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STUDY THE EFFECT OF THERMAL IMPACT ON THE MODELLING OF (TITANIUM-TITANIA) FUNCTIONALLY GRADED MATERIALS BY USING FINITE ELEMENT ANALYSIS

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ABSTRACT

The developing of the composite materials produce a new generations Functionally graded material (FGM) where the materials characteristics are changing linearly depending to the composition materials variations. However, this piece of research presents an attemp to design, manufacturing and multi Ti/TiO_2 combined characterization into each functionally graded materials. The supposed in this design is to better the general Ti/TiO_2 characteristics. These materials were designed in order to contain a compositional differences or a gradually microstructure within the body in one piece or single material.

Keywords: Composite Materials, Functionally Graded Material, Ti/TiO₂.

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1. INTRODUCTION

One of the virtually advanced ideas in Japan during the early 1980s which is the Functionally Graded Materials (FGMs), the materials are introduced this new concept in order to improve the adhesion and decrease thermal stresses in metal-ceramic composites materials which have been developed for reusing them in rocket engines [1]. At the same time, the concepts of FGMs have been promoting a wide world researches activities which can apply on metals,

organic and ceramics composites to produce an improvement with superior physical characteristics [2].

Nowadays, the production of FGMs are considered the next step in the development of composite materials. Where the FGMs are comparatively new engineering materials type in which the microstructure and/or composition changes in one specified direction. It is made of constant change in structure and does not have a specific interface. Subsequently, it is generally supposed that these composite structures must have a better resistance for the mechanical and thermal differences [3].

In metallurgy of powder, the technique of producing FGM is by placing the desired powder layer layer after layer, followed by pressing powder and then sintering. During the process of sintering, some mineral powders will interplay to produce a various compounds and chemical phases, which may be varying, depending on spatial location within the functionally graded material [4].

Titanium is applied for fixing the fractures of bones in the devices of spinal fusion, pins, screws and bone-plates. Another advantage for applying titanium in medicine is that the non-magnetic characteristics, so it poses no risk on patients with implants during MRI and exposure to electronical equipment, [5].

Titanium dioxide is also named titania (TiO₂), a safe and inert material which still represents one of the most popular and substantial materials that have many applications in different fields, due to the favaurable optical characteristics such as having a great reflection index 7.2 which is higher than the diamond refractive index (4.2) but less solid than diamonds, and this can be prepared with titanium and titanium dioxide. This could bring the hiding powder, chemical stability, whiteness and relatively cheaper production cost, [6-8]

More recently, several researches are directed to standardize titanium dioxide with inorganic crystals, particularly with biomimetic and biocompatible materials to get a composite materials of interest to biomedicine or have a synergistic inflence and increase image catalyst efficiency against bacteria and contaminants. Amongst these substances one of the most commonly used is hydroxyapatite. In fact, this substance has been studied, in addition to its use in the field of biomedicine, to be used also in the getting of rid of bacteria, [9] and [10]. HA was also found to replace the Ag^+ and Ti^{4+} ions showing excellent antimicrobial effects [11] and [12]. Thus, the combination of hydroxyapatite with TiO_2 to get substances that have the ability to decompose and absorb appears very promising.

Hideaki Tsukamoto, 2014 [13], fabricated samples of titanium-Zirconia functionally graded materials using of a spark plasma sintering (SPS). The results can be also of considerable use to understand thermo-mechanical behaviour of ZrO_2/Ti FGMs depending on a mean-field model of micromechanics-based.

Jayachandran, et al. 2013, [14], a mixed powder dye technique was proposed for the production of functionally graded materials (FGMs) with the favouable gradient composite. The green body was sintered by the spark plasma plating technique (SPS). The starting of the particle-settling process using powder ice was strictly controlled as a suspension medium. The FGMs of Ti-ZrO₂ were produced in this research, Vickers hardness the compositional gradient in FGMs production.

Nabaa S. Radhi, 2018, [15], prepared functionally graded samples multi layers of (100% Titanium-50% Titanium-50% Hydroxyapatite-100% Hydroxyapatite), and prepared each layer singly sample to investigated behaviour of each layer and total functionally graded. and tested the XRD of powder, density, porosity, particle size analyser and micro hardness.

2. MODEL CHARACTERISTICS

In order to simulate the behavior FGM under the change in temperature, a full model of the test specimen was developed. Model containing the geometry of the 3D solid component partitions, their assembly, and the mesh characteristics in addition to boundary conditions, were carried out using Abaqus-CAE software [16].

Because the samples consist of different regions with different material properties, the modelled specimens had cylindrical shape and composed of three and five different parts (layers) respectively, as seen in the sample configuration shown in Figure 1. The geometry and dimensions used for each part in the model were identical to the dimensions used to produce the samples in the experimental work. The dimensions of the layers for each sample are listed in Table.

The connections between layers were assumed to be idealised and free from any defects, such as voids or partial bonding.



Figure 1 Geometry definition of the different material partition zones used for model of the samples with: (a) five layers, (b) three layers

3. MATERIAL PROPERTIES

As stated earlier the samples were divided into three and five distinct regions, in terms of their material properties. It is difficult to evaluate the material properties of transition regions because they consist of mixture of titanium and TiO_2 with different ratios. However, to simulate the material properties in these regions in the finite-element model, the local properties could be calculated using the rule of mixture. Tables 1and2 show the material properties for each layer in the samples.

Layer No.	Chemical analysis	Thickness (cm)	Thermal expansion (μm ⁻¹ K ⁻¹)	Thermal conductivity (Wm ⁻¹ K ⁻¹)	Young modulus (GPs)	Poisson ratio
1 st	(100% wt Ti)	0.2	8.9	17.15	103	0.36
2 nd	(50% wt Ti-50% wt TiO ₂)	0.2	9.5	12.73	176.5	0.32
3 rd	(100% wt TiO ₂)	0.25	10.1	8.3	250	0.28

Table (1) material properties used in FGM₁ profile Model

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Layers	Chemical composition	Thickness (mm)	Thermal expansion (µm ⁻¹ K ⁻¹)	Thermal conductivity (Wm ⁻¹ K ⁻¹)	Young modulus (GPs)	Poisson ratio
1^{st}	(100% wt Ti)	2	8.9	17.15	103	0.36
2^{nd}	(75% wt Ti-25% wt TiO ₂)	1.8	9.2	14.94	139.75	0.34
3^{rd}	(50% wt Ti-50% wt TiO ₂)	1.5	9.5	12.73	176.5	0.32
4^{th}	(25% wt Ti-75% wt TiO ₂)	2	9.8	10.51	213.25	0.3
5 th	(100% wt TiO ₂)	2.2	10.1	8.3	250	0.28

Table (2) material properties used in Model of FGM₂ profile

4. BOUNDARY CONDITIONS IN THE MODEL

To simulate the actual situation of the effect of thermal impact, the model was assumed to be subjected to a change in temperature of 100 $^{\circ}$ C type boundary condition. The sample were assumed free of gripping to show the temperature change influence on the thermal stress resulted from the thermal expansion variation between the layers alone, and eliminate the effect of other factors. It should be noted that the effect of gravity was neglected because it was very small compared to the other affecting factors during the test.

5. MESH BUILDING

A tetrahedral structured mesh was created in all the regions of the samples. Ten-node C3D10M elements were used (see Figure 2). The tetrahedral elements were used because they are geometrically versatile and the software did not allow the use of a simpler hexahedral structured mesh, due to the presence of the concave interfaces.



Figure 2 Mesh distribution for the samples with: (a) five layers, (b) three layers.

6. RESULTS AND DISCUSSION

It is important to understand how using dissimilar materials with different properties (e.g. thermal expansion coefficients) affects the resulted properties of different mechanical parts. For instance, in the FGM, the investigation of the stress distribution resulted from the thermal impact and deformation at the interface between the layers are important things in the process of improving the quality of the component and predict the mechanical properties.

Figure 3 demonstrates the distribution of Von-Mises equivalent stress at the final stage of the analysis for the three layers sample. The figure also shows the Von-Mises corresponding stress in the vertical cross-section. It can be noted that the stress mostly concentrated at the

interface (bonding zone) between the lower layer (Ti) and the next one (Ti + 50 %TiO₂). The stress concentrated in this region due to the sharp change in material properties and this may be affected the development of the failure of the FGM. By moving away from this region, the stress shows clear decrease. On the other hand, increasing the number of FGM layers (with decreasing the sharpness in the material properties change) reduces the level of stress concentration at this region as can be observed in Figure 4, that shows the Von-Mises equivalent stress distribution for the five layers sample. However, the highest stress concentrated in this case located at the interface between (TiO₂) which is the upper layer and (Ti+75 TiO₂) which is the adjacent layer.



Figure 3 The Von-Mises corresponding stress distribution on the sample with three layers affect by temperature change of 100°K (a) full sample and (b) vertical cross-section through all layers.

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Figure 4 The Von-Mises corresponding stress distribution on the sample with five layers affect by temperature change of 100° K (a) full sample and (b) vertical cross-section through all layers.

The effect of transition between two layers with different material properties can be clearly seen in Figures 5 and 6. In these two figures, the stress shows very high concentration near the interfaces between the layers. However, the three-layers sample shows much higher peak stress than the peaks seen in the five-layers sample, especially at the outer surface of the samples.



Figure 5 Comparison of the stress distribution predicted in two lines of nodes passing through the vertical cross-section at outer surface and the centre line of the sample with three layers.



Figure 6 Comparison of the stress distribution predicted in two lines of nodes passing through the vertical cross-section at outer surface and the centre line of the sample with five layers.

The stress distributions shown in Figures 3-6 provide evidence of the failure path resulted from thermal impact, which was found to be through the interface between the layers rather than through thickness of the FGM. A second evidence can be clearly seen in Figures 7 and 8, which show strain distribution through the same samples. The two figures show very high difference in strain value when moving from the Ti layer to the adjacent layer, because titanium has lower young modulus than TiO2. However the three-layers sample still show much higher strain concentration near the interface due to the high difference in material properties between the adjacent layers (especially young modulus)



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Figure 7 The Von-Mises corresponding stress distribution on the sample with five layers affect by a temperature change of 100°K (a) full sample and (b) vertical cross-section through all layers.



Figure 8 The distribution of Von-Mises equivalent stress on the sample with five layers affect by temperature change of 100°K (a) full sample and (b) vertical cross-section through all layers.

7. CONCLUSIONS

Depending on the numerical results, the following assumptions could be described:

- Proposing of a non-symmetrical design which consists of three and five layer of functionally graded materials to achieve a linear variation along the layers of (TiO2& Ti) constituents.
- The developed FE model was successful in increasing understanding of the behaviour of the FGM when subjected to thermal impact.
- The stress and strain distribution in the modelled FGM samples showed approximately the same overall behaviour with the highest concentration occurring at the regions near the interfaces between the layers
- With increasing the number of layers or in other words by decreasing the difference in material properties between each two adjacent layers, the peak stress and strain will reduce.

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