number of iterations in the simulation that can take a long time to complete, the nanoindentation model is made 1/8 of the original model. This is permitted because of the properties of symmetry and isotropic of the indenter and materials. Furthermore, the model developed is in the form of three dimensions (3D). The use of 2D models is easier and faster to get results, but in obtaining a more precise distribution of stress, the 3D model is used because according to Misha et al., (2014), 3D models can make much better results than 2D models although it takes longer time and complicated.

Two criteria that need to be fulfilled in this nanoindentation simulation are i) the gradient of release loads and ii) the maximum load value for the curvature against the displacement curve (dP / dh) (Deng et al., 2019; Zamri et al., 2012). Both of criteria need to be met by ensuring the percentage difference is less than 1%. Both of these criteria are shown in the equations below.

$$\frac{P_{max,EXP} - P_{max,FEM}}{P_{max,EXP}} < 1\% \tag{1}$$

$$\frac{\left(\frac{dP}{dh}\right)_{EXP} - \left(\frac{dP}{dh}\right)_{FEM}}{\left(\frac{dP}{dh}\right)_{EXP}} < 1\% \tag{2}$$

To compare differences in hardness and elasticity, each coating has the same coating thickness of 3 μm. This thickness is selected based on past studies that have been performed on the application of the punches where the thickness used is within the range of 1-5 μm (Kumar et al., 2014; Willey et al., 2007). Therefore, in order to avoid the impractical thickness, the average thickness is calculated and the value is as mentioned earlier. To demonstrate the FEM simulation ability for nanoindentation tests, the validation of nanoindentation simulation results were compared to the previous study results. The results of nanoindentation studies by Kumar et al., (2014) were compared to the results of the FEM simulation study for the TiAlN, AlCrN single coating layers and TiAlN / AlCrN coated coatings. The constants for the indenters and substrate are shown in Table 1. The coating model used for layered is shown in Figure 3. The overall thickness for all coating combinations is 3 μm.

However, for AlCrN / TiAlN coated layers the arrangement is in different shapes and thickness given as shown in Table 2 and Figure 4. The name of the first coating that touches with the indenter (top coating) is placed in front. In addition, the indentation depth used is 400 nm.

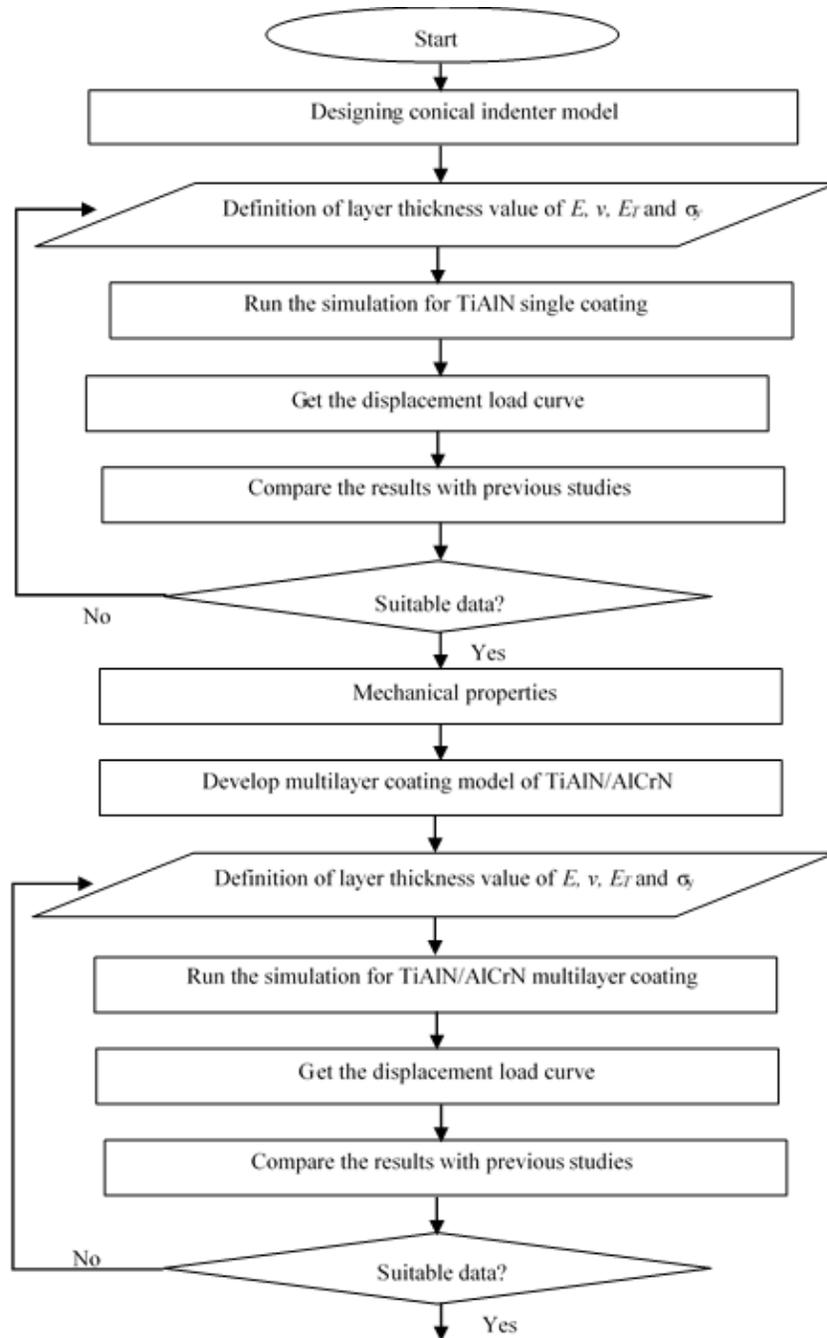


Figure 1: The flow chart for the experiment to be performed on the model of the coating.

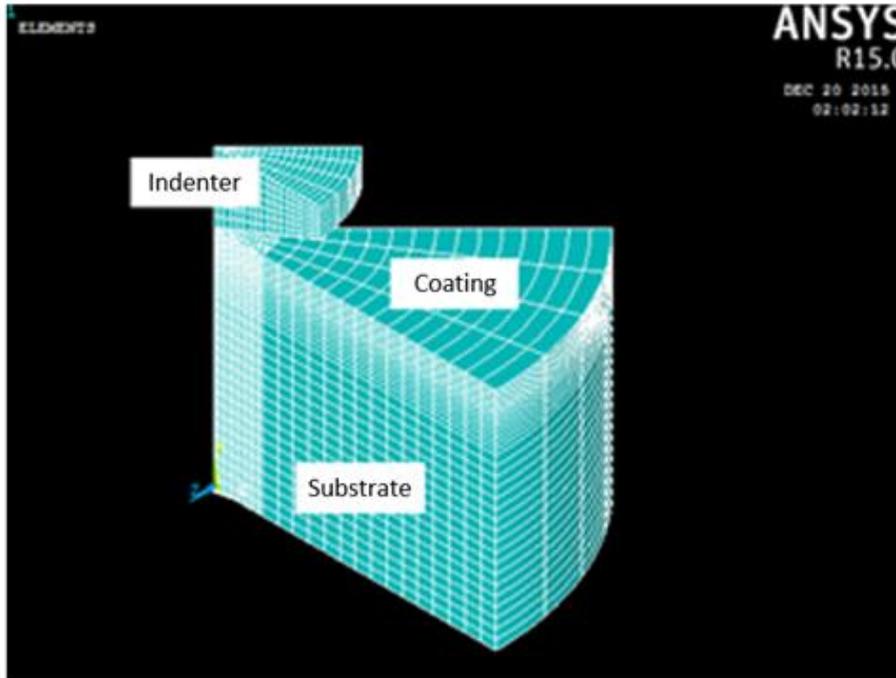


Figure 2: FE nanoindentation model.

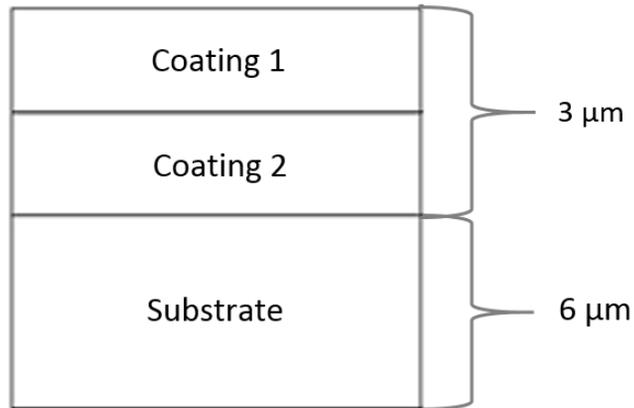


Figure 3: Multilayer coating model.

Table 1: The properties of HSS and diamond materials used in FEM simulation.

	Young Modulus, E (GPa)	Poisson's Ratio, ν	Yield Strength, σ_y (GPa)
Steel M2 (Substrate)	210	0.30	1.896
Diamond (Indenter)	1141	0.07	35.7

Table 2: AlCrN and TiAlN coatings layer arrangement and thickness.

Category	Arrangement	Label	AlCrN Thickness (μm)	TiAlN Thickness (μm)
A	AlCrN/TiAlN	A1	0.75	2.25
		A2	1.50	1.50
		A3	2.25	0.75
		A4	2.50	2.50
		B1	0.75	2.25
B	TiAlN/AlCrN	B2	1.50	1.50
		B3	2.25	0.75
		C1	1.00	1.00x2
D	TiAlN/AlCrN/TiAlN/AlCrN	D1	0.75x2	0.75x2
E	AlCrN/TiAlN/AlCrN	E1	1.00x2	1.00
F	AlCrN/TiAlN/AlCrN/TiAlN	F1	0.75x2	0.75x2

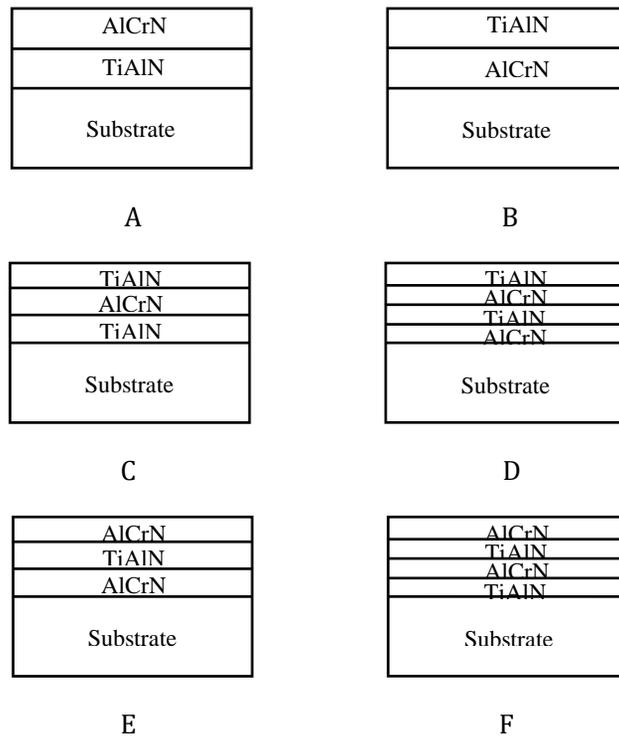


Figure 4: Coating model category that used for all multilayer coating.

3.0 RESULTS AND DISCUSSION

3.1 Verification of Nanoindentation Simulation Model

Before the simulation of the coating was conducted as the initial test of the model to be used was first verified by comparing the result of a load-displacement curve with a study by Kumar et al., (2014) uses a layered coating model to ensure that the model is appropriate. Comparisons made have errors of less than 1% complying with the conditions stated by Zamri et al., (2012). Furthermore, the initial tests on layered layers of different arrangements and thickness are carried out.

The findings of nanoindentation simulation for TiAlN and AlCrN single layers show mechanical properties of hardness, H and elasticity, E are still in the range of previous study findings (TiAlN: 139 -383 GPa; AlCrN: 277 – 474.6 GPa) (Fox-Rabonovich et al., 2006; Wang et al., 2008; Mo et al., 2007). This indicates other mechanical properties of tangential modulus, E_T , Poisson ratio, ν and yield stress, σ_y can be applied (Zamri et al., 2016). Previous elasticity, E and hardness, H values were different due to different parameters such as temperature, coating composition and type of coil. Then, the mechanical properties of these two single coating are used in the nanoindentation simulation of the coating of model A, AlCrN / TiAlN (Table 3). The load-displacement curves for the AlCrN / TiAlN coating experiment and simulation are shown in Figure 5. The simulation gave good results which was almost similar to the experimental result. The differences in the unloading gradient (unloading curve) and the maximum load for the experiments and the simulations were less than 10%. The results showed that simulation results of the model A coated coating showed the hardness of H enclosed in the range of previous studies by Kumar et al., (2014). The H/E ratio is to assess the degree of a substance wear resistance. The higher the H/E value, the higher the wear resistance level (Leyland and Matthews, 2000). The comparison of AlCrN/TiAlN coating mechanical properties of previous simulation and studies is shown in Table 4.

Based on Figure 6, the hardness value of model A layered coating (AlCrN/TiAlN) is the highest as described in Hassan et al., (2017). High hardness increases the wear resistance because the coating can accommodate higher stresses (Zamri et al., 2016). In terms of elasticity, E, the TiAlN coating has the highest value compared to the other coating. The value of elasticity, E helps in determining the stress value for a plastic moulding coating. Therefore, TiAlN coating can accommodate larger stresses than other coating before undergoing plastic changes. Further, the layered coating has the highest H/E ratio (around 20% higher than single coatings). This shows that the layered coating has the best wear resistance and can improve the performance of the punch tool if applied.

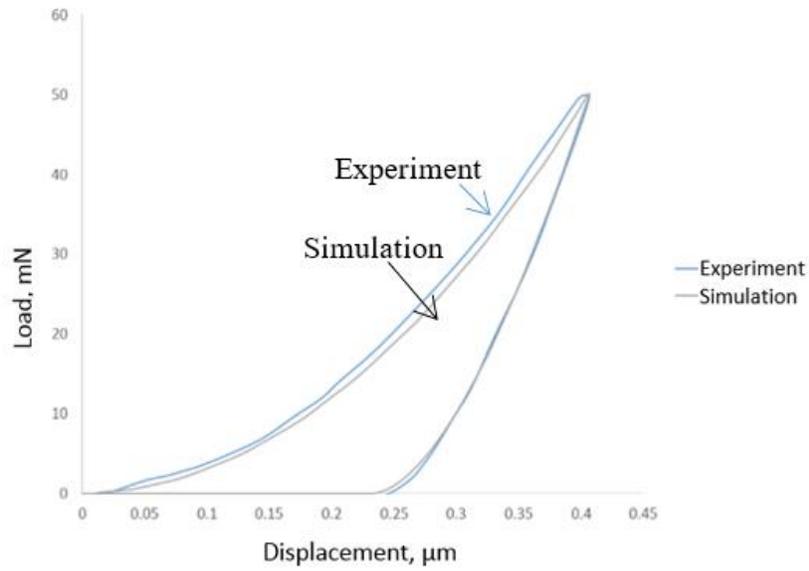


Figure 5: Comparison of load-displacement curves graphs from previous simulation and studies for AlCrN / TiAlN layers.

Table 3: The mechanical properties of AlCrN and TiAlN coatings from the simulation (model A).

Material	Hardness, H (GPa)	Elasticity, E (GPa)	Tangent Modulus, E_T (GPa)	Poisson Ratio, ν	Yield Stress, σ_y (GPa)	Ratio H/E
AlCrN	33.71	370	90	0.3	3.0	0.091
TiAlN	31.83	380	65	0.3	3.4	0.084

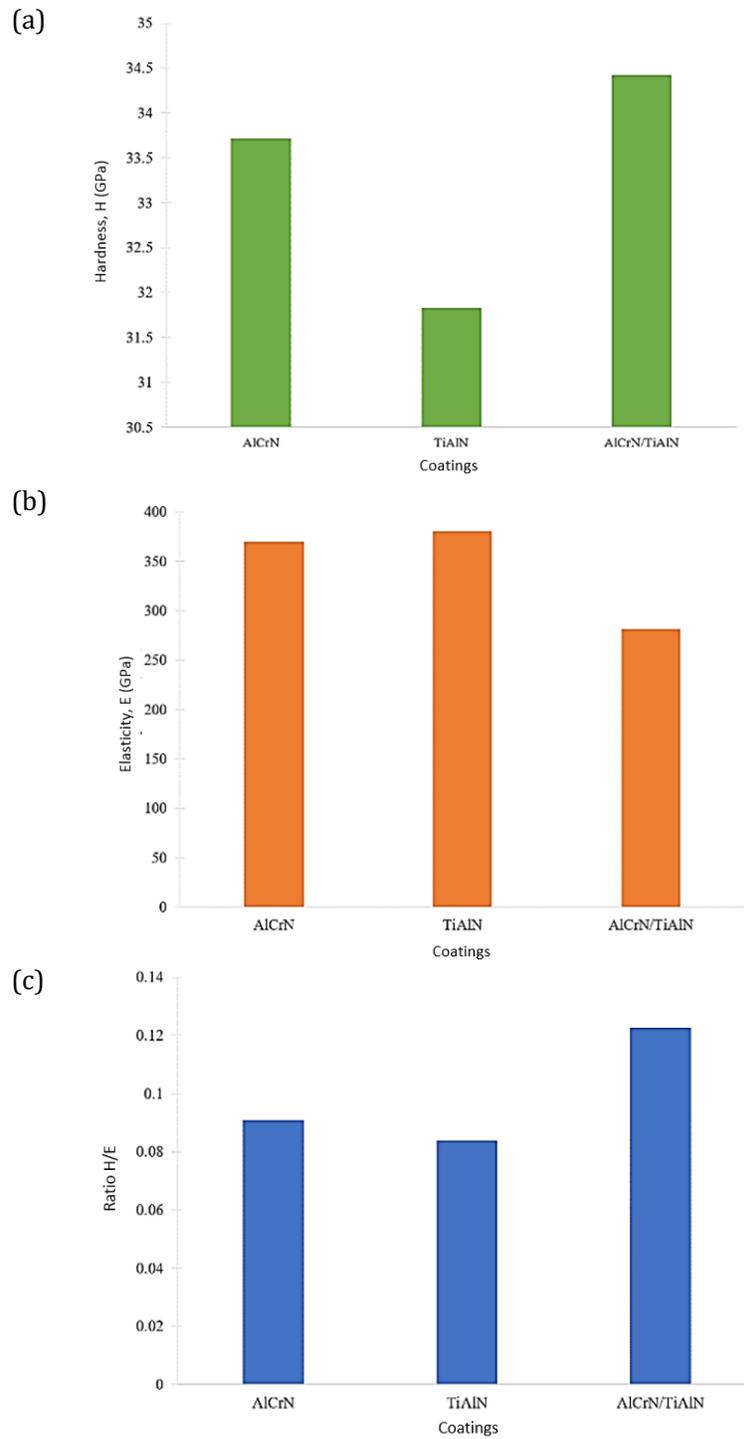


Figure 6: Comparison of mechanical properties (a) H and (b) E and (c) H/E ratio for single layer and multilayer AlCrN and TiAlN.

3.2 The Simulation Results of Coated Layers Nanoindentation Vary in Order and Thickness

Using the simulation, various types of coating arrangement and coating thickness can be developed as well as to identify the mechanical properties of the coating. There are six categories of coating that have different orders and number of layers. In addition, model A and B each use four and three different thickness. The total number of layers order is eleven and each layer is labelled to ease the reference starting from A1 to F1 (Table 5). For example, the arrangement of model A (AlCrN/TiAlN), it is divided into 4 types of thickness i.e. A1 up to A4. Although it has the same two-layer arrangement in which the top layer is AlCrN and the second layer is TiAlN, but the characterization of A1 up to A4 gives a difference to the thickness of both coating. Thickness effects are also identified in this study. Results of nanoindentation simulation of the load-displacement curves for different arrangements layered coatings are shown in Figure 7. All mechanical properties obtained through load-displacement curves such as hardness, H and elasticity and E for the purpose of comparative wear resistance are described in the next subtopic.

Table 5: The nanoindentation simulation results of multilayer coating vary layer arrangement and thickness.

Category	Layer Arrangement	Label	AlCrN Thickness (µm)	TiAlN Thickness (µm)	Hardnes, H (GPa)	Elasticity, E (GPa)	Ratio H/E
A	AlCrN/TiAlN	A1	0.75	2.25	36.37	372.98	0.0975
		A2	1.50	1.50	37.04	379.92	0.0975
		A3	2.25	0.75	37.03	379.90	0.0975
		A4	2.50	2.50	37.45	384.09	0.0975
B	TiAlN/AlCrN	B1	0.75	2.25	33.35	386.28	0.0863
		B2	1.50	1.50	32.59	377.45	0.0863
		B3	2.25	0.75	32.65	378.19	0.0863
C	TiAlN/AlCrN/TiAlN	C1	1.00	1.00x2	32.78	379.66	0.0863
D	TiAlN/AlCrN/TiAlN/AlCrN	D1	0.75x2	0.75x2	33.48	387.75	0.0863
E	AlCrN/TiAlN/AlCrN	E1	1.00x2	1.00	36.37	372.98	0.0975
F	AlCrN/TiAlN/AlCrN/TiAlN	F1	0.75x2	0.75x2	36.43	373.67	0.0975

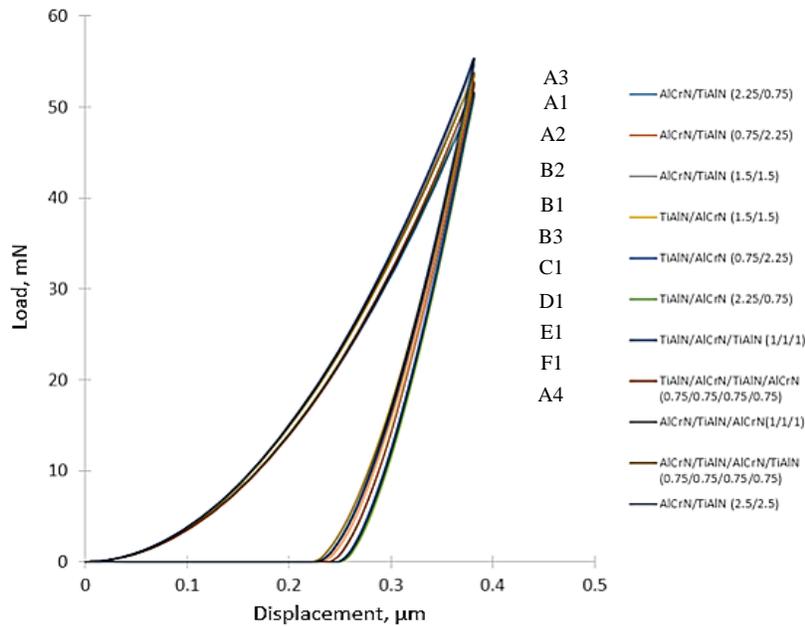


Figure 7: The load-displacement curve graph of multilayer coating of different arrangement and thickness.

3.3 Comparison of Hardness, H

Figure 8 shows that A4 coating has the highest hardness value of 37.45 GPa. If seen in terms of category A, thickness plays a role in increasing the value of hardness. Comparisons between A2 and A4 that have the same coating thickness distribution can indicate the difference when the thickness value is increased. Therefore, the thicker the coating, the higher the hardness value. In addition, hardness values are found to be higher when the first coating that touches the indenter is AlCrN. Furthermore, the increased layer can also increase the value of hardness Kumar et al., (2014). This can be seen in the coating labelled C1, D1, E1 and F1 where the layer is enhanced from three (C1 and E1) to four layers (E1 and F1). However, the coating with four layers has a lower hardness than two-layered coatings. This can be attributed to the thickness and type of coating. It is found that if the surface layer used is AlCrN and its thickness is high, the coating hardness value will be high. This shows that AlCrN coating is best used as a surface layer for punches applications in increasing its lifespan.

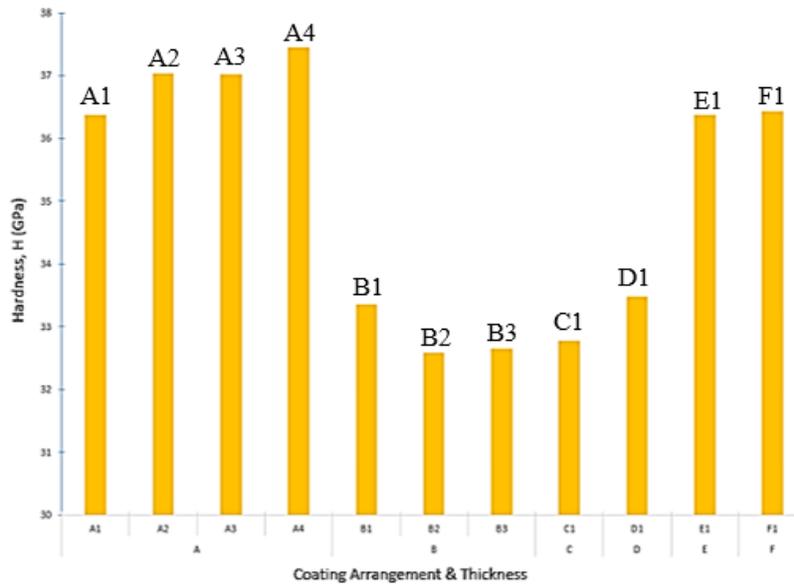


Figure 8: Hardness multilayer coating vary in arrangement and thickness.

3.4 Comparison of Elasticity, E

In addition to hardness, the maximum load value can also be attributed to the elasticity of a material. In achieving the specified indentation depth, the value of elasticity can affect the maximum load required. Referring to Figure 9, the coating with the highest elasticity is the labelled D1 coating which is TiAlN/AlCrN/TiAlN/AlCrN layer arrangement. High elasticity shows that this coating has a high elasticity and hard to change shape. In addition, Figure 9 also shows the surface coating using the TiAlN coating has a higher elasticity value than the AlCrN coating. Furthermore, TiAlN thickness also affects the value of elasticity. It is found that the increased thickness of TiAlN increases the elasticity of the coating. However, coating that uses TiAlN coating as surface layer has a low hardness value. Therefore, the thickness of both AlCrN and TiAlN coating plays a role to produce layered layers of high hardness and elasticity.

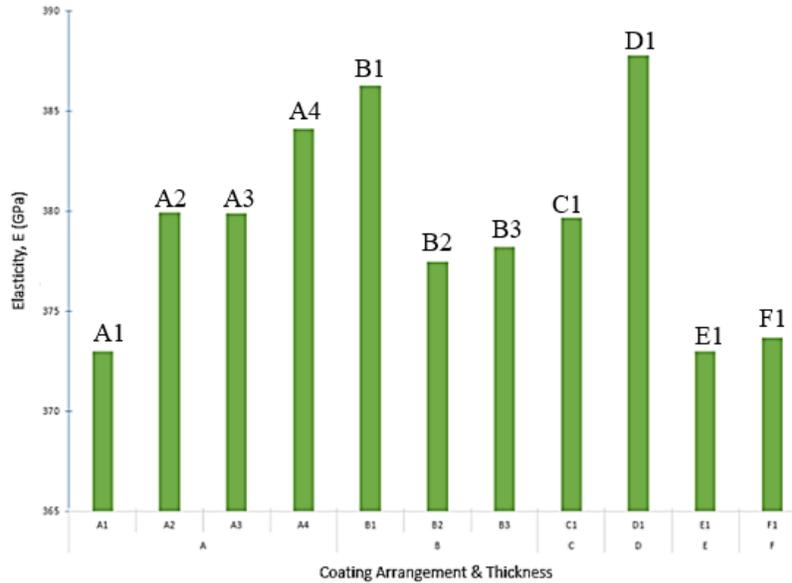


Figure 9: Elasticity multilayer coating vary in arrangement and thickness.

4.0 CONCLUSION

The results of the study show that simulation of nanoindentation using finite element method can give more mechanical properties value as well as hardness and elasticity such as tangential modulus, E_T , yield stress, σ_y and Poisson ratio, ν . It can be seen that the comparison between single and multi-layered coating of TiAlN and AlCrN materials shows a good result. Multi layered coatings provide better mechanical properties than single coatings. In addition, layered coating also has a higher H/E ratio indicating this coating has a better wear resistance. AlCrN works to increase the value of hardness while TiAlN contributes to the value of elasticity. Therefore, AlCrN is more suitable to be used as a surface layer which is directly applied to the tool because it has higher hardness. For punch tool applications, A4 labelled coating shows the most optimum and excellent results as it has an optimum hardness and elasticity compared to other architectural layer structures. Other factors such as temperature need to be taken into account in future research in developing nanoindentation model because the temperature can affect the production of load-displacement graph and elasticity will vary due to different indentation. Therefore, the depth of the indentation should be increased in the simulation to see the effect of the load on the lower layer apart from the surface layer. This can give the same stress distribution for the application of the punch tool as it may be exposed to higher load.

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