Design and Modelling of (Fe /Zro_2) Functionally Graded Materials (Part I)

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ABSTRACT

It is hoped to design and modeling of five layers Fe/ZrO_2 functionally graded materials for high temperature applications in this paper. The design part, were started with the supposing of connecting two distinct material layers. The two layers were associated by a graded interface composing of three layers. Thickness of graded layer (i.e. RF) was designed and tested with the FEM method through the COMSOL package. The software was used extensively to examine the best graded part thickness percentage (i.e.RF %) that connecting the two different material layers. Two parameters were examined such as N and RF% to determine the best value of (N) and (RF %) that imparts low residual stresses. Thermal stresses that developed as a result of exposing of material to high temperature environments also calculated. The simulation indicates that the sample with (RF= 80% and N = 0. 7) Provides minimum residual stress at high working temperature 1000℃ with good mechanical properties.

Keywords: Design of Iron / Zirconia functionally graded materials, Simulation of residual stresses, Thermal stresses.

تصميم ونمذجة مادة متدرجة بالخواص ذات اساس (حديد /زركوينا) (الجزء الاول)

الخلاصه

نأمل في هذا البحث التوصل الى نمذجة ماده متدرجه بالخواص ذات اساس (حديد / زركونيا) مكونه من خمس طبقات جرى تصميمها للعمل في في تطبيقات درجات الحراره العاليه. ان هذا الجزء من البحث بدأ بأفتراض ان من الممكن ربط طبقتين مكونتين من مادتين مختلفتين. وهاتان الطبقتان يتم ربطهما من خلال ثلاثة طبقات متدرجه. إن سمك هذه الطبقات الثلاثه (RF) قد تم تصميمه واختياره بأستخدام طريقة العناصر المحدده من خلال برنامج (COMSOL). ولقد تم استخدام هذا البرنامج بعمق لأختبار افضل نسبة سمك للطبقات الوسطيه المتدرجه (RF%) التي تربط كما اشرنا طبقة الحديد من الاسفل مع طبقة الزركونيا من الاعلى. تم دراسة تأثير عاملين مهمين وهما المعامل (n) وكذلك (RF%) اللتان تعطيان اقل اجهادات متبقيه بين الطبقات. تم إحتساب الاجهادات الحراريه التي تنتج عن تعرض الماده الى درجات حراريه عاليه. ان النمذجه ببرنامج COMSOLاثبتت ان نسبة RF% = 80% و N = 0.7) سوف

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تعطيان اجهادات متبقيه منخفضه عندما تعمل الماده في درجات حراره عاليه (1000 مئوي) وخواص ميكانيكيه عاليه.

INTRODUCTION:

Functionally Graded Material (FGM), a revolutionary material, belongs to a class of advanced materials with varying properties over a changing dimension [1,2]. Functionally graded materials occur in nature as bones; teeth etc. [3].Nature designed these materials to meet their expected service requirements. Functionally graded material, eliminates the sharp interfaces existing in composite material where failure is initiated [4]. It replaces this sharp interface with a gradient interface which produces a smooth transition from one material to the next [5, 6]. Ahmadian, et.al,(2005),studied, the size-dependent static behavior of micro-beams made of (FGMs) analytically on the basis of the modified couple stress theory in the elastic range [7].Xin Jin , et al, (2009) studied the microstructure and mechanical properties of ZrO_2/NiCr functionally graded materials (FGMs) fabricated by powder metallurgy [8]. Ali Bouchafa, et.al, examined the thermal stresses in exponential FGM called (E- FGM) [9].Kyung Su Na, et.al,(2010) studied the volume fraction optimization of functionally graded (FGM) composite panels considering the stress reduction and thermo-mechanical buckling, [10]. Noor S. Ghafil, (2010)fabricated five-layered stepwise Cu/Ni functionally graded materials using pressure less sintering under vacuum; she used an ANSYS code for simulation of temperature and thermal stress distribution across the FGM [11].

Dheya N. Abdulameer, (2012)has used the COMSOL package for simulation of temperature distribution, displacement, and stress distribution for five- layered FGM of Al_2O_3 /Ti [12]. Ali Rizah nateghai, et. al, (2013) studied the thermal effect on buckling and the free vibration behavior of functionally graded (FG) micro beams based on modified couple stress theory, Numerical results show that the modified couple stress theory predicts higher values of buckling load and natural frequency for FG micro beams [13].The aim of this paperwork is to employ the FE method to study the distribution of thermal induced displacements, stresses within the functionally graded materials that result from the working these materials at high temperature applications. Parameter study will be performed. For instance, the influence of mixing ratio variation index (i.e. N) and graded layer thickness (i.e. RF %) on the resulting thermally induced stresses will be investigated.

Design of Functionally Graded Materials

Starting materials:

Commercially available ZrO_2 (Y_2O_3-PSZ) with low thermal conductivity which can be used as a thermal barrier and pure iron with high ductility and thermal expansion close to that of Zirconia are used as a starting material. The characteristics of two starting materials are listed in table (1).

Table 1 :(Y_2O_3 -PS Zirconia) and pure iron properties [14]

Property	Symbol	Units	Zro2	Fe
Thermal conductivity	K	W/K.m	2.2	80.4
Density	ρ	Kg/m^3	6000	7874
Specific heat	Cp	J/kg.K	400	444
Modulus of elasticity	E	Gpa	205	211
Poisson ratio	ν		0.23	0.29
Thermal expansion	α*E-6	1/k	10.3	11.8
Microhardness		HV	1200	60-80
Yield stress	σy	Mpa	-	120-150
Flexural stress	σ	Mpa	1000	-

Geometric of models& Assumptions:

Cylindrical Fe/ZrO_2functionally graded materials were considered. The material is of diameter d and thickness H. Further, h indicates the thicknesses of each FGM layers. The thickness ratio of FGM layers is denoted by RF that expressed as RF=h/H

The samples consist of five layers; the bottom layer is pure iron, while the top layer is pure Zirconia, and three intermediate layers represented the graded region as shown in figure (2). Different samples with different (RF=40%, 45%, 50%, 55%, 60%, 80%) were conceived in this work paper.

The amount of applied load is (256000 N/mm^2) for mechanical testing (i.e. Compression) and 1000 ^0C for thermal test. Residual stresses represented by a Von miss's stress, Z-displacement, and temperature distribution throughout the thickness of the model are examined as well.

In order to design FGMs a model must be created describing the use of composition throughout the material. The volume fraction, V, which describes the volume of ceramic at any point, z, throughout the thickness (h) according to a parameter N, which controls the shape of the function as can be seen in figure (1) and equation (1) below:

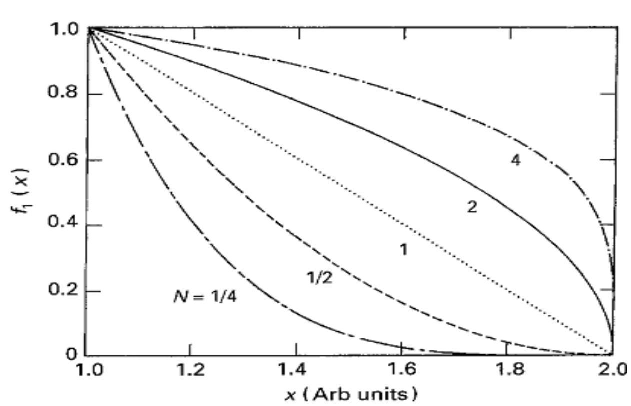


Figure (1): Plot of ceramic volume fraction versus Z for selected values of N.

$$Vc = \left(0.5 + {}^{Z}\!/_{H}\right)^{N} \qquad \text{..... (1)}$$

It follows that the volume fraction of metal is

$$Vm = 1 - Vc \qquad \text{........ (2)}$$

Where,

(V_m) is the volume fraction of ceramic and (Vc) is the volume fraction of metal. The values of N that depended in this study are (0.7, 1, and 1.5). The material properties through the thickness vary as a function of the volume fraction and can be seen in equation (3) below [14].

$$P = Vc * Pc + Vm * Pm \qquad \text{...... (3)}$$

Where, (P) is the material property, (Pc): property of ceramic, (Pm): property of the metal, (Vc): volume fraction of ceramic and (V_m) isthe volume fraction of metal. This equation holds true for the modulus of elasticity, density, thermal expansion, thermal conductivity, heat capacity and Poisson's ratio.

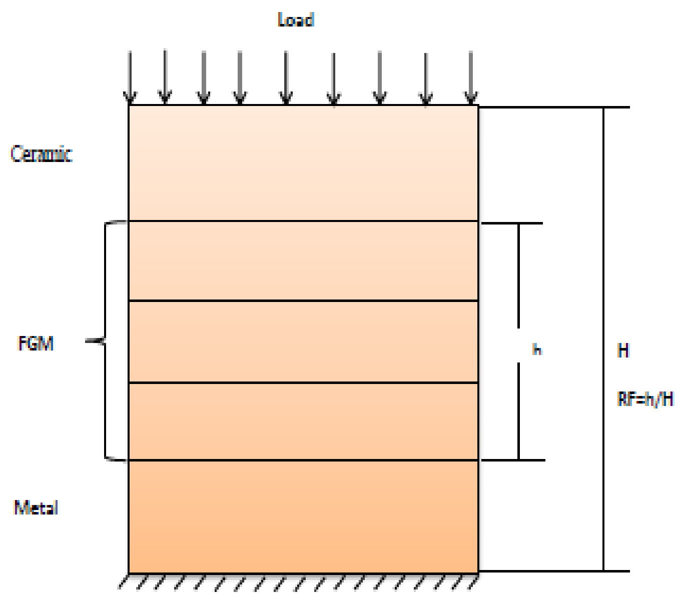


Figure (2): geometry of prepared FGM samples.

Displacements &the Von Misses stress:

The aim of this section work is to employ the finite element method to analyze the displacements and distribution of maximum Von misses stresses within the functionally graded materials that result from compression loading process. The parameters of study that performed are the influence of mixing ratio variation (i.e. N-parameter) and graded layer thickness (i.e. RF %) on the resulting induced displacements and stresses.

At the outset, it is considered a three dimensional infinitesimal element in Cartesian coordinates and considering the tetrahedral element. The total potential energy is given by: [15].

$$\pi p = U + \cap s \quad \text{……. (4)}$$

Where, (πp): is the total potential energy, (U): strain energy and$(\cap s)$: potential energy of distributed load?

$$[K] = [B]^T[D][B]\,V \quad \text{…. (5)}$$

Where, [K] stiffness matrix B: gradient matrix, [D] constitutive matrix, the stresses relate to the element strain by

$$\{\varepsilon\} = [B]\{d\} \quad \text{….. (6)}$$

$$\{\sigma\} = [\boldsymbol{D}]\{\boldsymbol{\varepsilon}\} \quad \text{…….. (7)}$$

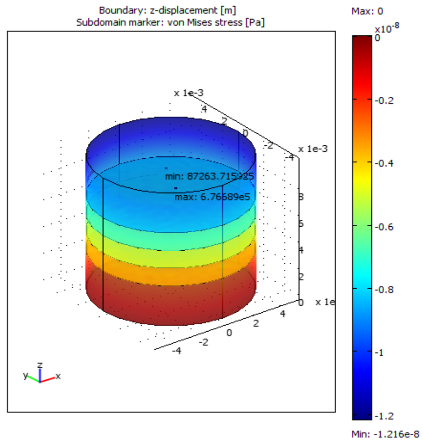
$$[D] = \frac{E}{(1+v)(1-2v)}\begin{bmatrix} 1-v & v & v & 0 & 0 & 0 \\ v & 1-v & v & 0 & 0 & 0 \\ v & v & 1-v & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2v}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2v}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2v}{2} \end{bmatrix} \quad \text{….. (8)}$$

(E): modulus of elasticity, (v): Poisson's ratio, which are calculated from the equation (3), [16]. FGM samples are subjected to uniform compression load of amount 256 KN/m^2 as mentioned above. The generated stresses and displacement has been calculated using Comsol package. The legend in the right (see figures 3 to 4) refers to z-direction displacement which starts from zero at the top (red color) and ends to the maximum compressive displacement at the bottom (blue color), the sub marker refers to maximum & minimum Von Misses stresses that generated in the FGM samples

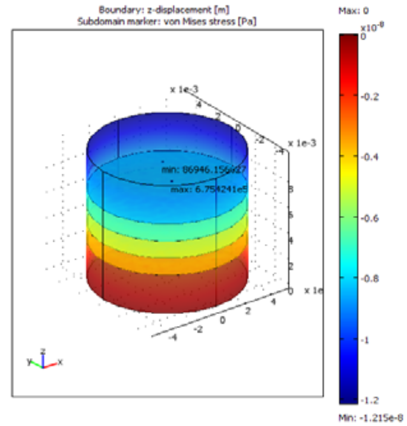
Results and Discussions:

In Fe-ZrO_2 FGMs, the two constituents have different thermal expansion coefficients. Hence, as the material cools down from the sintering as well as operating temperature, the contraction of the different layers will not be uniform but will vary with the mixing ratio. This effect will in turn cause thermal residual stresses in the material, and this may cause delamination and hence the failure of the material. Therefore, it is necessary to analyze and optimize the distribution of these thermal residual stresses in order to construct a sound FGMs. Distribution of Von Misses stresses and displacements within the metal-ceramic FGM have been analyzed. The finite element package Comsol has been used to study the displacements and stresses induced and result from compression loading process. Moreover, the material has been assumed to be solid, piecewise homogenous, isotropic and elastic.

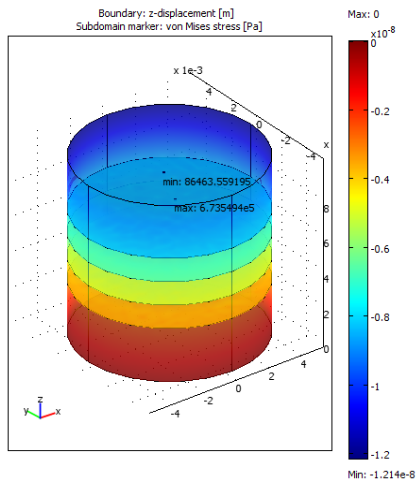
In all samples, when the volume fraction index (N) is increased at each value of RF%, the compressive stress decreases generally and reaches minimum values at RF% = 60%:



(a): RF%=40% & N=0. 7

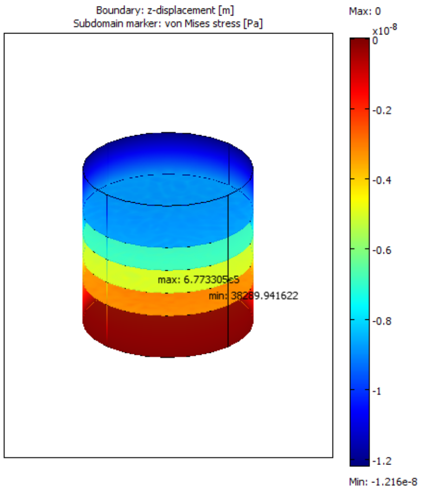


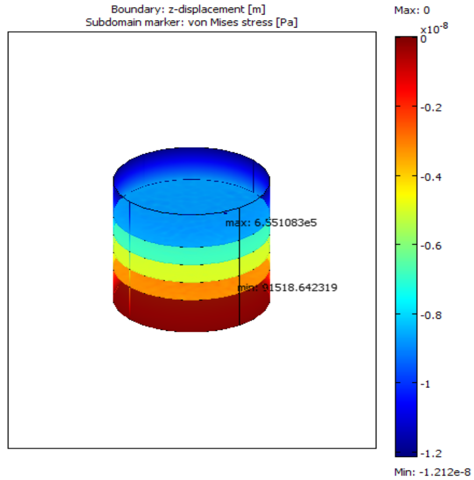
(b): RF% = 40% & N= 1



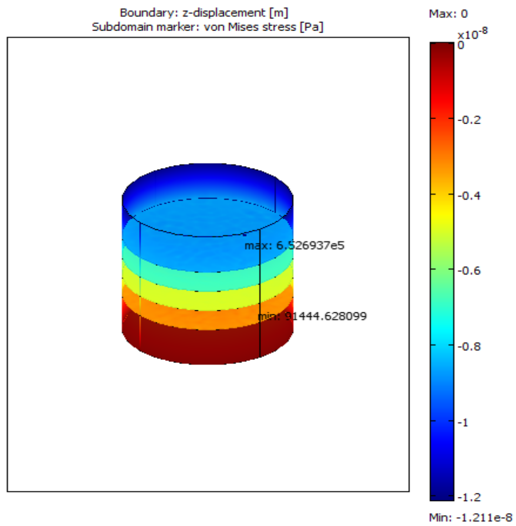
(c) RF%=40% & N=1. 5

Figure (3): Z- direction displacement contours under compression load at RF = 40% and (N = 0.7 1 and 1.5 respectively).



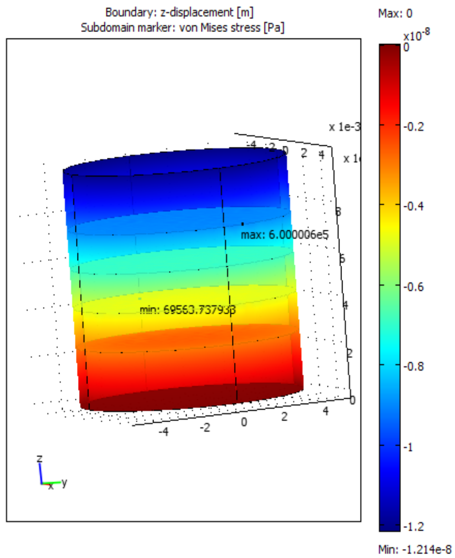


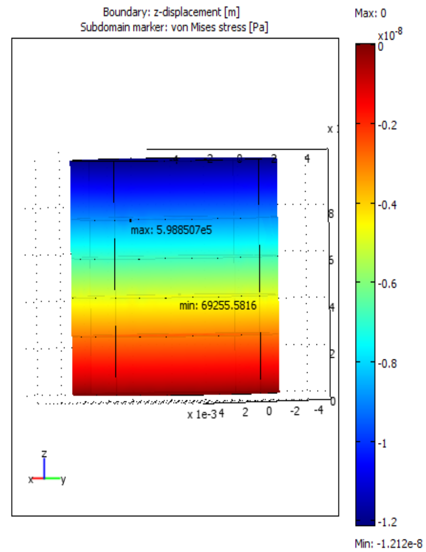
(a):RF%=45% & N=0.7 **(b): RF% = 45% & N= 1**



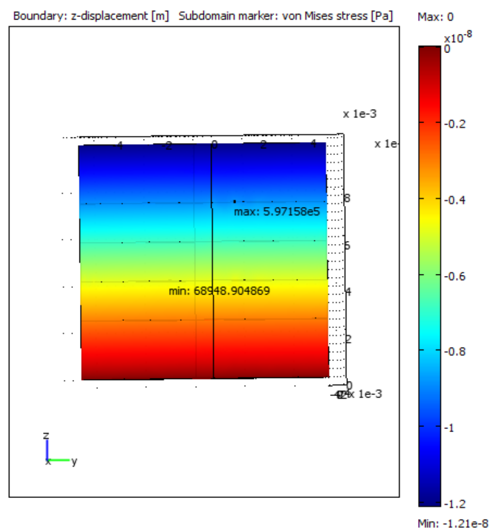
(c): RF% = 45% & N= 1.5

Figure (4): Z- direction displacement contours under compression load at RF = 45% and (N = 0.7, 1 and 1.5 respectively).



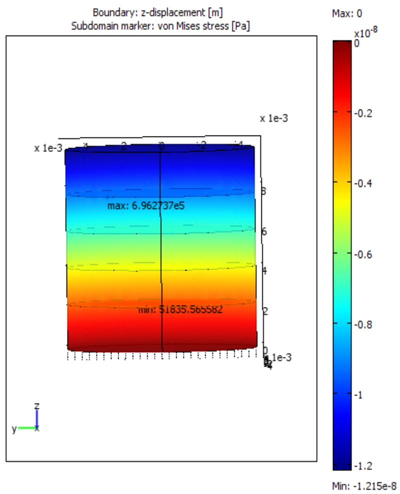


(a): RF%=50% & N=0.7 **(b): RF% = 50% & N= 1**

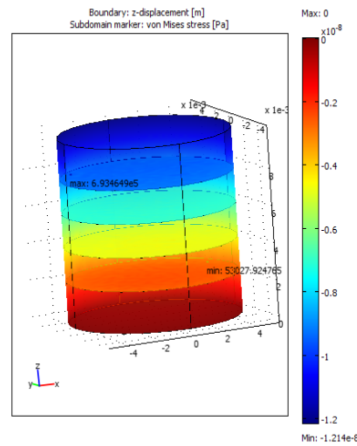


(c): RF%=50% & N=1.5

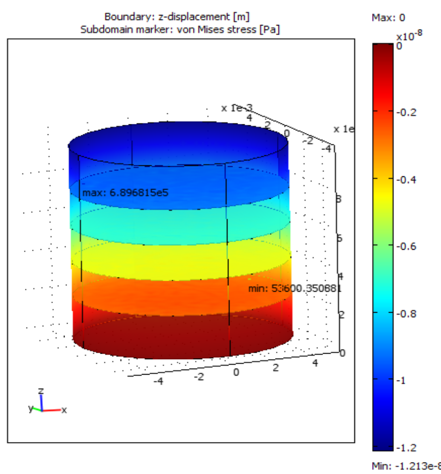
Figure (5): Z- direction displacement contours under compression load at RF = 50% and (N = 0.7, 1 and 1.5 respectively).



(a): RF% = 55% & N= 0.7

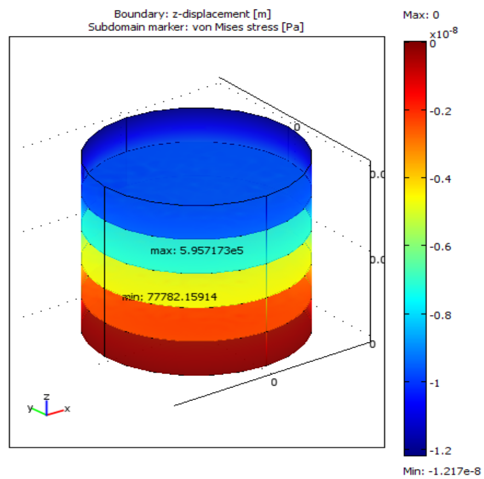


(b): RF%=55% & N=1

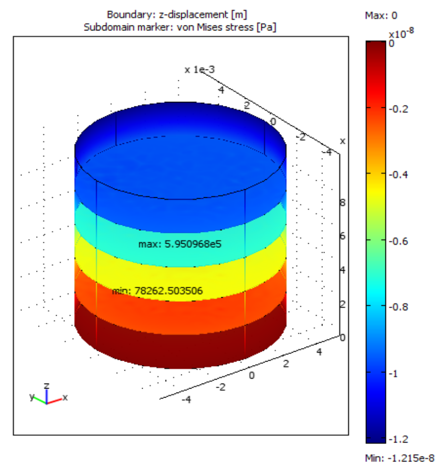


(c): RF% = 55% & N= 1.5

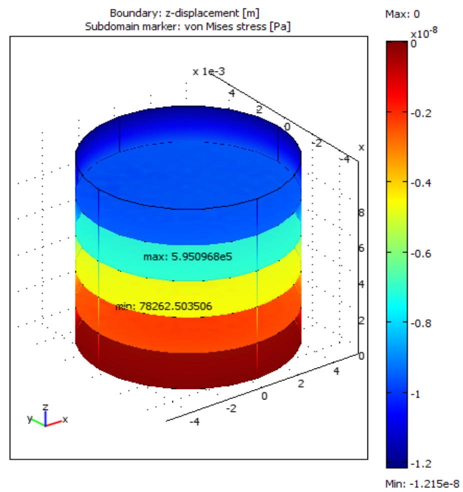
Figure (6): Z- direction displacement contours under compression load at RF = 55% and (N = 0.7, 1 and 1.5 respectively).



(a): RF%=60% & N=0.7

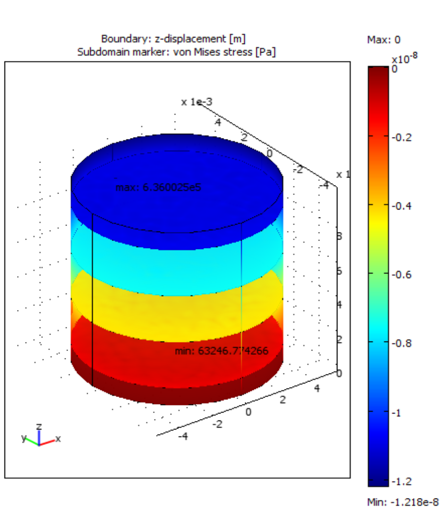


(b): RF% = 60% & N= 1

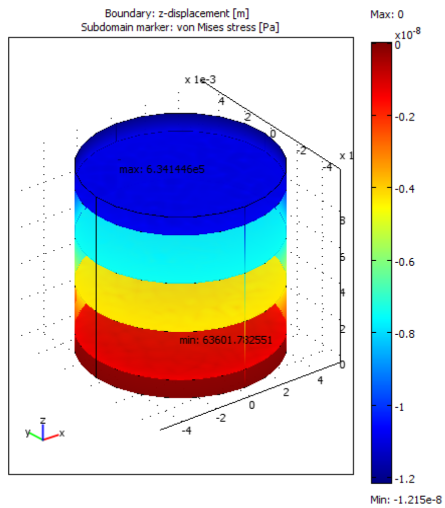


(c): RF%=60% & N=1.5

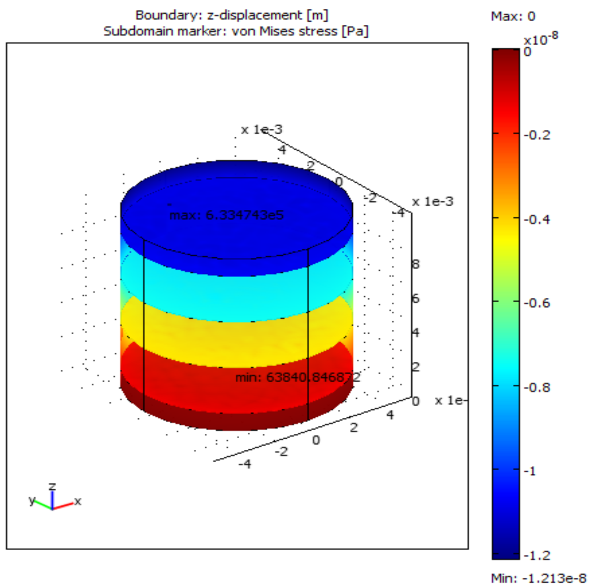
Figure (7): Z- direction displacement contours under compression load at RF = 60% and (N = 0.7, 1 and 1.5 respectively).



(a): RF% = 80% & N= 0.7



(b): RF% = 80% & N= 1



(c): RF%=80% & N= 1.5

Figure (8): Z- direction displacement contours under compression load at RF = 80% and (N = 0.7, 1 and 1.5 respectively).

It is obviously shown from above contours and the concluding figure (9) that, as the index ratio of different RF% increased, Von misses stresses are decreased. The reasons behind such behavior are that, as the modulus of elasticity (E)was increasing as the volume fraction index (N) is increased. That lends a less displacement as well as less residual stresses was achieved. When RF= 60% minimum residual stresses are documented at each value of (N). The highest residual stresses of all samples are documented with RF= 55%, and N=0. 7. These results are very important to consider during the manufacturing process of this kind of FGMs.

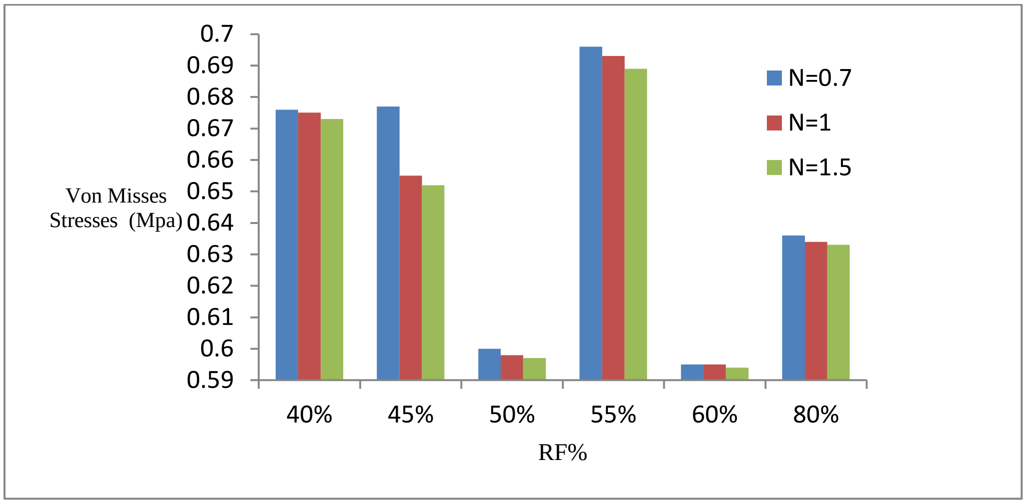


Figure (9): Residual stresses as a function of RF% at different values of N index.

Thermal behavior modeling:

Temperature changes in a structure can result in large stresses if not viewed properly in design step. Residual stresses after cooling or heating of FGM system involves two principal contributions, one arising from stress equilibrium due to the contraction or expansion and the other coming from the moment equilibrium due to asymmetric stress distribution [9].

The latter arises from the asymmetric variation in the proportions of the constituents, and hence the elastic and thermal expansion characteristics, across the thickness.

Boundary conditions:

The samples have been tested thermally by subjecting the models to a thermal load of about 1000℃ at the top and 25℃ at the bottom which also fixed.The accompanying figure shows boundary conditions of the samples. Only the FGMs with RF%=80% at N=0.7 was documented in this section.

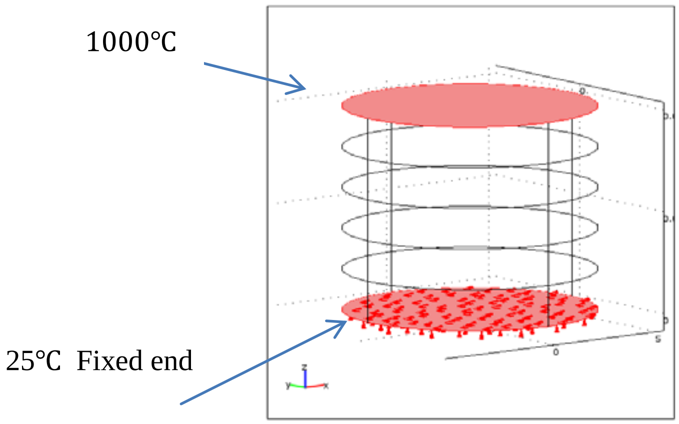


Figure (10): Thermal model of FGM boundary conditions.

For simplicity it can be consider our models as an axisymmetric element. According to finite element method, the thermal strain matrix is

$$\{\varepsilon_T\} = \begin{Bmatrix} \varepsilon_{rT} \\ \varepsilon_{zT} \\ \varepsilon_{\theta T} \\ \gamma_{rzT} \end{Bmatrix} = \begin{Bmatrix} \alpha T \\ \alpha T \\ \alpha T \\ 0 \end{Bmatrix} \qquad \ldots\ldots (9)$$

The thermal force matrix is given by

$$\{f_T\} = 2\pi\bar{r}A[\bar{B}]^T[D]\{\varepsilon_T\} \qquad \ldots\ldots. (10)$$

Where $\bar{r}$is the centroid, A is the surface area of the element, $\bar{B}$ is the matrix gradient at the centroid, the [D] constitutive matrix which is given by [15]

$$[D] = \frac{E}{(1+v)(1-2v)} \begin{bmatrix} 1-v & v & v & 0 \\ v & 1-v & v & 0 \\ v & v & 1-v & 0 \\ 0 & 0 & 0 & \frac{1-2v}{2} \end{bmatrix} \qquad \ldots\ldots.. (11)$$

$$\{\sigma\} = [D][\bar{B}]\{d\} - [D]\{\varepsilon_T\} \qquad \ldots\ldots. (12)$$

Two models will be presented in thermal test; displacement and temperature distribution models. Knowing that, the temperature distribution across the FGM section is depends mainly on the thickness of the top ceramic layer. Furthermore, there was a slight difference in the temperature distribution for FGMs models of same top layer thickness. So an image and diagram will be presented at the models end of similar RF.

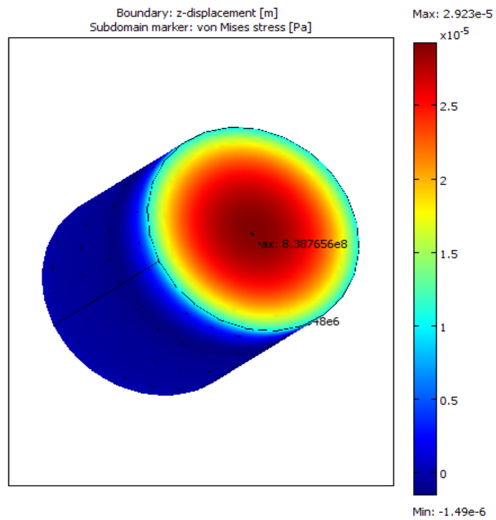


Figure (11): z- displacement contour and max Von Misses under thermal load for RF= 80%, N=0.7

The temperature distribution contour and curve for RF=80%, N=0.7, is represented in the figure (12/a and b) respectively.

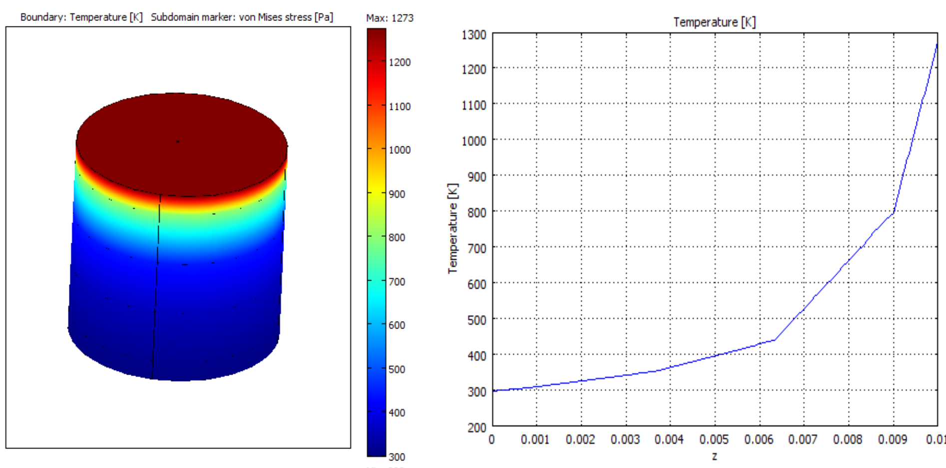


Figure (12): Temperature distribution contour in RF= 80%, N=0.7; (b): Temperature distribution curve of RF=80%, N=0.7.

Figure (12/a) shows a slight decreasing of temperature across the thickness. The behavior of temperature decreasing starting from the monolithic ZrO_2 layer to the monolithic Fe layer is an exponential behavior. The slight and smooth behavior across the FGMs layers is obviously proven, that indicated the graded and smooth chemical compositions were obtained.

Thermal models discussion:

The effect of graded region size (RF %) at different volume fraction index (N) on the residual stresses is summarized as shown in figure below. Knowing that, as the RF% decreased, the monolithic ceramic regions as well as the metal regions are increased that imparts an increasing in the layers of thermal residual stresses as shown below. As RF increases above 50%, thermal residual stresses are going to fall significantly due to the homogenous gradation of the interlayer.

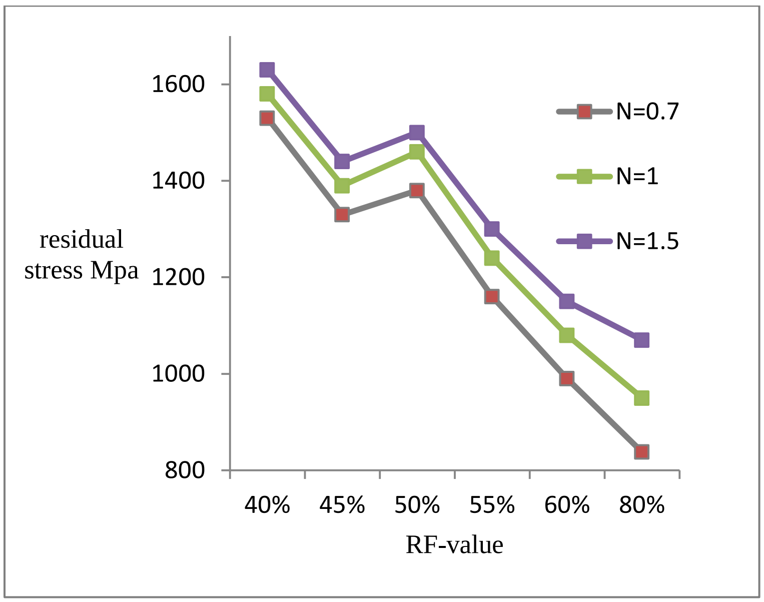


Figure (15): Thermal residual stresses vs. RF values at different N.

CONCLUSIONS:

According to results obtained, the following points can be concluded:

1. Appling distributed compression load of about 256 KN/m^2 showed minimum (Von misses stress=594,000 pa) is when RF= 60%.
2. The FGMs will have best thermal resistance when the index (N) is (0.7) i.e. when the ceramic properties in the FGM are dominating.
3. At RF= 80% higher FGM thickness showed minimum residual stress (838Mpa) in the Zirconia layer which in turn considered acceptable from the design point of view.
4. Temperature distribution through a material depends on the size of fully ceramic layer.
5. An exponential temperature distribution across the FGMs thickness with RF% = 80%.

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