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Minimizing the Formation of Thermal Residual Stresses of the Elastic Zone in Functionally Graded Materials

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Abstract: ***Functionally graded materials (FGM's) are advanced composites consisting of two or more materials whose composition and structure changes gradually over the volume, leading to gradual change in its property. Typically one component is a ceramic, while the other is metal or metal alloy. In common embodiments, the composition can change gradually from all ceramic on one side to all metal on the other side, the ceramic contributing high resistance to temperature with the metal contributing high ductility. It's a way to incorporate favorable properties of two materials into different locations of a single structure. In ideal cases the composition changes gradually but for manufacturing reasons, the changes occurs in homogeneous layers. The boundaries between the layers cause thermal residual stresses to arise, especially during material processing and in cases of cyclic loading. These thermal residual stresses are a result of differences in the thermal expansion coefficient of the varying compositions of materials. Thermal residual stresses may lead to cracking and ultimate failure of FGM's. This study investigates the formation of thermal residual stresses for a Nickel-Alumina Ni-Al_2O_3 FGM. The Ni-Al_2O_3 system is chosen because it is one of the most common systems used in practice. This work explores the formation, impact and minimization of thermal residual stresses for a number of practical conditions that may arise during processing. All relevant properties are calculated using the rule of mixture equations. Abaqus, a non-linear FEA solver, is used for all the simulation work. In addition, the study highlights the need for examining elasto-plastic analysis to illuminate the process of crack development which is our future research goal.***

I. INTRODUCTION

The use of functionally graded materials is a relatively new phenomenon in industry. The control of thermal residual stresses (TRSs) in functionally graded materials (FGMs) is critical. The change in material properties lead to the possibility of residual stresses due to the variation in material properties. In this research we use finite element analysis (ABAQUS) as a numerical technique to predict the formation of residual stresses. "Functionally graded materials are engineered materials that are made of two or more materials in such a way that properties of these composites vary along one dimension [1]. Possible applications of this type of materials are diesel internal combustion engines (top surface of a piston), outer skin of space reentry vehicles, inner linings of nuclear power plants and turbine blades in jet engines. In the case of the latter, the two ends of the turbine blades are exposed to extreme temperatures and stresses, thus needing to have a wide variation in properties for optimal functionality. This wide variation in properties may be achieved by using thermal barrier coating system (TBC) and/or using functionally graded materials (FGM). In a traditional thermal barrier coating a ceramic layer is applied as a coating on a metal substrate where the properties change abruptly between the two layers. In a functionally graded material (FGM) the fraction of each material (and therefore, the properties) vary continuously or stepwise over the interface region between the two materials. A fundamental understanding of these composites is needed both for designing them as well as for manufacturing. During manufacturing, residual stresses in these types of materials is a typical problem that could cause early failure during their use [2], [3].The purpose of this research is to develop a fundamental understanding of how residual stresses are formed and developed in these types of materials during their thermo-mechanical processing and then to optimize process parameters and design parameters to minimize these stresses.

In this paper, the study of the formation, concentration and how to minimize the thermal residual stresses at the interface surface between layers of the two constituents, which is called the nickel-Alumina (Ni-Al_2O_3) system in 50 mm length and 10 mm thick plate is investigated and the parameter such as volume fraction is used to compute mechanical and physical properties such as Young's module (E), Poisson ratio (ν), thermal expansion coefficients (α), thermal conductivity(k) and heat capacity (C) of each layer of stepwise of Functionally Graded Material(FGM).

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This is accomplished through rule of mixture equations, number of layers such as two, three and ten layers. The Functionally graded Material (FGM) can consist of two; three and ten layers are subjected to transient of 300 ˚K as initial temperature and cool dawn to 100˚K as a sink temperature. Finally based on finite element as numerical analysis model and an Abaqus technique software is used as numerical model for simulation." [14], [15].

II. MATERIAL PROPERTIES

A combination of various rules of mixture are used to estimate the various mechanical and physical material properties required to carry out the finite elements modeling. The elastic modulus E is given by [1], [2], [3]

$$E = \frac{aV_m E_m + V_c E_c}{aV_m + V_c}, \qquad (1)$$

Where E and V denote the elastic modulus and volume fractions and the subscripts m and c denote metallic and ceramic materials, respectively. The parameter a is given by

$$a = \frac{q + E_c}{q + E_m}, \qquad (2)$$

Where q is known as the stress-strain transfer ratio and given by

$$q = \frac{\sigma_m - \sigma_c}{\varepsilon_c - \varepsilon_m}, \qquad (3)$$

With σ and ε being the customary notation for stress and strain, respectively. The stress-strain transfer ratio is a positive quantity that vary between zero and infinity. A q value of zero indicates the condition where the metal and ceramic carry equal stress while q tending to infinity indicates equal strain for both constituent materials. For the combination of nickel and alumina, a typical value of q is 500 GPa. The modulus of elasticity for the nickel is taken as 199.5 GPa and that of the alumina is 393 GPa.

The thermal conductivity k of the FGM is given by [1]

$$k = k_m + \frac{k_m V_c (k_c - k_m)}{k_m + (k_m - k_c)\frac{V_m}{3}}, \qquad (4)$$

Where k and V are the thermal conductivities and volume fractions and the subscripts m and c indicate the metallic and ceramic components, respectively. The nickel thermal conductivity, k_m, is 90.7 W/mºK and that for the alumina, k_c, is 30.1 W/mºK.

The thermal expansion coefficient α of the FGM is given by [1]

$$\alpha = \alpha_m V_m + \alpha_c V_c - \left[\frac{\frac{1}{B_L} - \frac{1}{\hat{B}}}{\frac{1}{B_m} - \frac{1}{B_c}}\right](\alpha_m - \alpha_c), \qquad (5)$$

Where α, V, B and σ are the thermal expansion coefficients, volume fractions and bulk moduli, respectively. The subscripts m and c denote the metallic and ceramic compositions. The thermal expansion of the nickel, α_m, is 15.4E-6 ºK^{-1} and that of the alumina, α_c, is 7.4E-6 ºK^{-1}. The bulk modulus of the nickel, B_m, is 180 GPa and that of the alumina, B_c, is 230 GPa. The thermal expansion of alumina, B_c, is 10^3 ºK^{-1}

The term B_L is the bulk modulus of the combined material obtained by a simple rule of mixture and given by

$$\frac{1}{B_L} = \frac{V_m}{B_m} + \frac{V_c}{B_c}. \qquad (6)$$

The term $\hat{B}$ relates the bulk moduli and volume fractions as well as the shear modulus of the ceramic G_c in the following

$$\hat{B} = V_m B_m + V_c B_c + V_c V_m \left[\frac{(B_c - B_m)\left\{\frac{1}{B_c} - \frac{1}{B_m}\right\}}{\frac{V_m}{B_m} + \frac{V_c}{B_c} + \left(\frac{4G_c}{3B_c B_m}\right)}\right]. \qquad (7)$$

The shear modulus of the alumina, G_c is taken at 190 MPa.

The densityρ, Poisson's ratio ν and specific heat C of the material are given by a straight rule of mixture, in direct relation to the volume fractions by

$$\rho = \rho_c V_c + \rho_m V_m, \quad (8)$$

$$\nu = \nu_c V_c + \nu_m V_m, \quad (9)$$

And

$$C = C_c V_c + C_m V_m. \quad (10)$$

The density of nickel, ρ_m, is taken as 8900 kg/m^3 and that of the alumina, ρ_c, is taken as 3950 kg/m^3. The Poisson's ratio of nickel, ν_m, is taken as 0.3 while that of the alumina, ν_c, is taken as 0.23. The specific heat of nickel, C_m, is taken as 440 J/g^{o}K and that of alumina, C_m, is taken as 840 J/g^{o}K.

III. DISCUSSION OF PARAMETERS

The most basic way to determine the material properties of a two-phase material such as the nickel-alumina FGM is the standard rule of mixture. The rule mixture stipulates that property A of a metal-ceramic composite is related to the properties of the constitutive materials A_c and A_m, and the volume fractions V_c and V_m, by

$$A = A_c V_c + A_m V_m. \quad (11)$$

The form of Equation 9 is only exact for the most basic properties such as density but only offers an approximation for the more complex ones such as the modulus of elasticity, the thermal conductivity and the coefficient of thermal expansion.

A comparison of the thermal conductivity given by Equations 4 and 11 is shown in Figure 1. The law of mixture seems to under predict this property by about 5% at the point of equal fraction of metal and ceramic. Figure 2 shows the law of mixture over predicting the coefficient of thermal expansion, given by Equation 5, by about 2.5%.

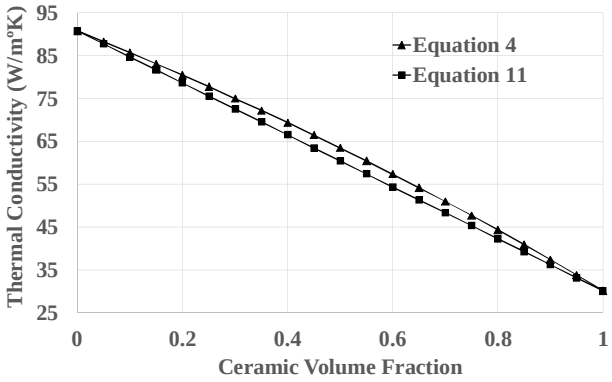

Figure 1. Thermal conductivity of nickel-alumina material using the model from Equation 4 and that from a proportional law of mixtures, given in Equation 11

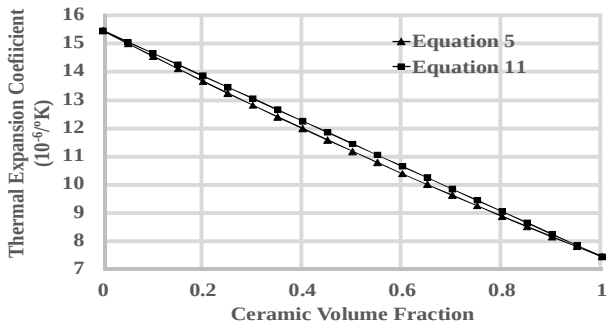

Figure 2. Thermal expansion coefficient of nickel-alumina material using the model from Equation 5 and that from a proportional law of mixtures, given in Equation 11

Figures 1 and 2 are shown to illustrate the relative accuracy of the law of mixture for thermal properties. Using the law of mixture for the mechanical properties, on the other hand, can lead to significant errors. Referring to Equation 1, parameter a, which depends on the stress-strain transfer ratio q, can dramatically alter the modulus of elasticity. A q value of zero implies that the two phases carry equal stress, which in turn implies that both phases of the material are acting as springs in series. For q equaling zero, Equation 1 reduces to

$$E = \frac{E_c E_m}{E_c V_m + E_m V_c} \quad or \quad \frac{1}{E} = \frac{V_m}{E_m} + \frac{V_c}{E_c}. \qquad (12)$$

The other extreme is q tending to infinity, which is the case that both phases of the material are subjected to equal strain. In that case, Equation 1 transforms into the law of mixture given by the form of Equation 11. This scenario represents the case of two springs acting in parallel.

The modulus of elasticity is shown in Figure 3 as a function of ceramic volume fraction for q values of 0, 500 and tending to infinity. The case of q equals zero (springs in series) leads to a significantly lower modulus than large values of q (springs in parallel).

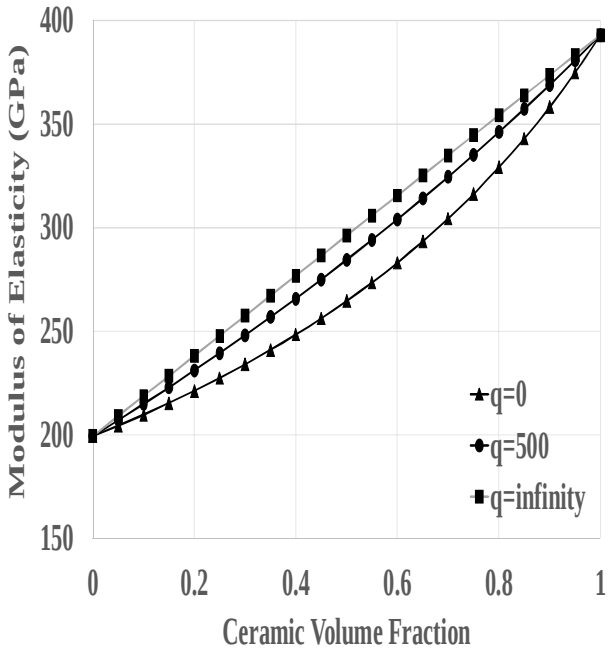

Figure 3. Predicted modulus of elasticity of nickel-alumina material using Equation 15 for q equaling 0, 500 and tending to infinity

An understanding of the physics behind the modeling of the modulus of elasticity is important, particularly for the elastic deformation modeling in the subsequent section

IV. FINITE ELEMENTS MODEL

Numerical modeling of FGM has been approached by recent studies. See references [5] to [9], [10] and [12]. In this study, we will demonstrate the effectiveness of utilizing Finite element modeling of FGM to capture the behavior within the elastic zone of Nickel-alumina FGM. The advantage of Finite Element modeling in identifying the behavior of thermal residual stresses at the partition zones is the point of focus. The thermal residual stresses are modeled in a rectangular block of height H of 10 mm and length L of 50 mm. Two dimensional modeling was used in order to simplify the model, which is an accurate approximation for the conditions away from the edges. The mechanical boundary conditions, shown in Figure 4 (a), consist of a clamped boundary conditions on the left side and a slider on the right bottom corner. The thermal boundary conditions consist of a uniform initial temperature of 300ºC throughout the body and a uniform heat sink temperature on all external edges. The film coefficient h, which relates the heat flux to the temperature difference is taken as 3000 J/s/m^2/ºC.

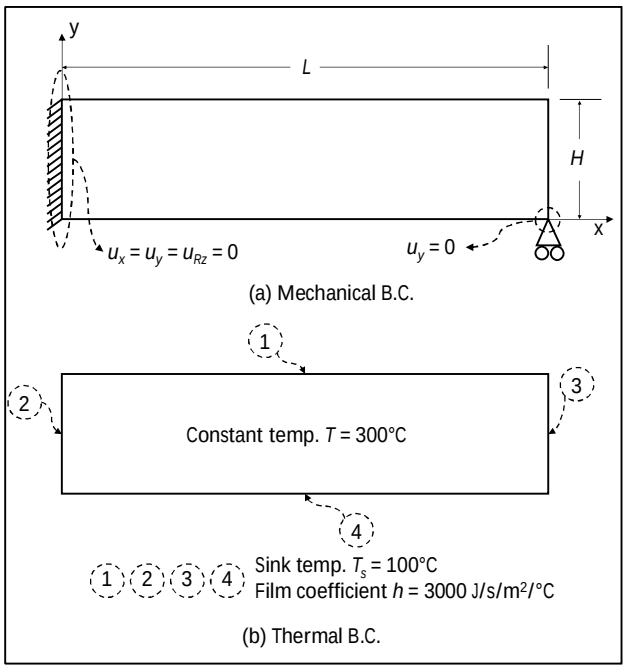

Figure 4. Simplified suspension model of the FGM study sample

A fully coupled thermal-stress analysis was conducted using the first order Abaqus/Standard element CPE4T of size 0.1 mm.

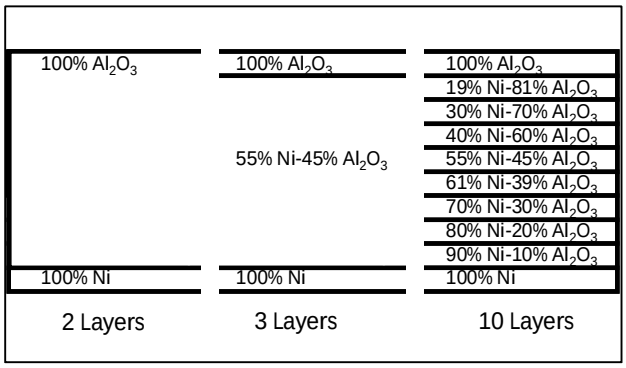

Figure 5. Arrangements of layers in the FGM in the three cases studied.

V. FUNCTIONALLY GRADED MATERIAL IN NATURE

FGM are abundant in nature. Examples are the microstructure of human bones, see Fig. 6 [1], microstructure of human tooth, see Fig. 7 [1], bamboo, see Fig. 8 [1], mollusk shells, Fig. 9 [1],

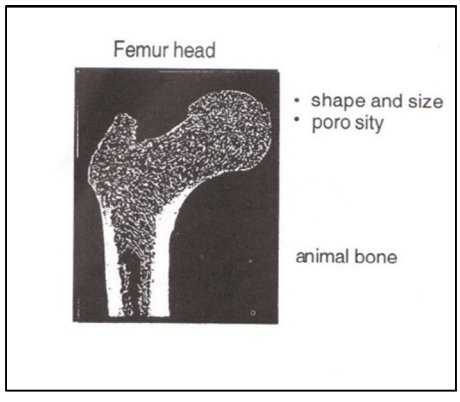

Figure 6. FGM in human femur head bone

Figure 7. FGM in human tooth

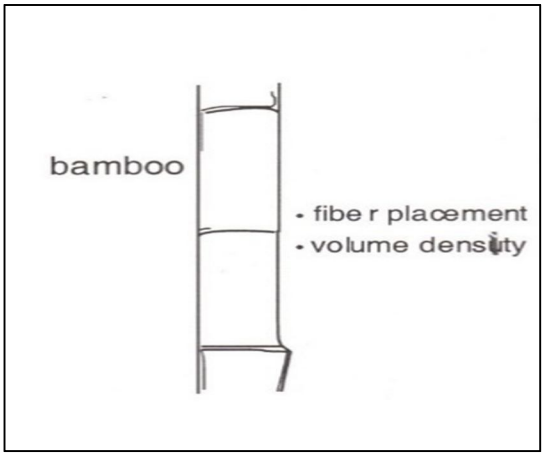

Figure 8. FGM in bamboo tree

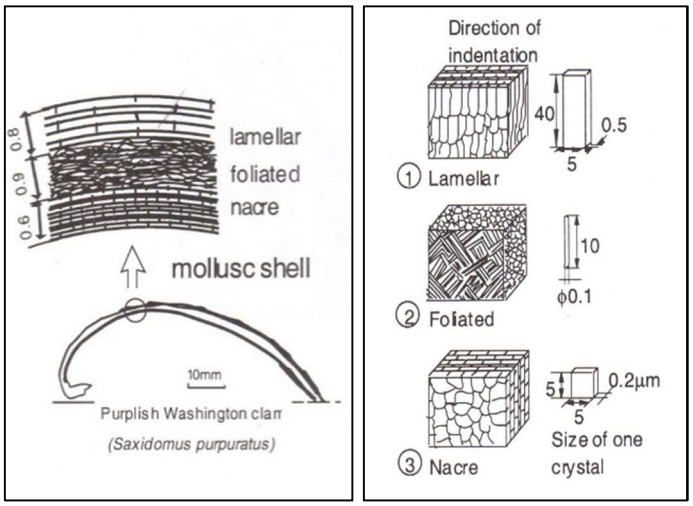

Figure 9. FGM in Mollusk Shells

FGM and residual stresses are illustrated in Figure 10 below. The illustration shows the difference between classic layer composites (CLC), Thermal Barrier Coating and FGM. Figure 10 shows also residual stresses in a substrate and FGM & coating.

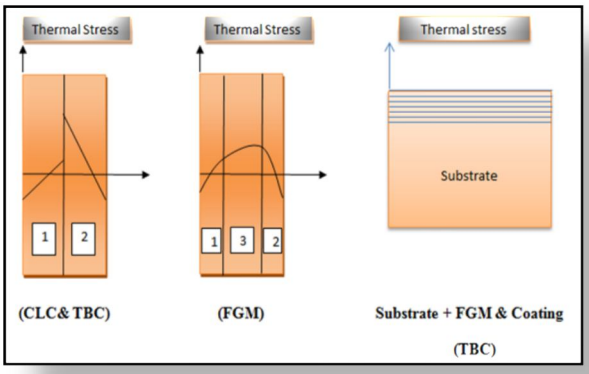

Figure 10. FGM and residual stresses

VI. RESULTS

The minimization of the formation thermal residual stresses resulting from the functionally graded nickel-alumina material cooling from 300ºC to 100ºC are computed for the cases of two, three and ten layers.

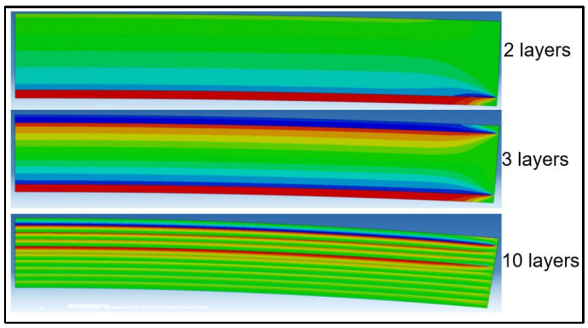

Figure 11. S_{11} (x dir.) Stress contours – elastic material properties.

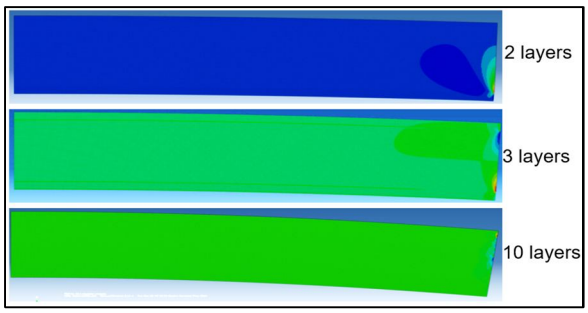

Figure 12. S_{22} (y dir.) Stress contours – elastic material properties

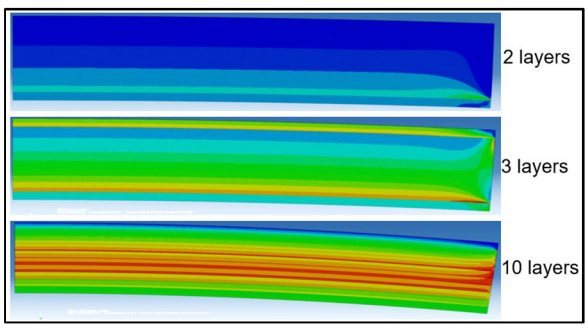

Figure 13. S_{vm} (Von Mises) Stress contours – elastic material properties.

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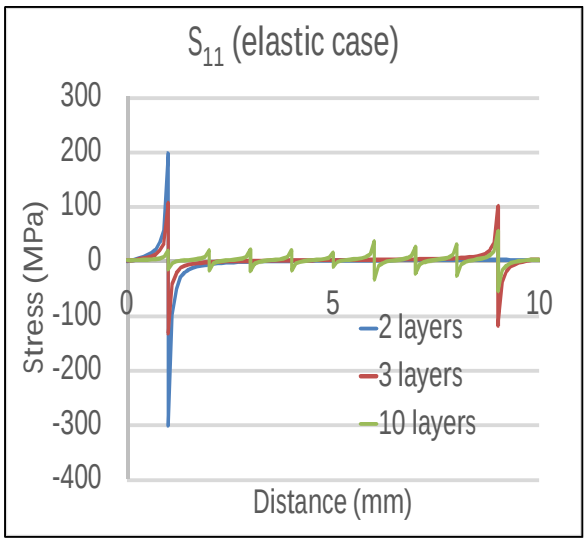

Figure 14 S_{11} (x dir.) Stress plot vs. thickness – elastic case

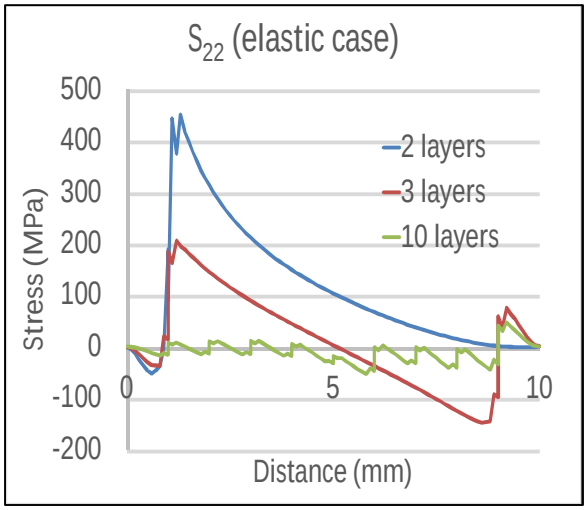

Figure 15 S_{22} (y dir.) Stress plot vs. thickness – elastic case

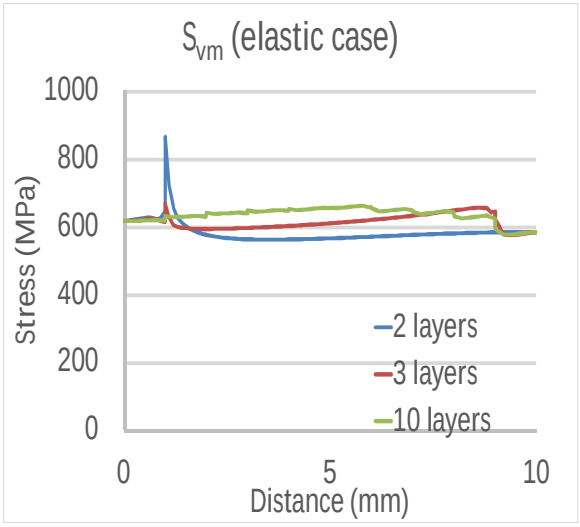

Figure 16 S_{vm} (Von Mises) Stress plot vs. thickness – elastic case

VII. CONCLUSION

The Finite Element modeling of the Functionally Graded Material FGM was analyzed in the elastic zone to study the minimization of formation of thermal residual stresses in FGM. In this study, Alumina and Nickel FGM was considered in the analysis. The stress-strain curves for thermal residual stresses of Alumina Nickel were produced, it is evident in the outcome of the Finite Element modeling that as the percentage of ceramic increases (i.e. the percentage of Nickel decreases), the thermal residual stresses are increasing. It is concluded from this study that the thermal residual stresses in the Alumina Nickel FGM is behaving smoothly except at the partitions between ductile component (in this case Nickel) and brittle material (in this case the alumina).

This conclusion is helpful in designing arrangements of layers of FGM to minimize fluctuation of residual thermal stresses in across material thickness emphasizing the conclusion of our previous work. Please see references [14] and [15].

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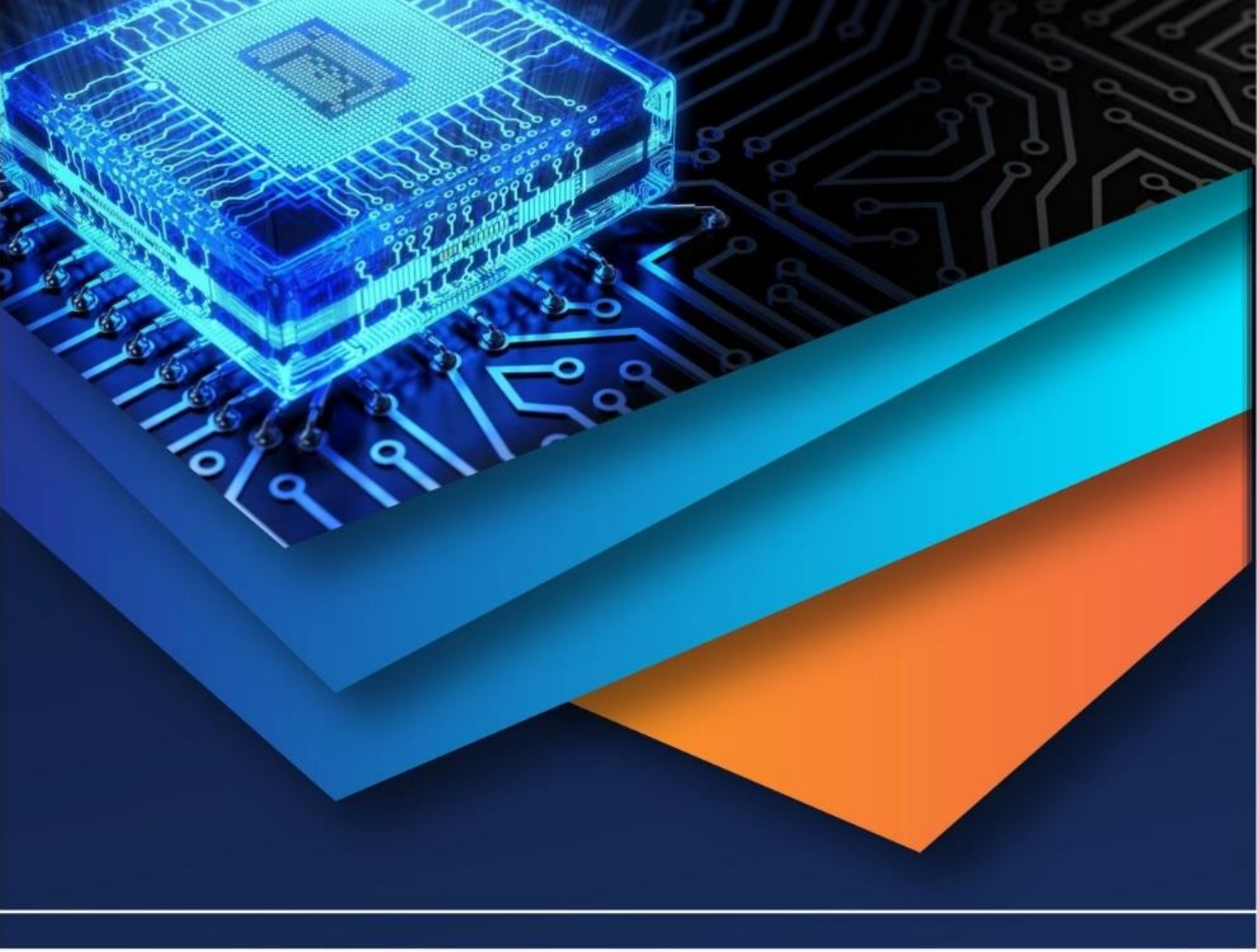

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