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Optimization Study on Simulation Technique of Bismuth Telluride(Bi_2Te_3) Thermal Barrier Coating Fabrication by Finite Element Method

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***Abstract*— Bismuth Telluride (Bi_2Te_3) is basically known for its unique properties for various ranges of several device applications. Now in nanotechnology, as devices are migrating to the level of nanometer scale, the significant amount of experiments are being progressed to keep it up with the rapidly growing research field of nanotechnology. The surface coatings of Bismuth Telluride (Bi_2Te_3) films supply superior surface thermal barrier coating on substrate. With the support of finite element simulation technique, the performance of surface coating under various load can be calculated and thus provided useful information, for the design and the use of the surface coatings for different applications. The purpose of present study is to model and simulate Bismuth Telluride (Bi_2Te_3) thermal barrier coating nano-fabrication process on Bismuth Telluride coated high speed material by finite element method and to compare its results with experimental other barrier coating nano-fabrication results. A two- dimensional and three-dimensional axisymmetric model is simulated in sequential and iterative application using MATLAB. The finite element simulation is modeled as stiff structure of Bismuth Telluride (Bi_2Te_3) material. The designed models have the aptitude and ability for simulation of the observed loading and unloading curves and the occurrence of coating distortion during indentation. Developed load-displacement curve obtained from finite element simulations are compared with the other load- displacement curves estimated by the experimental result. Finally, the outcome of finite element simulation presents that there is excellent performance with the experiment results.**

Keywords*— Bismuth Telluride, Thermal Barrier Coating, Finite Element Method, Finite Element Simulation.

I. INTRODUCTION

The progressive improvement in the characterized performance of various useful material systems has been carried out by the application of thin films of different substances on nearly all kinds of substrates, to meet the advanced industrial needs. Coating is a controlled process at the nano-scale level to significantly enhance the ability of surface properties of substrate like hardness and elastic modulus [1]. The failure of thin coated substrate is related to the failure of coating itself or deformation of the substrate. It has been noted that coated surface very often fails due to the tensile fracture. Tensile fracture generally occurs at the surface contact edge of a surface contact due to the high tensile stresses [2]. So, it is essential to analyze the capabilities of coated surfaces. There are many different techniques that are used for measurement of its mechanical as well as physical properties of the coated surfaces of material. Among all these techniques, nano-indentation method is one of the fundamental technique [3][4]. But the test and analysis results are complicated to analyze because of the high complexity of triaxle stress. Recently, many numerical methods and techniques have been proposed in the area of various engineering, technology and applied sciences, for purpose of simulation and exploring the indentation issues and problems. The finite element model give solution of high complex stress-strain field of hard and solid coated surfaces. Environmental, economical, safety aspects and energy saving emphasize the significance of friction control and wear in the machineries, tools and devices [4]. Lubrication with oil is the most common way to control friction and wear. The use of liquid lubricant is usually not so advantageous for environmental reason, problems with to keep it in the contact area, ageing, circulating, storing, and contamination [5]. Surface engineering, where the surface property of affecting contacts are basically changed in a favorable way by deposition of a different material or surface treatments, is an effective and efficient way to control friction and wear.

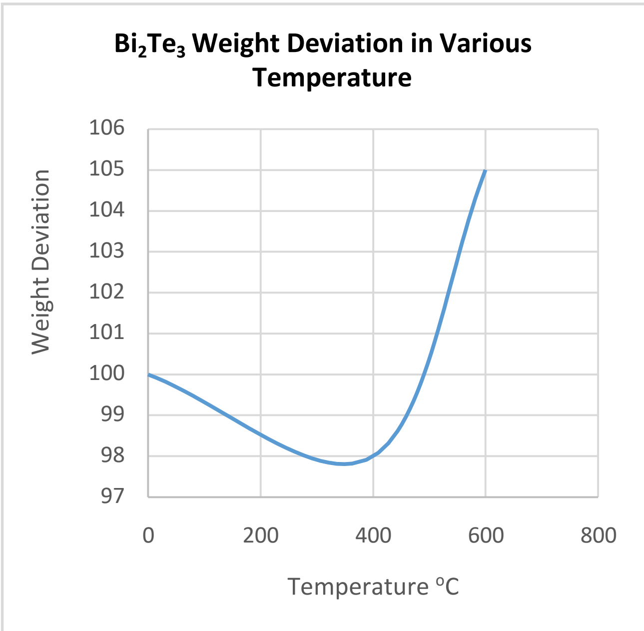

Figure 1: Bi_2Te_3 Weight Deviation Thermal Effect

Figure 1 presents some mass loss as temperature varies. There is also a slope in the mass loss and mass gain. This is due to desorption from surface and evaporation of the absorbed residues like moisture [6].The slope of mass loss is more gradual from 160 to 400 °C and this is due to sublimation of tellurium. At temperature of 400 °C the graph presents relatively high weight gain. Usually, some chemical reactions occur from the surroundings environment. If tellurium (Te) exceeds, then oxidation of bismuth (Bi) is a candidate for reaction [7]. The heating rate of around 10 °C per minute presents the upward direction of the curve and the oxidation reaction does not carry out during the time. The relative studies of Bismuth Telluride (Bi_2Te_3) thermal barrier coating fabrication procedure by experimental and finite element analysis demonstrates that the finite element analysis is capable of generating the loading-unloading behavior of thermal barrier coating fabrication test. So far, the finite element analysis is an effective method for simulating hardness computations and its confirmation[8]. There is the ratio of coating thickness to its indentation depth, on which this property has a minor effect on the force with respect to displacement curve.

The intention of this research is to simulate the process of nano-indentation on the surface coatings of Bismuth Telluride (Bi_2Te_3) films as a thermal barrier coating on substrate. This simulation includes the modeling of the system in terms of two-dimensional (2D) and also three dimensional (3D) axisymmetric models [9]. The finite element results are compared with experimental results of nano indentation process. The simulation is compared with ball indenter of carbon material, and other substrate by the inductively coupled plasma intensive deposition technique [10]. The simulation procedure is carried out in sequential and iterative application using MATLAB.

II. LITERATURE REVIEW

In this paper we reviewed, explored and analyzed some modern finite element simulation on surface of some nano-materials.

A. *Finite Element Simulation of Shot Peening Coverage with the Special Attention on Surface Nanocrystallization*

The purpose of the simulation study to challenge the present finite element technique in the conditions of the most significant experimental parameters, which is the coverage. Important production and models from the previous work are again re-simulated and its result of treated surfaces are explicitly examined [11]. The outcome of this analysis presents that existing finite element models do not reflect the actual practical coverage. in order to obtain full practical coverage and simultaneously dropping the computational cost, the symmetry of variable dimension cell is developed. This analytical model presents successful simulation of the surface nano-crystallization process by shot peening which results the amount of coverage which is much higher than the conventional shot peening[11].

This simulation of finite element method of shot peening have been evaluated in terms of resulted coverage that is practically the most significant measurable variable of this shot peening procedure. Results of this simulation study presents the existing methods have the limitations of either not capturing a practical coverage or very cost effective to simulate the high coverage [12]. A symmetry cell of various dimensions have been launched to conceal both shortcomings. This model illustrated to have the capability of simulating severe shot peening for which coverage is often high.

B. *A Finite Element Model of Carbon Composites*

Carbon fiber-reinforced polymer composites are extensively used in automobile industries, aerospace technology and many structural applications for their higher physical and mechanical properties [13]. It outperforms structural metals in durability, high strength to-weight ratio, stiffness and density. Although, aside these advantages, the machining carbon fiber-reinforced polymer is unmanageable due to extremely abrasive carbon fibers, low thermal heat conductivity of epoxy as well as a weak inter-surface bond created between reinforced fibers and matrix. Parts made of carbon fiber-reinforced polymer material are fabricated to the necessary final shape, however fabrication cannot be ignored to congregate individual components. To assist bolting and riveting of mechanical components, holes need to be drilled, for this purpose, traditional drilling methods are often adopted. Apart from low quality surface finish and geometric tolerance, conventional drilling can begin various damage modes in carbon fiber-reinforced polymer such as burr formation, matrix cracking, delamination, interfacial de-bonding and fiber pull-out. Therefore, the load-carrying ability of composite construction is affected [13][14]. The rapid tool wear is due to abrasive carbon fibers which results in frequent replacement of tools. To handle these problems, an alternative drilling method is required.

The drilling method by ultrasonic supported is a modern machining technique which is capable for drilling difficult machine materials like carbon based composites, here ultrasonic vibrations are imposed upon the tip of revolving drill bit. Now, ultrasonically supported drilling has been revealed to possess numerous benefits in comparison to traditional drilling, with a reduced torque and thrust force, minimum drilling-induced impairment and complete enhancement in surface finish and roundness of the drilled hole. A finite element method of ultrasonically supported drilling in carbon based composite is offered. This method accounts for volumetric as well as thermal softening process in the work piece substantial under the impact of localized vibroimpacts, that is the typical feature of ultrasonically supported drilling [15]. This method was applied in explicit and confirmed with results from experimentations, representing a reasonable connection between them. A parametric analysis is also carried out to observe the effect of dissimilarity in intensity of ultrasonic energy on the amount of softening in the carbon based composite for ultrasonically supported drilling.

C. Constitutive material model using Finite Element Simulation

In the model of constitutive material, the work piece material applied is quasi-isotropic laminate M21/T700 of thickness 10 mm and individual ply thickness of 0.25 mm which is commercially available. The specifics on the stack arrangement and mechanical properties of carbon fibre-reinforced polymer laminate employed in present simulations is found by experimental and numerical investigations in ultrasonically supported drilling [16][17]. The thermo-mechanical plasticity method proposed in present work is constructed on the quadratic yield principle for anisotropic materials and the hardening rule ofnon-linear isotropic for rate-independent plasticity. The model equations of this method for uni-axial loading are:

The entire strain tensor for throughout deformation is the summation of elastic strain tensor and plastic strain tensor, which is given by,

$$\varepsilon = \varepsilon^{el} + \varepsilon^{pl}$$

The elastic part of stresses is calculated using a constitutive stress-strain relationship:

$$\sigma = C.\varepsilon$$

$$\varepsilon = C(\varepsilon^{el} + \varepsilon^{pl})$$

where, σ and ε are the second-order elastic stress and strain tensors while C is the fourth-order stiffness tensor. The yield function for orthotropic carbon fiber-reinforced polymer material in rectangular Cartesian stress components [18].

III. PROPOSED METHOD

Bismuth Telluride (Bi_2Te_3) films are fabricated by using a standard inductively coupled plasma-enhanced chemical vapor deposition reaction chamber powered by a high RF power source. For simulation of thermal barrier coating fabrication, a high speed Bismuth Telluride (Bi_2Te_3) thin films of 1.5 cm x 1.5 cm square area with thickness of 2 mm was taken as a substrate for depositing Bismuth Telluride (Bi_2Te_3) thermal barrier coating film. The pressure in MATLAB simulation is varied with the help of closing and opening the throttle valve. The total flow rate was maintained as a constant by varying the composition of the precursor gases. The curve of load-displacement within finite element modeling is obtained by the nano-hardness tester fitted with an integrated optical atomic microscope which is equipped with some material, having a triangular-pyramid shape. There is a comparison graph of the load-displacement curve obtained from carbon based material and Bismuth Telluride (Bi_2Te_3) thin films.

Finite Element Modeling:

For expressing axisymmetric model, two-dimensional and three-dimensional axisymmetric case are performed to simulate the process of indentation [19]. The model is designated by master and slave surfaces. These models were meshed in model and analyzed in finite element using MATLAB. In these models, ball indenter was considered as rigid of Bismuth Telluride (Bi_2Te_3) thermal barrier coating material having tip radius of 200μm. The specimen sample is modeled with the help of plane 82 different element type. The indentation is basically very small with compared to size of the specimen sample. The volume of substrate involved into consideration is taken as 12×4×2 cube mm, as height, width, and thickness. Input material properties required for modeling is shown in table 1.

Table 1: Mechanical properties of ball indenter, coating and substrate materials

S.No.	Name of the Modelling parts	Properties
1.	Ball indenter	(a) Material = Bismuth Telluride
		(b) Young's modulus = 1140GPa
		(c) Poisson's ratio= 0.07
2.	Coating	(a) Material= Bismuth Telluride
		(b) Young's modulus= 70GPa
		(c) Poisson's ratio= 0.22
3.	Substrate	(a) Material= Bismuth Telluride
		(b) Young's modulus = 200GPa
		(c) Poisson's ratio= 0.29
		(d) Yield strength = 4100MPa
		(e) Strain hardening coefficient = 20

The substrate distortion behavior is categorized as elasticity. Two dimensional and three dimensional models are mesh with the help of MATLAB simulation. After that these models are analyzed in finite elemenmethod. A fine mesh is applied around the contact area of film and near the tip of indenter in both two-dimensional and three-dimensional models and these models are generally of second order.

The connection restriction is defined by master (ball indenter) and slave (substrate) surfaces. The ball indenter can usually penetrate the substrate. The process of indentation is simulated during both loading and unloading period. The values of load applied by the ball indenter upon coated substrate are within the minimum range of 0 N and maximum rangeof 5 mN. During loading process, the simulation is performed to a depth, which is 75% of thickness (10 μm) of Bismuth Telluride (Bi_2Te_3) thermal barrier coating in the y-direction, the indenter tip penetrates through the specimen, while during the process of unloading the indenter tip returns back to the initial position at (0, 0, 0) coordinate. When the ball indenter arises in contact with coated substrate then the load value is 0 mN. During the process of loading the velocity of indenter is 1 mN per second and the maximum value of load become up to 5 mN. The boundary surroundings are applied sideways with the original point, centerline and also bottom of specimen by setting the sample at horizontal axis. The nano- indentation model was developed based on the following assumptions:

(i). Materials are considered to be fully homogeneous and free from contaminates, pinholes and defects,

(ii). The surface in the simulation model are preferably smooth, which presents that surface irregularity effects are not measured, residual stress is not considered in modelling,

(iii). Coating/substrate interference is perfectly bonded. During indentation process decently elastic distortion takes place only throughout the starting of the indentation process. In order to calculate occurrence of plastic deformation, Mises yield criterion is applied.The equation of Mises stress is given by the expression,

$$\sigma_{mises} = \sqrt{\frac{(\sigma_1-\sigma_2)^2 + (\sigma_2-\sigma_3)^2 + (\sigma_3-\sigma_1)^2}{2}}$$

Where σ_1, σ_2 and σ_3 are the three principal stresses. Whenever σ_{mises} reaches the yield strength σ_0, the material begins to distort plastically.

IV. Simulation And Result Evaluation

We used MATLAB as a simulator for our implementation and performance evaluation of our proposed method. The curve of load-displacement obtained for thermal barrier coating fabrication by finite element method is shown in figure 2.

An indentation curve is obtained on one sample. The amount of loading and unloading rate is same with the value of 1 mN/sec. The maximum depth of indentation of 100 nm and the maximum load of 5 mN and are applied over 500 seconds. So, the total distortion is confined within the thin film. The residual displacement is 50 to 150 nm for a total displacement of 200 nm is estimated. Thus, the thin film underwent 60% elastic deformation and 40% plastic deformation. By using two-dimensional (2-D) simulation models the development of plastic deformation in Bismuth Telluride (Bi_2Te_3) thermal barrier coating fabrication by finite element method is investigated in order to know the better understanding of the elasticity deformation behavior in the material as the indentation depth is enlarged.

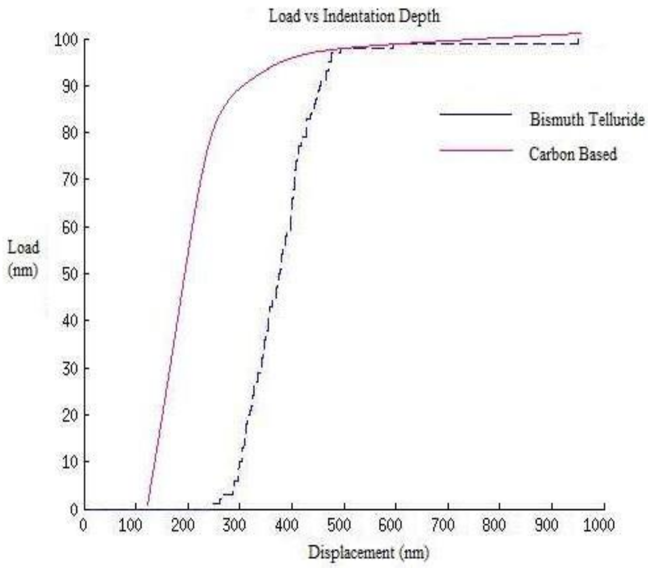

Figure 2: Load-displacement curve of Bismuth Telliride film

V. CONCLUSION

Finite element method is a powerful implementation method and precedure to simulate the indentation process at the nanoscale level. This simulation study presents two-dimensional as well as three-dimensional axis-symmetric finite element model to estimate the nano-indentation procedures. The finite element model has been developed to simulate the nano- indentation response of surface coatings of Bismuth Telluride (Bi_2Te_3) thin films as a thermal barrier coating on substrate. The model is capable of simulating the loading and unloading stages of the plastic deformation behavior during the indentation process. The applicability of the model has been investigated by experimental nano-indentation test of surface coatings of Bismuth Telluride (Bi_2Te_3) filmsas a thermal barrier coating on substrate. The simulation result is in decent agreement with the experimental results.

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