

DESIGN OPTIMIZATION OF FUNCTIONALLY GRADED HYDROXYAPATITE/TITANIUM CIRCULAR PLATE USING TWO-DIMENSIONAL FINITE ELEMENT MODELLING

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Abstract

Functionally graded Hydroxyapatite/Titanium (HA/Ti) structure shows the combination of two superior properties such as high strength-to-weight ratio of the Ti (metal phase) and good heat resistance of HA (ceramic phase) in a unit structure. The main intention of this combination is to highlight the significance of the extremely low thermal conductivity of HA in enhancing the performance of the advanced material. This paper aims to determine the optimum design parameters of the HA/Ti FGM. The optimization of design parameters which considered the number of layers, grading index and thickness, was achieved through the evaluation of the residual stress distribution along the compositional gradient plane at the circumference surface of the cylindrical FGM plate. Optimization analysis was performed by assuming that the residual stress occurred because of a temperature drop during the sintering process due to a variation in the thermal and elastic properties along the transverse direction of the FGM structure. Since the effective properties vary with the variation in the number of layers, grading index and thickness of the FGM plate, an evaluation of the residual stress distribution was significant when determining the optimal geometrical parameters of the structure. The convergence properties of the present results were examined thoroughly in order to assess the accuracy of the theory applied and to compare them with the established research results.

1.0 INTRODUCTION

Developing applications in bioengineering, biomedical engineering, aerospace and electronics demands properties that are unobtainable in any single material. These properties should include resistance against high mechanical and thermal stresses. Combining ceramic and metallic materials may have the potential to overcome the aforementioned situation. In situations where the operating temperature is extremely high, structural ceramic materials are used because of their refractory qualities, their resistance to corrosion and their resistance to wear in situations where metallic materials cannot survive. However, ceramic materials cannot withstand the mechanical stresses that metals easily overcome. Metals offer properties such as fracture toughness, resistance to wear and resistance to corrosion, but they should be shielded from excessive or extreme heat under operating conditions.

Various metal and ceramic pairs have been considered in the development of Functionally Graded Materials (FGMs) for several advanced engineering applications. Among the various pairs, HA and Ti materials were among the well-known combinations, but so far their applications are limited to biomedical engineering and human implants. Looking at the advantages of HA and Ti materials from a different perspective, this thesis highlights the potential of HA/Ti FGMs in high thermal barrier applications. The FGM's mechanical properties, such as its high strength-to-weight ratio, high resistance to corrosion and the lower density of Ti material, have been thoroughly analyzed as it is widely utilized in industrial aerospace applications. However the low thermal conductivity of HA has not often been considered for applications that require good heat resistance.

In order to develop an FGM model, the material properties such as thermal conductivity, Young's modulus, Poisson's ratio, thermal expansion coefficient and etc. gradient along the transverse plane of the

structure need to be accurately estimated. The prediction methods of the entire effective properties within the framework of single continuum mechanics can be divided into three main approaches known as direct, variational and approximation approaches. Based on the direct approach described in Hill (1963), the FGM material properties are estimated by seeking the closed-form analytical solutions to the overall properties of ideal composites.

The variational approach which implements the variational principles of thermo-mechanics for the bounds derivation which directed to the determination of the FGM's effective thermo-physical properties. This method assumes that the properties of each layer inside the FGM is homogeneous and isotropic. Hashin and Shtrikman (1963) have shown the relationship between the effective bulk modulus and shear modulus of the upper and lower bounds of the material. Besides the direct and variational approaches, another approach which is commonly used for the prediction of the material properties of FGMs is based on a rule of mixture (Lee et al., 2008; Park et al., 2009; Ryu et al., 2009; Alshorbagy et al., 2013). By using this rule, the material properties of FGM are estimated by taking into account the individual properties and compositional percentage of the constituents. The constituent particles are assumed to uniformly dispersed while remain separately without react one another.

This paper is primarily concerned with data predicted using FEA. The computational work started with a 2-D FE analysis to optimize the grading parameters, the number of layers and the thickness parameters of a pre-designed HA/Ti FGM plate. Its primary aim is to provide a greater understanding of the effects of some of the important influencing parameters on the behaviour of the FGM.

2.0 THEORETICAL FORMULATIONS

The design of an FGM can be considered in different physical parameters, such as its thickness, the number of layers, grading index, grain size and porosity. Each of these parameters has its own significant effect on FGM design. In this study, the optimum thickness, number of layers and grading index of the cylindrical FGM specimen used in the experimental work were determined using a 2-D FE model. The effects of these parameters on the FGM were studied by evaluating the computed thermal residual stresses distribution of FGM structures with varying design parameters.

The typical properties of the base materials, HA and Ti, used throughout the numerical modelling are given in Table 1 (Chu et al., 2003). The properties of the stepwise layers at intermediate locations on the FGM models were calculated based on a ROM formulation shown in Equation 3.3. When analyzing an FGM containing a HA constituent, it is important to realize

that the elastic modulus of this material varies in a range between 73 to 120 MPa depending on the sintering temperature (Ruseska et al., 2006). Therefore the selection of properties shown in Table 1 was made by taking into account the sintering temperature used for the preparation of the FGM samples, which is shown and discussed in the next section.

Table 1. Properties of materials. Source: *Chu et al., 2003
**Moroi et al., 1993

| Material | (*) E (GPa) | (*) Y | (*) $\alpha \times 10^{-6}$ (/°C) | (**) K (W/mK) |
|----------|----------------|----------|--------------------------------------|------------------|
| HA | 110.89 | 0.28 | 14.87 | 2.16 |
| Ti | 107.95 | 0.34 | 10.9 | 17.5293 |

3.0 FINITE ELEMENT MODELLING

The development of the model began with the identification of the FGM's cross-sectional area in order to analyze and calculate the material properties at distinctive layers of the FGM structure. In this study, the cylindrical shape of the FGM specimen was transformed into 2-D axisymmetric model as depicted in Figure 1. In addition, by assuming that the two constituents' particles are well-dispersed and ideally joined, the position-dependent material properties were calculated based on a ROM formulation. The geometry of the cross-sectional area selected for the analysis and the typical material properties at different FGM layers were defined as the inputs for the analysis. Before defining the boundary conditions, the model was discretised into 8-node SOLID273 elements, as defined in ANSYS library with a 0.1 mm mesh size.

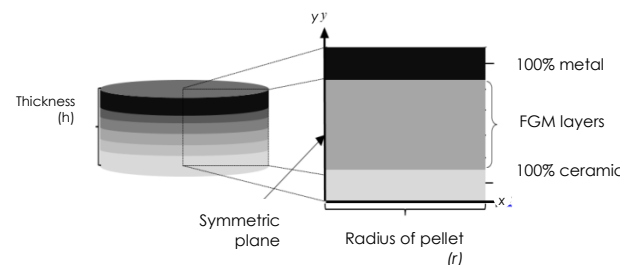


Figure 1. Transformation of the cylindrical FGM plate into a 2-D axisymmetric model.

Although only the axisymmetric cross-sectional area of the cylindrical FGM was considered during the analysis, deformations at certain coordinates on the structure can be non-axisymmetric. SOLID273 was selected for this analysis since it can support all nonlinearities existing in the analysis. In addition to the displacement boundary, thermal boundary conditions were also defined based on the assumption that the thermal residual stresses occurred during the cooling stage of the sintering process. Finally, by taking into account the behaviors of the metal and ceramic compositions in FGMs, the residual stresses were

interpreted in terms of von-Mises and principal stresses. For the optimization of the FGM design parameters, the FE analysis had to be repeated with different design parameters as the inputs. The parameters used in the design of the FGM with the smallest thermal residual stress peak and the maximum relaxation in thermal residual stresses distribution were considered the optimum design parameters.

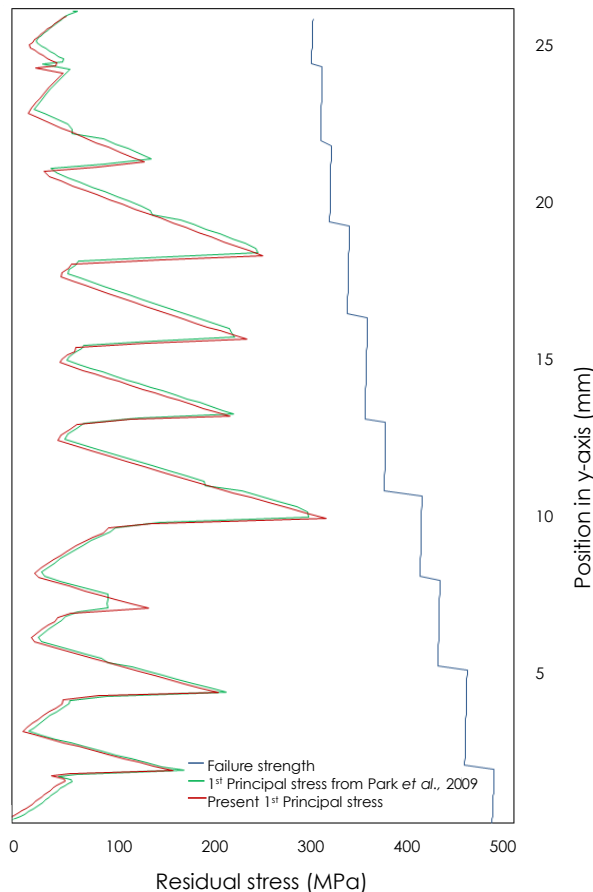


Figure 2. Verification of 2-D modelling method

In order to ensure the reliability of the FE models developed to predict the various characteristics of the FGM, verification of the FE calculations was obtained by comparing the present results with established results. The 2-D FE model for the FGM design optimization analysis was confirmed by taking into account the results reported by Park *et al.* (2009). This research team developed a crack-free Ni/Al₂O₃ FGM model with a total thickness of 26.1 mm and with 10 layers by considering the maximum principal stress theory. Figure 2 indicates the distribution of the first principal stress through the outer surface of the specimen simulated from both calculations.

4.0 RESULTS AND DISCUSSION

4.1 Evaluation of the Grading Index

The compositional distribution of the FGM plates with various grading indices is shown in Figure 3. The FGM plates with a grading index number $n=0$ and ∞ have homogeneous ceramic and metallic ingredients respectively. The properties' variation along the thickness direction of the plate is only possible when the grading parameter is between these two values. This parameter led to either ceramic or metal phase domination in terms of the volume fraction in the FGM plate. The grading parameter $n=1$ showed the balance or linear mixing ratio of the constituents' differences between adjacent FGM layers.

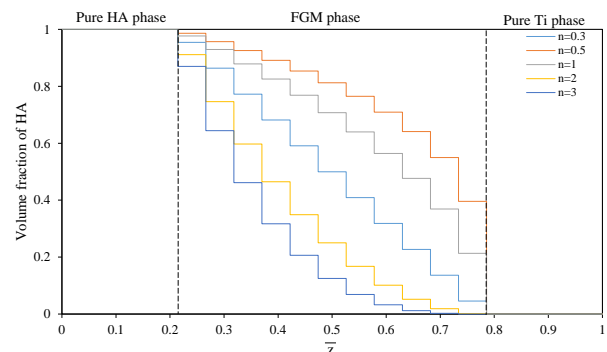


Figure 3. Compositional distribution profiles of the HA/Ti FGM plates with a variation of the grading parameter.

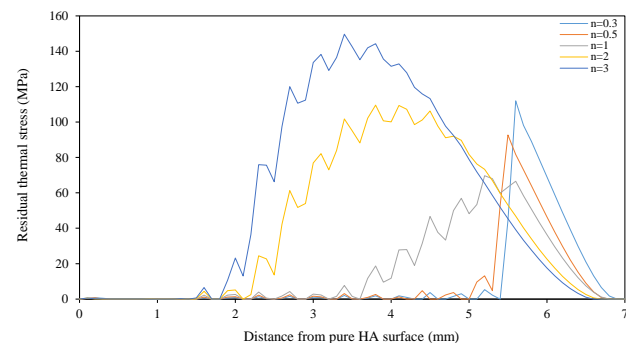


Figure 4. Residual thermal stress distribution along the thickness of the HA/Ti FGMs with various grading indices ($L=11$, thicknesses of pure Ti, FGM and pure HA layers: 1.5mm, 4mm, 1.5mm, respectively).

The residual stress distributions for different grading indices along the gradient plane of the FGM plates are represented by the teeterboard plots shown in Figure 4, where the lowest stress peak is found in the FGM plate with $n=1$. The linear variation in the compositional distribution of the constituents led to better stress relaxation in this plate. The higher stress peaks in the FGM plates with $n \neq 1$ need to be avoided in order to produce less stress intensity which cause failures in the FGM structure. The results shown in Figure 4 conclude that $n=1$ is the optimum grading index number for the pre-designed FGM plate analyzed in this study.

4.2 Evaluation of the Number of Layers

Figure 5 shows the residual stress distributions along the thickness of the HA/Ti FGM plates between 2 and 11 layers. The thermal relaxation in the FGM plates can be evaluated by considering the maximum residual stresses and the maximum stress peaks given in Table 2. The results indicate that with a higher number of layers inside the plate, the highest stress difference and highest residual stress of the respective FGM plates gradually reduced, most probably due to the lower significance of the component concentration variation between adjacent layers.

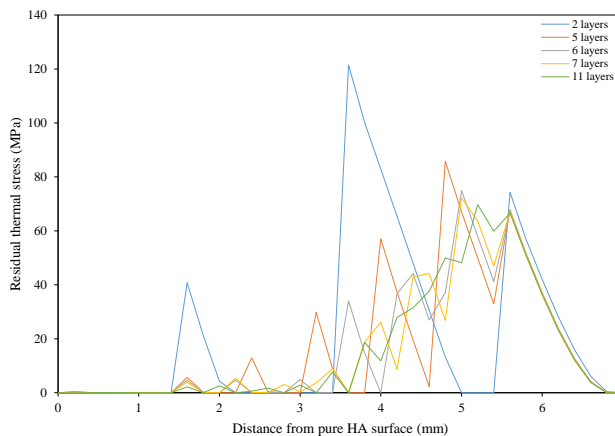


Figure 5: Residual thermal stress distribution along the thickness of HA/Ti FGM plates with various number of layers ($n=1$, thickness of pure layers, FGM layer: 1.5mm, 0.007m)

Table 2: Maximum thermal residual stress and the maximum thermal stresses differences of the HA/Ti FGM plates with different number of layers

| Model | Maximum residual thermal stress (MPa) | Maximum thermal stress jump at the interfaces between the adjacent layers (MPa) |
|---------------|---------------------------------------|---|
| FGM 2 layers | 121.49 | 121.49 |
| FGM 5 layers | 85.78 | 83.47 |
| FGM 6 layers | 74.89 | 53.67 |
| FGM 7 layers | 72.14 | 45.33 |
| FGM 11 layers | 68.04 | 27.75 |

Furthermore, the highest stress differences decreased rapidly when compared to the highest residual stresses. Since the worst bonding regions in the FGM plates are located at the interfaces, the drastic decrease in the highest stress differences is advantageous for the structural integrity of the plates. Even from a theoretical perspective, a greater number of layers is advantageous for the relaxation of the residual stresses (Zhang *et al.*, 2008). The decision whether to add more layers to the FGM plate should be included when considering fabrication. From this result the maximum residual stress relaxation was found on the FGM containing six layers. Thus $L \geq 6$ is selected as the optimum number of layers for the HA/Ti FGM.

4.3 Evaluation of the FGM's Thickness

A correlation between the FGM's thickness and the residual stress distribution was investigated for FGM plates with graded layers between 0.1 to 12 mm. The thickness of the upper and lower pure layers remained similar for all FGM plates. From Figure 6, it is evident that the stress peaks decrease within increasing thickness. For FGM plates with a thickness in the range 0.1 mm to 2 mm, the residual stress increased rapidly from the pure HA surface before decreasing towards the pure Ti surface. The same trends were found in FGM plates with moderate thickness ($t=4, 6, 8$ mm) except in drastic stress differences. A gradual variation in the residual stress found in FGM plates with a moderate thickness still could be found in an FGM plate with greater thickness ($t=10, 12$ mm). However the stress kept increasing towards the pure Ti surfaces without decreasing back to the lowest value.

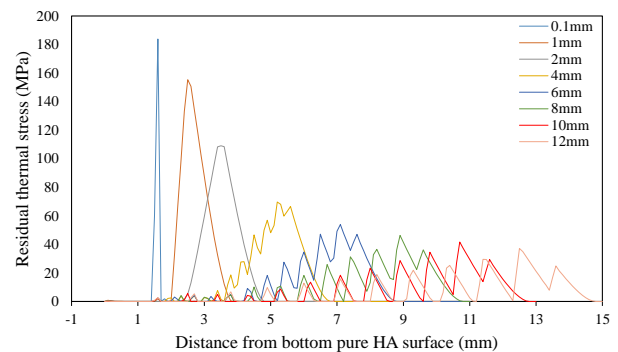


Figure 6: Residual thermal stress distribution of the HA/Ti FGM plates with various graded layers' thicknesses ($L=11$, $n=1$, thickness of the pure Ti and HA layers: 1.5mm)

Table 3: Maximum thermal residual stresses and jumps in HA/Ti FGM plates with different thicknesses of the FGM phase

| Thickness of FGM (mm) | Peak Stress (MPa) | Different of current with previous peak stresses (MPa) |
|-----------------------|-------------------|--|
| 2 | 109.16 | 41.55 |
| 4 | 68.04 | 41.12 |
| 6 | 54 | 14.04 |
| 8 | 46.35 | 7.65 |
| 10 | 37.36 | 8.99 |
| 12 | 25.37 | 22.99 |

In order to find the optimum thickness, the maximum residual stresses and the difference between the adjacent stress peaks of the FGM plates (given in Table 3) were considered. The minimum difference in the adjacent stress peaks of the FGM plate by thickness ($t=8$ mm) represented the greatest stress relaxation in this plate when compared to others. From this result, the optimum thickness of FGM layers was taken as $t=8$ mm. The optimum thickness of each layer inside the FGM plate can be calculated by dividing the FGM thickness

by the number of layers inside the FGM plate. In the current case, the optimum thickness for the single FGM layer was ± 0.7 mm.

5.0 CONCLUSION

The study outlined in this paper includes an in-depth 2-D FEA study into the effects of the parameters that influence the property distribution of the design and various responses of the HA/Ti FGM. The optimization of the grading index, the number of layers and the thickness acquired by the maximum residual stress relaxation have been successfully computed using a 2-D axisymmetric FE model. The results of the 2-D analysis showed that the optimum cylindrical HA/Ti FGM plate consisted of a minimum of six layers with linear property variation ($n=1$) and a specific thickness that can preserve the property gradation function.

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