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M. J. Hernandez[a], S. E. White[a], J. F. Chessa[a] & C. V. Ramana[a]
[a] Department of Mechanical Engineering, University of Texas at El Paso, El Paso, Texas, USA
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M. J. HERNANDEZ, S. E. WHITE, J. F. CHESSA, and C. V. RAMANA

Department of Mechanical Engineering, University of Texas at El Paso, El Paso, Texas, USA

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The thermal residual stress and associated effects in TiN coatings with planar and nonplanar surface roughness on silicon (100) substrates were analyzed using both analytical and finite element (FE) modeling. The effect of growth temperature (T_s), thickness, and the modulus of elasticity on the stress evolution in TiN coatings is reported. The results indicate that the variable thermal stress in the TiN coatings is due to the existence of both positive and negative temperature gradients and thus the resultant existence of disparity of the coefficient of thermal expansion between the substrate and the coating.

Keywords: TiN coatings, thermal stress, finite element analysis axisymmetric geometry, interfacial mechanics

1. Introduction

Titanium (Ti) compounds, especially nitrides, find widespread use in various scientific and technological applications. Due to their exceptional physical and mechanical properties, TiN coatings have been used as protective and wear- and corrosion-resistant coatings for industrial machinery tools [1–4] and as biocompatible wear-resistant coatings for implants and surgical components in biomedical engineering [5, 6].

Titanium nitride coatings can be produced by a wide variety of physical and chemical deposition methods. During the growth or deposition of TiN coatings, residual stresses arise as a result of the following, however, not limited to: energetic particle bombardment, applied boundary conditions or constraints on the geometry, microstructure variability and progression with each successive layer, and thermal loading. The residual stresses can be further categorized into two specific types of stresses, which are intrinsic and thermal [7–9]. Intrinsic stress arises due to the deposition process itself [7]. Specifically, the coatings' microstructure undergoes progressive and continuous variability during growth as each successive layer is deposited. Furthermore, intrinsic and thermal stresses can be both tensile and compressive in directionality [8]. Considering the intrinsic (microstructure) stress, the directionality of stress is dependent on the level of micro void formations and its changes and, hence, the coatings' density and microstructure. These physical characteristics of the coatings are in turn affected by several processing parameters, such as bias voltage, partial pressure of gases, substrate materials, growth temperature, and the deposition rate itself. If tensile stress is observed, then it is expected that there exists a low atomic density, which possibly could be due to large quantities of micro voids. However, if there is an opposite sense of directionality (i.e., the intrinsic stress is compressive), the conditions mentioned above are no longer valid. In a compressive state there exists a high atomic density with smaller quantities of micro voids in the coating. Intrinsic stresses are most evident when sputter-deposition of the coating is at room temperature and decreases in dominance as the growth temperature increases. The thermal stress begins to show full dominance over intrinsic stresses as the main component of the residual stresses for coatings deposited at elevated temperatures.

The thermal stresses are a direct result of the existence of either positive and/or negative temperature gradients and thus the resultant existence of disparity of the coefficient of thermal expansion (CTE) between the substrate and coating, which affects the entire system [8]. This CTE mismatch between substrate and that of the coating is extremely vital, since the mismatch is proportional to the magnitude and the direction of resultant thermal stress on the coating-substrate system as a whole. Thus, a thermal stress that is tensile will correspond to a resultant positive difference in CTE between coating and substrate, and hence the negative corresponds to the resultant negative mismatch in CTE [8]. Therefore, if the deposition parameters, such as temperature and the CTE disparity, are substantially different, thermal stress plays an important role and can affect the mechanical properties, reliability, durability, and hence the overall performance of the system.

Reliability and the state of use of the coatings for desired structural, mechanical, and tribology applications are highly sensitive to these residual stresses. Specifically, if depositing coatings at higher temperatures, the systems' mechanical prop-

Address correspondence to C. V. Ramana, Department of Mechanical Engineering, University of Texas at El Paso, 500 W. University Avenue, El Paso, TX 79968, USA. E-mail: rvchintalapalle@utep.edu
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erties can be affected in such a way that could possibly lead to crack initiation, propagation, and ultimately failure [8]. It has been well established that the coatings' surface and interface along with the constrained section of the composite system is usually the locations of high thermal stress. These thermal stresses (residual stress component) can cause various failure modes, such as cracking of either coating or substrate, and debonding of interface of the two materials due to various stress states in the geometry, which directly impacts reliability and durability. It is then vital to understand the underlying physics of the deposition process and its resulting stresses, specifically a concentration on the thermal stresses on a coating–substrate system.

The present work was performed on the TiN coatings employing analytical and finite element (FE) modeling. The impetus is to investigate the thermal residual stresses at the nano and micro scale of TiN coatings on silicon (100) substrates inclusive of planar and nonplanar surface roughness. While the attention paid towards nano-layered coatings is scarce in the literature, attention has been directed in this work to derive an understanding of the stress evolution from nanometer dimensions to the bulk of TiN coatings.

2. Modeling

2.1. *Analytical Formulation of Thermal (Residual) Stresses*

The thermal stresses induced by the successive deposition of layers to form a coating under a temperature gradient (thermal load) can be approximated via the coalescence of Tsui and Clyne's model [9] with the well-established Stoney's formulation [10]. This analytical model is applicable for metallic coatings and for a planar geometry. The planar geometrical setting utilized in this work is shown in Figure 1.

The combined analytical model yields the thermal stress of the coating and its formulation is presented as:

$$\sigma \mathrm{f} = \frac{\left[Eef * \int_{Trm.}^{Tdep.} (\alpha \mathrm{sub} - \alpha \mathrm{film}) dT \right]}{\left[1 + 4 \left(\frac{Eef}{Ees} \right) \left(\frac{h}{H} \right) \right]}, \tag{1}$$

where α_{sub}, α_{film}, ν_s, ν_f, T_{rm}, T_{dep}, h, H, $E_{es} = [E_s/(1-\nu_s)]$, and $E_{ef} = [E_f/(1-\nu_f)]$, are the coefficients of thermal expansion of the substrate and the film, Poisson's ratio of the substrate and the film, room temperature and deposition temperature, coating and substrate thickness, and the effective Young's modulus

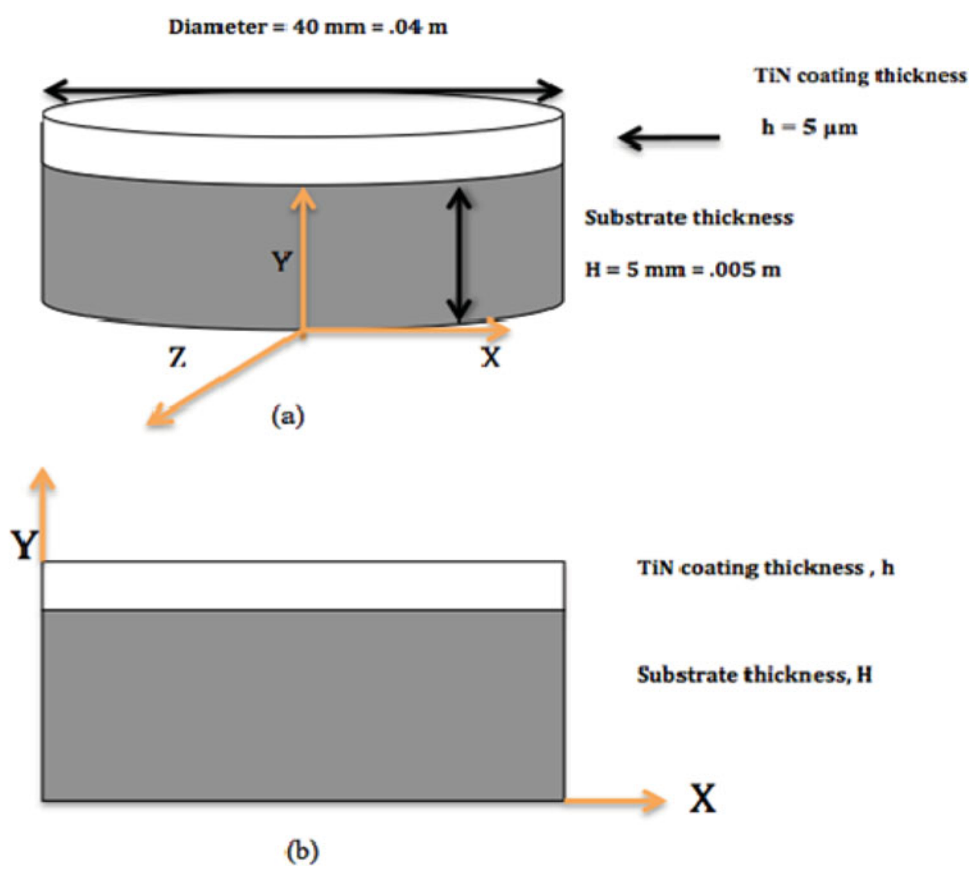

Fig. 1. (a) Three-dimensional cylindrical coating and substrate system depicting substrate thickness, TiN coating thickness, diameter, and axisymmetric axis (Y). (b) Extracted axisymmetric two-dimensional planar geometry for both analytical computations and finite element analysis (FEA).

Table 1. Material properties of both the substrates (silicon and sapphire) and the film

	Properties		
Material	Young's modulus (GPa)	Coefficient of thermal expansion ($\times 10^{-6}$ 1/°C)	Poisson's ratio
TiN	600	9.4	0.25
Si	167	2.33	0.3

of both the substrate and film, respectively. As is evident from Eq. (1), the thermal stress is a function of the material properties of the constituents (i.e., substrate and coating) and the geometrical configuration or setting parameters. For both the analytical computations and the FE component of the study, the mechanical and thermal material properties that were required were the following: Young's modulus, coefficient of thermal expansion (CTE), and the corresponding Poisson's ratio for TiN and Si materials. Modeling was performed considering the following assumptions: (i) coating was considered to be thin in terms of height as compared with the height of the substrate, and (ii) that the coating-substrate system under investigation was taken to be a composite beam, allowing an equivalent biaxial state of plane stress.

The deposition technique and the deposition parameters of the coating are highly variable in terms of manufacturing quality, then so are the coatings' material properties due to this dependence. The mechanical and thermal material properties for TiN coating and Si substrate employed in the present work are listed in Table 1.

2.2. *Finite Element (FE) Model Formulation*

2.2.1. *Geometric Model and Assumptions*

For simplicity, several simplifications were made to form a model that can be implemented in a FE analysis. First, a planar (2D) geometry was extracted from the original 3D cylindrical setting. Thus, specifically the local XY plane has an origin at the center of the cylinder and is under a right hand Cartesian coordinate system by convention. This is perfectly acceptable since there exists an asymmetry within the geometry about the Y-axis. Second, the TiN coating and Si substrate system were considered to have a certain cylindrical geometrical configuration specifically with a diameter, coating thickness, and substrate thickness of 0.04 m, 5 microns, and 0.005 m, respectively. The logic behind these physical parameter selections was twofold: (1) to maintain a geometric setting that allows thin film coating classification, and (2) to allow bending in the composite beam of the free end side while constrained on the axisymmetric axis, which will be a closer approximation to reality. Third, the contact plane (interface) of the coating and the substrate composite is perfectly bonded, which means no variation of bonding exists along this plane. Finally, both of the composite constituents (TiN and Si) were assumed to be isotropic materials. Furthermore, the composite constituents were considered to exhibit thermoelastic behavior in a linear sense and under a set influential temperature difference (thermal load).

2.2.2. *FE Model Description*

The FE of the thermal stresses in the composite beam (TiN-Si) after sputtering at elevated temperatures was performed in an axisymmetric 2D code created within MATLAB. The composite beam was discretized into a mesh of four-node quadrilateral elements with a constant element size of 0.000125 m from the bottom surface of the substrate to the top surface of the film consistently. To show the mesh of the specified element size and the output after one numerical simulation in MATLAB, Figure 2 illustrates a plot of the thermal stress. Both plots are for a TiN-Si system with the following parameters: substrate thickness of 0.005 m, coating thickness of 5000 nm (5 microns), and a thermal gradient load of 475 C. However, the first and second plots illustrate the planar surface roughness and the sinusoidal surface roughness on the coating substrate system mentioned.

The boundary conditions or constraints imposed on the beam were to be pinned completely on the left edge of the coating-substrate system, the axisymmetric y-axis, and all other nodes were then able to be dynamic in terms of degrees of freedom, which allowed bending. The loads that were imposed in the numerical simulation only consisted of a uniform thermal gradient load (room temperature of 25°C and the preset deposition temperature of 500°C). The thermal stresses in the beam were reported as the effective stress or Von Mises stress.

2.3. *Thermal Stress Analysis Methodology*

The evaluation of the thermal stresses for each of the interested parameters (i.e., growth temperature, coating thickness, substrate thickness, and coating Young's modulus) was carried out by fixing all other variables at the time (i.e., film and substrate moduli, Poisson's ratio of both film and substrate, geometric parameters h and H, etc.). For instance, while utilizing the combined analytical model presented in Eq. (1) for evaluating the thermal stress variability with growth temperature for Si, T_{dep} is varied for the selected range (i.e., room temperature to 500°C), while h, H, E_{ef}, E_{es}, α_{film}, α_{sub}, and T_{rm} are held at its predetermined and fixed values.

This procedure was also utilized once again in the finite element analysis (FEA) component of the report, but the analytical calculations served as some insight or approximate values for comparison, thus this is the pre-processing phase for the FE modeling. Numerical simulation results were verified point to point and macroscopically in terms of shape and directionality of thermal stress behavior with the analytical calculations. The thermal stress analysis sequence was performed on all the aforementioned parameters of interest for the TiN–Si system.

The effects of thermal stress on a select finite number of parameters, which are substrate temperature, coating thickness, substrate thickness, and the TiN Young's modulus variability, was analyzed. Thermal stress behavior plots were generated for each of the parameters by holding all other parameters

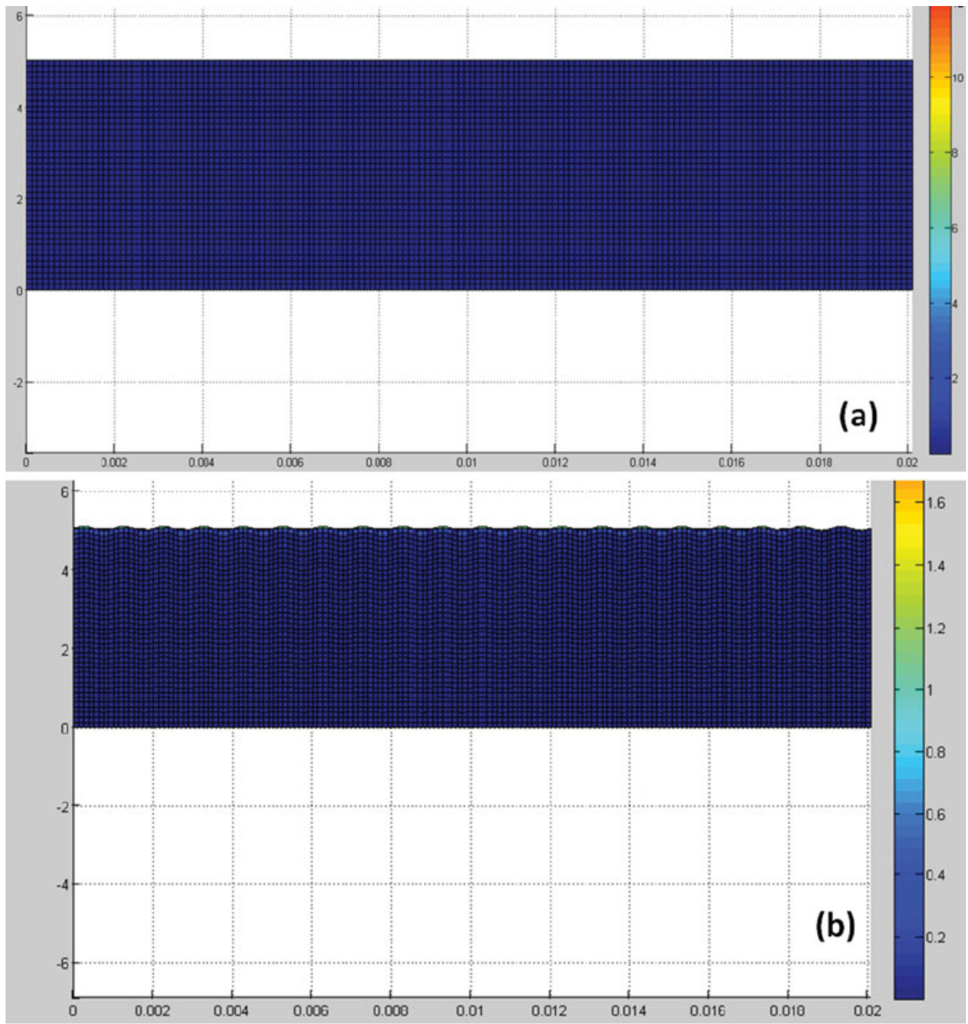

Fig. 2. Depiction of the element size and the construction of the mesh of the TiN-Si system using MatLAB for the FE method. (a) FE planar surface roughness thermal mesh. (b) FE sinusoidal surface roughness mesh (wave amplitude of 0.00005 m and wavelength of 0.001 m).

constant and varying only one parameter of interest at the time. The typical constant values for deposition temperature, coating thickness, substrate thickness, and coating Young's modulus were 500°C, 5 microns, 0.005 m, and 600 GPa, respectively. The parameter numerical ranges of variability are as follows: the deposition temperature in the range 25–500°C, coating thickness in the range 0–5000 nm, substrate thickness in the range 0.001–0.005 m, and the coating's Young's modulus from 350 to 600 GPa.

3. Results and Discussion

3.1. *Thermal Stress Behavior for the TiN-Si*

The results obtained on the TiN-Si system are shown in Figures 3–5. The variation of thermal stress with substrate temperature, coating thickness, substrate thickness, and Young's modulus of the coating is shown via all three modeling types (analytical and via FE method for both surface roughness types). During the sputtering process, considering both planar and sinusoidal surface roughness (Figure 3), the thermal stress increases linearly with increasing substrate temperature in magnitude and is compressive. As the temperature increases, the thermal stress tends to a higher compressive state, which is partly due to a proportional increase in the energy of the bombarding ions on the film with temperature. The maximum thermal stress values for the analytical and the planar surface roughness are −2.654 and −2.298 GPa, respectively. Therefore, the maximum error between the two methods is quite reasonable, and it can be explicitly seen that the FE method agrees with the combined analytical formulation. This compressive state is due to the magnitude of the mismatch between the CTE of the Si substrate and TiN coating. However, considering the sinusoidal roughness type, the maximum thermal stress occurs at the same substrate temperature of 500°C and has a corresponding value of −26.074 GPa. Thus, the sinusoidal roughness type has a much higher compressive thermal stress behavior overall. The absolute difference in thermal stress at this maximum point of

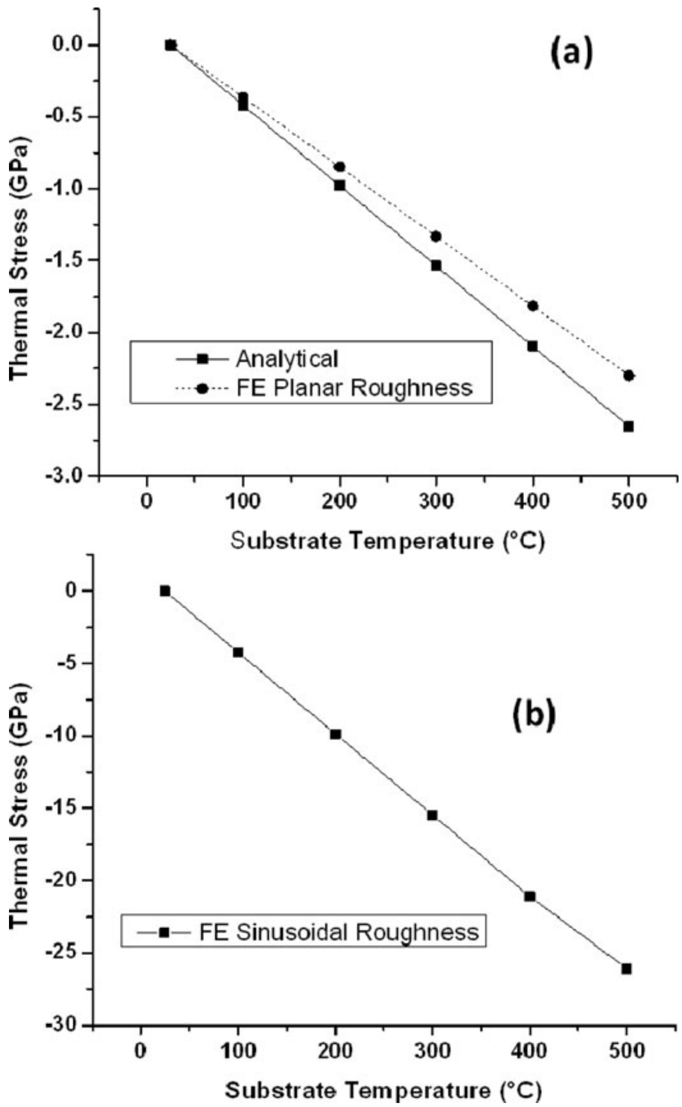

Fig. 3. The thermal stress behavior with substrate temperature for both methods, analytical and FE method. The stress evolution for both types of surface roughness is presented. (a) Analytical and planar surface roughness with FE model. (b) Sinusoidal surface roughness with FE model.

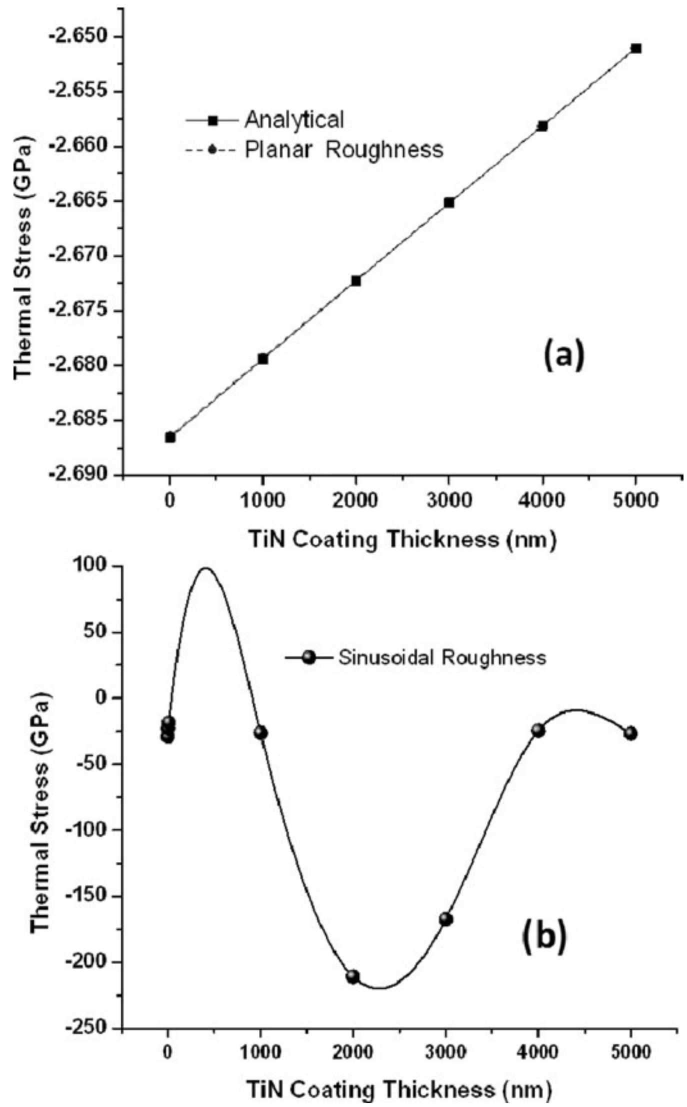

Fig. 4. The thermal stress variation with TiN coating thickness in analytical and FE methods. The effect of both types of surface roughness is presented. (a) Analytical and planar surface roughness with FE model. (b) Sinusoidal surface roughness with FE model.

substrate temperature is approximately 23.78 GPa while comparing both surface roughness types. Furthermore, it can be observed that roughly for every 100°C increase in substrate temperature, the thermal stress increases by ∼5 GPa.

The thermal stress variation of TiN coating with thickness for the analytical and planar roughness is shown in Figure 4. Thermal stress decreases in magnitude and approaches towards a positive scale as the coating thickness increases from 1 to 5000 nm. However, considering the sinusoidal surface roughness type, the thermal stress varies in a nonlinear fashion. There exists a significant and abrupt increase in the thermal stress from 1000 to 2000 nm and a change in directionality when increasing towards 4000 nm. The maximum thermal stress is found at the smallest coating thickness of 1 nm. The maximum stress values obtained are −2.68659, −2.6866, and −210.81 GPa for the analytical, planar, and sinusoidal analysis, respectively. Indeed, the compressive stress values obtained are close to that of experimentally determined value (∼2 GPa) of stoichiometric TiN coating by the cantilever laser technique [11]. In addition, the results are in good agreement with those reported for thick TiN coatings using FE modeling and analysis in the literature [12, 13]. However, the absolute difference between the two types of surface roughness is approximately 208 GPa, which is quite large. The minimum thermal stresses that occur at 5000 nm for the analytical, planar, and sinusoidal roughness are −2.65104, −2.65110, and −18.3680 GPa, respectively. Similarly, as with the last parameter substrate temperature, the analytical and planar roughness calculations via the FE method display similar results and are in correlation with each other.

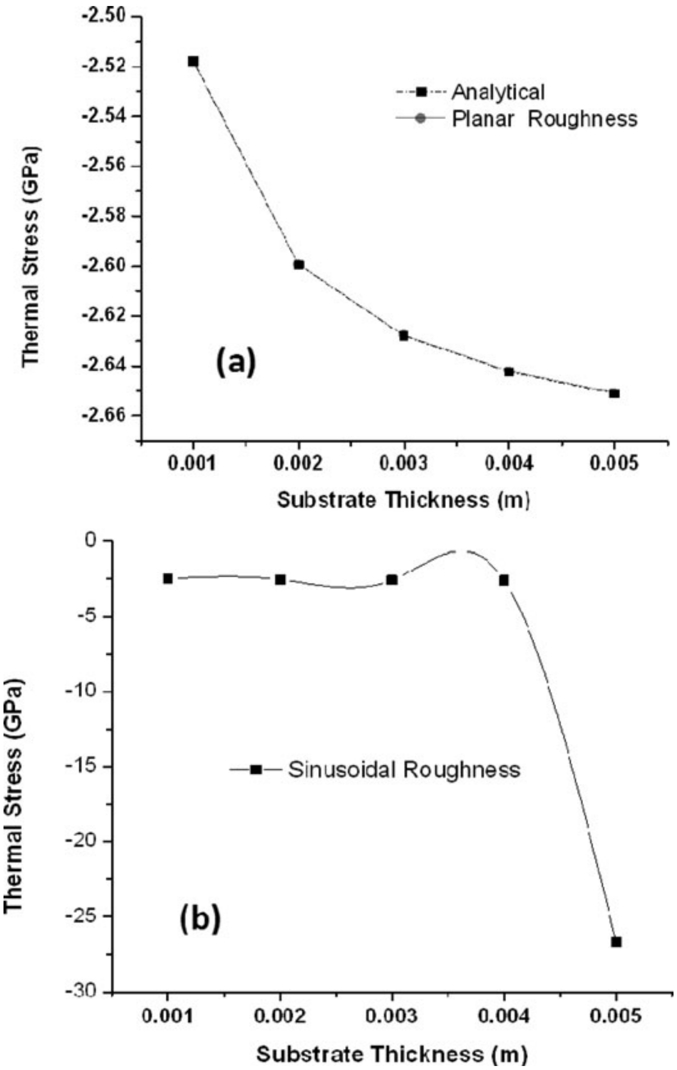

Fig. 5. The thermal stress variation as a function of substrate thickness for both methods, analytical and FE method inclusive of both types of surface roughness. (a) Analytical and planar surface roughness with FE model. (b) Sinusoidal surface roughness with FE model.

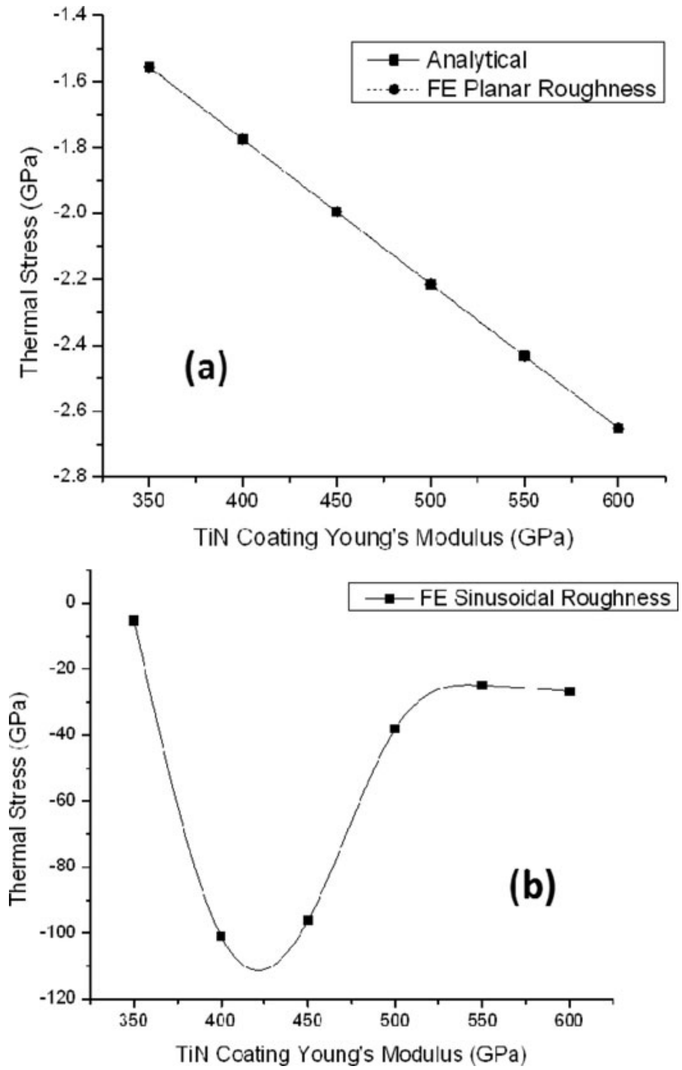

Fig. 6. The thermal stress behavior as a function of TiN coating Young's modulus for both methods, analytical and FE method inclusive of both types of surface roughness. (a) Analytical and planar surface roughness with FE model. (b) Sinusoidal surface roughness with FE model.

We now turn to the third parameter of interest for the TiN-Si system, which is the substrate thickness. The thermal stress on the system with a constant planar surface roughness varies in a nonlinear fashion (Figure 5) and approaches a maximum magnitude in a compressive state. The minimum and maximum thermal stress values are −2.5181 and −2.6511 GPa, which correspond to a substrate thickness of 0.001 and 0.005 m, respectively. As seen in the previous plots, the FE method is seen to be in agreement with the analytical solution with a maximum error of 0.002%. For the sinusoidal surface roughness, the composite exhibits a nonlinear thermal stress behavior. From 0.001 to 0.003, the thermal stress is seen to be approximately constant; however, after 0.004 m (4 mm) of substrate thickness, the thermal stress increases rapidly to the maximum value. Therefore, if the objective is to minimize the thermal stress, a thin film should be grown on a silicon wafer (100) with a substrate thickness of less than 0.004 m.

The effect of the variation of the coatings of Young's modulus of elasticity on the thermal stress evolution is shown in Figure 6. Since TiN coatings can be grown under various sputtering conditions, variations in TiN coatings' mechanical properties, especially the modulus of elasticity, is expected. Consequently, the effective modulus of the film (E_{ef}) becomes variable as well. The coatings of Young's modulus can vary from 350 to 600 GPa, which is due to this inconsistency in the coating; the thermal stress was examined under the various Young's modulus values, as stated above. It can be seen from Figure 6, that the thermal stress increases in a negative linear fashion and tends to be a more compressive state as the TiN Young's modulus increases to the maximum value of the range, 600 GPa, for the planar surface roughness. Thus, in order to minimize thermal stress, the TiN coating should be grown to have a much lower Young's modulus to constrain the thermal stress, but this can have a greater impact on the stiffness of the coating; thus, a trade-off exists if considering a planar surface roughness. The maximum values of thermal stress for the planar and sinusoidal surface roughness of the TiN-Si system are -2.6511 and -100.902 GPa, respectively. However, when a sinusoidal surface roughness is introduced on the coating substrate system, a nonlinear thermal stress behavior is induced (Figure 6). To minimize the thermal stress, a coating must be grown with an approximate Young's moduli of 300–350 or 500 to 600 GPa, if considering a sinusoidal surface roughness type. Similarly, as with the other parameters mentioned previously, the FE model of the effects of thermal stress on this particular coating substrate system with planar surface roughness is in agreement with the analytical calculations with minimal error.

4. Conclusions

Conclusions that can be made from both the analytical and FE analysis of the TiN-Si system as presented in this study are as follows:

(1) The existence of the compressive thermal stress is due to the CTE mismatch between the film and substrate.
(2) Thermal stress increases dramatically by more than 50% at a time if a sinusoidal surface roughness is observed in the film-substrate system.
(3) Nonlinearity of thermal stress occurs for either type of surface roughness (constant or sinusoidal) for Si substrates.
(4) The FE and analytical models, when considering a planar surface roughness for all parameters, have similar results.
(5) Variable stress occurs and was observed at the free edge side, which is not maximum but exists under variable thermal loading conditions.
(6) As the deposition temperature increases, so does the potential thermal difference, the thermal stress increases.
(7) It is important to note that as any of the processing parameters, i.e., substrate temperature, substrate thickness, and TiN coating modulus, increases to a higher value, the thermal stress also increases to a much higher compressive state in general. However, the maximum compressive thermal stress exists at the smaller TiN coating thickness of 1 nm and decreases if the thickness reaches towards bulk values (5000 nm).

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