Mechanical Performance and Analysis of Bismuth Telluride (Bi_2Te_3) Thermal Barrier Coating

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***Abstract*- In this experiment, we analysed the purpose of this dissertation is to model and simulate Bismuth Telluride (Bi2Te3) 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. This dissertation is presented to show the use of finite element analysis (FEA) for the thermoelectric performance of micro-scale and nano-scale, self-assembled devices. Previous research has demonstrated an optimal performance at scales inaccessible to pick and place manufacturing and thin film deposition methods. The finite element simulation is modeled as stiff structure of Bismuth Telluride (Bi2Te3) 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.**

Index Terms- Bismuth Telluride, Nanomaterial, Figure of Merit, Finite Element Method, Load-Displacement.

I. INTRODUCTION

The motivation for this dissertation work 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 carbon based barrier coating nano-fabrication results. Several researchers in the domain of nano-fabrication coating have addressed and proposed various methods and techniques for effective thermal barrier coating. Most of the researchers concentrate on processing and fabrication techniques for different materials. Generally, the present approaches and strategies focus on finite element method on Bismuth Telluride (Bi_2Te_3) thermal barrier coating nano-fabrication process.

1. Nano-Material and Nanotechnology

Nano-material is material science, engineering and technology conducted at the nanoscale of materials, which is about 1 to 100 nanometers. Nanoscience and nanotechnology are the study and application of extremely small things and can be used across all the other science fields, such as chemistry, biology, physics, materials science, and engineering. [1]

Fig. 1 - Attributes of Nanotechnology

2. Bismuth Telluride (Bi_2Te_3)

Bismuth Telluride (Bi_2Te_3) is a gray powder that is a compound of bismuth and tellurium also known as Bismuth (III) Telluride. It is a semiconductor which, when alloyed with antimony or selenium is an efficient thermoelectric material for refrigeration or portable power generation. Bi_2Te_3 is also known to be a topological insulator, and thus exhibits many thickness-dependent physical properties. Bismuth Telluride is known to wield unique properties for a wide range of device applications. [2]

- Bismuth telluride (Bi_2Te_3) as Thermoelectric Refrigeration
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II. LITERATURE REVIEW

Literature survey is an important part in the design and implementation of any system. Proper survey can be quite helpful in the various design phases of the overall system.

1. Exploratory Review and Analysis Process of Nano- Materials.
2. Review of Modeling of Nano-Materials. [3]
3. Atomistic Modeling of Nano-indentation of Multilayered Graphene-Reinforced Nanocomposites. [4]
4. Qualitative Evaluation of Diamond Like Carbon Coatings Using Molecular Dynamics Nano-indentation Simulations. [5]
5. Establishment of Numerical Modeling. [6]
6. Theoretical Models of Nano-Structure. [7]
7. Discrete Element Method. [8]
8. Finite Element Simulation of Shot Peening Coverage with the Special Attention on Surface Nano- Crystallization. [9]
9. A finite element model of carbon composites. [10]

III. TECHNICAL ASPECTS OF BISMUTH TELLURIDE

Table No. 1 - Basic Bi_2Te_3 Properties		
1.	Molecular Weight	800.67 g/mol
2.	Crystal Structure	Hexagonal-Rhombohedral
3.	Lattice Constant	a = 4.38 Å, c 30.45 Å
4.	Band Gap	0.21 eV
5.	Electron Mobility	1140 cm^2/V s
6.	Hole Mobility	680 cm^2/V s
7.	Thermal Conductivity	3 W/mK
8.	Density	7.73 g/cm3
9.	Melting Point	585°C

In this dissertation, a nanoparticle with reference to Bismuth Telluride (Bi_2Te_3) is analyzed. Bismuth telluride (Bi_2Te_3) basically is a gray powder which is a compound of elements bismuth (Bi) and tellurium (Te) [11].

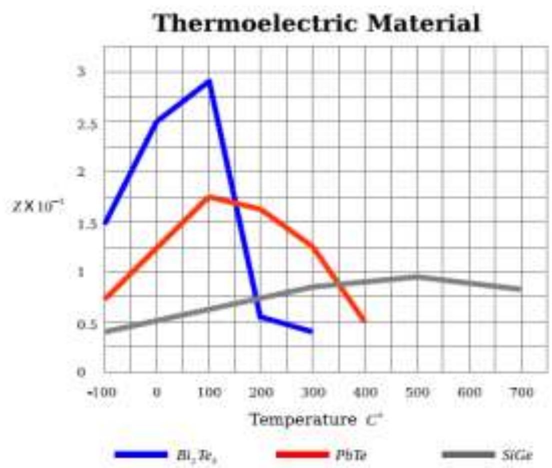

Fig. 2 - Performance of Thermoelectric Materials at Various Temperatures

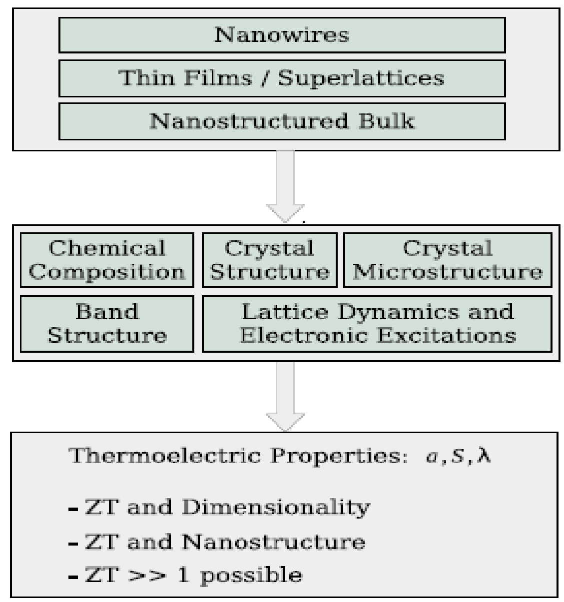

Fig. 3 Research Procedure to Improve the Thermoelectric Figure of Merit ZT in Bi_2Te_3 based Nanomaterial

The procedure described above is particularly useful for Bi_2Te_3 based compounds since these materials have a large number of structural and chemical degrees of freedom that affect thermoelectric properties of Bismuth Telluride (Bi_2Te_3) and require a systematic approach in terms of materials synthesis, structural characterization, thermoelectric characterization, and theory.

The performance evaluation of Bismuth Telluride (Bi_2Te_3), the parameter figure of merit (zT) is mostly used.

$$z = \frac{\sigma . S^2}{k}$$

where,
σ = electric conductivity,
S = Seebeck Coefficient,
k = thermal conductivity.

The total Seebeck coefficient as shown in Equation which can be calculated as

$$S = \frac{S_p \sigma_p + S_n \sigma_n}{\sigma_p + \sigma_n}$$

where,
S_p = Seebeck coefficients for p-type carriers,
S_n = Seebeck coefficients for n-type carriers,
σ_p = Electrical conductivities for the p-type carriers,
σ_n = Electrical conductivities for the n-type carriers.

IV. METHOD AND TECHNIQUE

For simulation of thermal barrier coating fabrication, a high speed Bismuth Telluride (Bi_2Te_3) thin films of 1.5cm x 1.5cm square area with thickness of 2 mm was taken as a substrate for depositing Bismuth Telluride (Bi_2Te_3) thermal barrier coating film.

The area of the residual indentation in the sample is measured and the hardness, H, is defined as the maximum load, P_{max}, divided by the residual indentation area, A_r:

$$H = \frac{P_{\max}}{A_r}$$

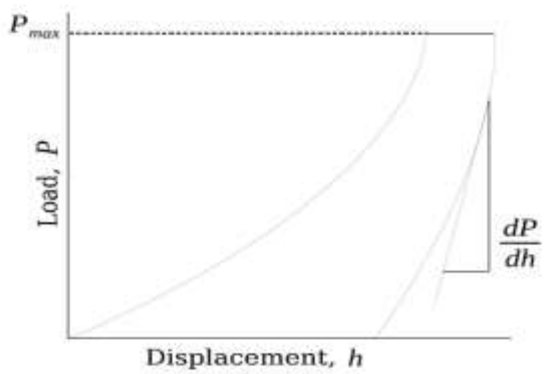

Fig. 4 - Load-Displacement Curve for a Nano-indentation Test

Young's Modulus of Bismuth Telluride (Bi_2Te_3) Nanomaterial:

$$E_r = \frac{1}{\beta} \frac{\sqrt{\pi}}{2} \frac{S}{\sqrt{A_p(h_c)}}$$

The strain-rate sensitivity of the flow stress m is defined as:

$$m = \frac{\partial \ln \sigma}{\partial \ln \dot{\varepsilon}}$$

where $\sigma = \sigma(\dot{\varepsilon})$ is the flow stress and $\dot{\varepsilon}$ is the strain rate produced under the indenter.

The optimization process can be performed step by step complying with the rules, from a simple case to a complicated case. On the one hand, the design and optimization processes from the aspect of residual stress of Bismuth Telluride (Bi_2Te_3) were performed.

As a simulator, MATLAB is used for the implementation and performance evaluation of the proposed method. The curve of load-displacement obtained for thermal barrier coating fabrication by finite element method.

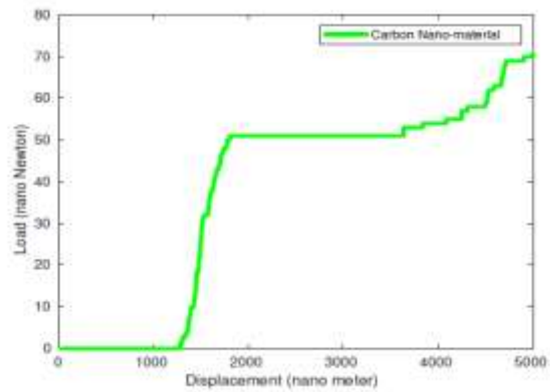

Fig. 5 - Load-displacement curve of Carbon based Material

The load displacement of Bismuth Telluride (Bi_2Te_3) is compared with carbon based material. For Bismuth Telluride (Bi_2Te_3), the red colored dashed line curve represents the load displacement in Nano-meter (nm) with respect to load applied in Nano-Newton (nN) range. The performance of load displacement calculation is estimated with reference to indentation depth with load, which is associated with stress and other physical properties of Bismuth Telluride (Bi_2Te_3).

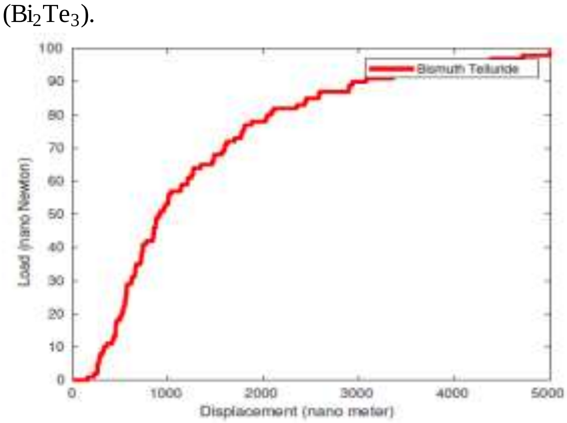

Fig. 6 -Load-displacement curve of Bismuth Telliride film

V. CONCLUSION AND FUTURE WORK

Conclusion: Finite element method is a powerful method and tool to simulate the indentation process at the nanoscale level. 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 work in this dissertation 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.

Future Work: There are many future possibilities and enhancements in nanotechnology and nanomaterial based mathematical analysis and experimental simulations which are as follows:

1. This simulation can further be investigated with thermoelectric property and electrical resistance of Bismuth Telluride (Bi_2Te_3) filled silicone matrix through the electro-spinning process.
2. In combination with nano-structuring and alloying, this may provide a promising route for further enhancements of the figure of merit. The methods used here can also be applied to other thermoelectric systems.

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