PERFORMANCE ANALYSIS OF FUNCTIONALLY GRADED THERMAL BARRIERS

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Abstract. *The development of Functionally Graded Materials (FGM), which are material composites in that the mechanical properties vary smoothly or continuously of a surface to the other, for energy-absorbing applications requires understanding of stress wave propagation in these structures in order to optimize their resistance to failure. The advantage of using these materials is that they are able to withstand high temperature gradient environments while maintaining their structural integrity with superior resistance to interfacial failure. In this present work, it presents a model to solve the coupled thermomechanical problem submitted to thermal solicitations. Traditional staggered algorithm without upsetting the unconditional stability property characteristic of fully implicit schemes is used. The proposed scheme is a fractional step method associated with a two phase operator split of the system of linearized thermoelasticity into an adiabatic elastodynamics phase, followed by a heat conduction phase. All dissipation is provided the heat conduction process. Numerical simulations are presented for one-dimensional case with FGM materials submitted to thermal shocks and analysis is accomplished for variation of its constitutive parameters.*

***Keywords**:* Functionally Graded Material (FGM), coupled thermomechanical problem, elastodynamics**,** thermal shocks.

1. Introduction

Composite materials, due to their thermal and mechanical merits compared to single-composed materials, have been widely used on a variety of engineering applications. However, the interfaces might represent regions of stress concentration and, due to that, risk of presenting failure mechanisms like loss of cohesion. For instance, linear elastic materials present stress singularities at the interfaces or at the free edges. In recent years, nonhomogeneous materials have been developed to attenuate the interfacial stresses under a new concept: Functionally Graded Materials (FGM). FGMs are composites whose mechanical properties vary smoothly and continuously along its domain. They have been used in Thermal Protection Systems (TPS) in order to decrease thermal stresses concentration without losing the capacity of standing the protection from heat. It is carried out by controlling the volume fractions of these materials to grade the thermomechanical response. The utilization of FGMs in the attenuation of stress wave propagation (Bruck, 2000) can be very useful in important engineering applications like, for instance, the re-entry motion of space vehicles, in which a rapidly changing temperature can lead to a dramatic failure scenario. In this type of situations the dynamic thermo elastic response should be considered. Dynamic thermoelastic problems have been studied, since several decades, in different structures (Shabana et al., 2001 and Suresh. and Mortensen, 1998).

The present work presents a numerical formulation to solve the strongly coupled thermomechanical problem submitted to thermal shock solicitations. A staggered algorithm without upsetting the unconditional stability property characteristic of fully implicit schemes is used. The proposed scheme is a fractional step method associated with a two phases operator split of the linearized thermoelasticity system into an adiabatic elastodynamics phase, followed by a heat conduction phase. Numerical simulations are presented for an FGM bar submitted to thermal flux and analysis is accomplished for cases in which FGM parameters are varied.

2. Mechanical modeling

Let the thermoelastic response of a body to be expressed by the displacement field **u** and the relative temperature field θ with respect to a constant reference value $\theta_{ref} > 0$, such that, the absolute temperature is given by $\Theta = \theta + \theta_{ref}$. Let $\boldsymbol{\varepsilon}[\mathbf{u}] = \mathrm{sym}[\nabla \mathbf{u}]$ the infinitesimal strain tensor associated with the displacement **u**, while the stress tensor, the heat flux, the entropy and the density in Ω are denoted by $\boldsymbol{\sigma}$, $\mathbf{q}$, η e ρ, respectively.

The local form of the balance of momentum and the balance of energy equations is cast as:

$$\rho \ddot{\mathbf{u}} = div[\sigma] + \rho \mathbf{b} \qquad \text{and} \qquad \Theta \dot{\eta} = -div[\mathbf{q}] + r \,, \tag{1}$$

where **b** e *r* are the body force and the heat source, respectively, assumed to be smooth functions in body domain. Superimposed dots denote time derivates.

The constitutive equations, which for infinitesimal thermoelasticity are defined by:

$$\boldsymbol{\sigma} = \mathbf{C}\boldsymbol{\varepsilon} - \theta \mathbf{m} \qquad \text{and} \qquad \eta = \bar{c}\,\theta + \mathbf{m} : \boldsymbol{\varepsilon} \quad , \tag{2}$$

and the Fourier´s law for heat conduction,

$$\Theta\, \dot{\eta} \cong \theta_{ref}\, \dot{\eta} \qquad \text{and} \qquad \mathbf{q} = -\,\mathbf{k}\,\nabla\Theta = -\,\mathbf{k}\,\nabla\theta \;\; , \text{ where } \bar{c} = \frac{c}{\theta_{ref}} \;\; \text{and } \bar{k} = \frac{k}{\theta_{ref}} . \tag{3}$$

where **k** is the conductivity tensor, the scalar $c > 0$ is the linearized volumetric heat capacity and **m** defines the structural properties reflecting thermomechanical coupling. The dilatation coefficient α is related to the thermoelastic coefficient **m** and the Bulk modulus **K** by $\mathbf{m}=3\mathbf{K}\alpha$, and **C** the elastic constants four rank tensor.

Substituting Fourier´s law (4) and relations (5) into the balance laws (1), yields the second order problem of evolution for linearized thermoelasticity:

$$\begin{aligned} &\rho\, \ddot{\mathbf{u}} = div[\mathbf{C}\boldsymbol{\varepsilon}[\mathbf{u}] - \mathbf{m}\theta] + \rho\, \mathbf{b} \\ &\bar{c}\,\dot{\theta} = div[\bar{\mathbf{k}}\nabla\theta] - \mathbf{m} : \nabla\dot{\mathbf{u}} \quad , \end{aligned} \tag{4}$$

3. Functionally graded materials thermoelastic response

Functionally graded materials are supposed to smoothly connect two base materials referred to here as 1 and 2, that posses quite different mechanical behavior. Indeed, the FGMs are composite materials resulting of an indicious combination of 1 and 2 controlled by the metal volume fraction V_m, here assumed as power-law function of the position, $V_m = \left(\frac{x}{d}\right)^n$, where x is a position of the material point in FGM, d is the length of FGM region and n is an exponent that can be varied in order to obtain specific microstructures distribution. The material properties can be depicted metal volume distribution associate to different values of n and their influence in the variation of the constitutive parameter n in the thermo elastic response is observed through numerical results.

In fact, in order to describe FGM behavior, it is necessary to estimate the properties such as thermal conductivity, the coefficient of thermal expansion, the Young's Modulus and Poisson's ratio. There are a number of micromechanical approaches that have been widely used for predicting the effective properties of FGM like, for instance: rule of mixture, mean field micromechanics (MFM) and self-consistent (SCM)(Hill, 1965). The progress in theoretical methods for the overall thermo mechanical properties is featured by Suresh and Mortensen (1998). In the present work, the modified rule of mixture is adopted. For the Young's modulus, Tamura, Tomota and Ozawa proposed the modified rule of mixtures. For that study, they consider each sub-layer in the graded layer are expressed in terms of the average axial stresses σ_i and deformations ε_i for each constituent material i, where this subscript assumes m or c refers to ceramic and metal respectively,

$$\sigma = V_m\,\sigma_m + V_c\,\sigma_c \qquad \varepsilon = V_m\,\varepsilon_m + V_c\,\varepsilon_c \tag{5}$$

In many practical situations, such as in two-phase composites in which one phase is discontinuous in a continuous matrix of the other phase, neither the Voigt model nor the Reuss model in simple rule of mixtures provides an accurate description of effective modulus of the composite (Suresh and Mortensen, 1998). An estimation of Young's modulus is obtained:

$$E = \left[\left(\frac{q+E_c}{q+E_m}\right)V_m\,E_m + V_c\,E_c\right] \Big/ \left[\left(\frac{q+E_c}{q+E_m}\right)V_m + V_c\right] \quad , \quad q = \frac{\sigma_c - \sigma_m}{\varepsilon_c - \varepsilon_m} \quad , \quad 0 < q < \infty \quad , \tag{6}$$

where the parameter q defines the ratio of stress to strain transfer. In practice, q may be approximately determined by tensile tests performed on monolithic specimens (Zhi-He *et al*., 2003 and Giannakopoulos et al., 1995). The exact nature of this dependence, however, it is not known (Williamson *et al.*, 1993). According to experiments with dual phase steels, within a wide range of volume fractions and loading condition, q = 4.5 GPa has been reported to be appropriate (Suresh and Mortensen, 1998).

Furthermore, the coefficient of thermal expansion is coupled with the bulk modulus through the relation

$$\alpha = \alpha_m + (\alpha_c - \alpha_m)\left(\frac{1}{K} - \frac{1}{K_m}\right) \Big/ \left(\frac{1}{K_c} - \frac{1}{K_m}\right) \quad , \qquad k = k_m + \frac{k_m V_c (k_c - k_m)}{k_m + \frac{1}{3}(k_m - k_c) V_m} \tag{7}$$

Moreover, specific heat and the specific mass is obtained by the rule of mixture, as follows:

$$c = V_m c_m + V_c c_c \qquad \rho = V_m \rho_m + V_c \rho_c \ , \tag{8}$$

4. Thermal Barriers Performance

The present section is devoted to improve the understanding of how FGM materials can impact the performance of thermal barriers. This goal is pursued by carrying out a numerical analysis involving a representative example in which consists of a one dimensional bar submitted to a thermal shock. The total length of the bar is 80 mm and the area of its cross section is 2.10^{-6} m^2. The bar contains a FGM layer providing a smooth transition between the ceramics insulation (SiC) and the metal component (Al 6061) to be protected. The situation is schematically depicted in Figure 1 and the materials' properties are presented in Table 1.

Figure 1. Schematic representation of the FGM bar lay-up and dimensions

Table1. Thermal and mechanical properties of metal and ceramic.

Material Properties	Al 6061	SiC ceramic
Density (10^3 Kg/m^3)	2.70	3.21
Young's modulus (GPa)	70	427
Poisson's ratio	0.30	0.17
Specific heat (J $Kg^{-1}K^{-1}$)	900	837
Thermal conductivity (W.$m^{-1}K^{-1}$)	233	65
Thermal expansion coefficient (10^{-6}/^{o}C)	23.4	4.3

The thermo elastic coupled system of partial differential equations resulting from the modeling in sections 2 and 3 is solved by combining the Finite Element Method with a time step staggered algorithm (Armero and Simo, 1992). This algorithm, which can be proven unconditional stable, splits each time step into two distinct phases corresponding to a linear thermo elastic adiabatic problem followed by a heat conduction one.

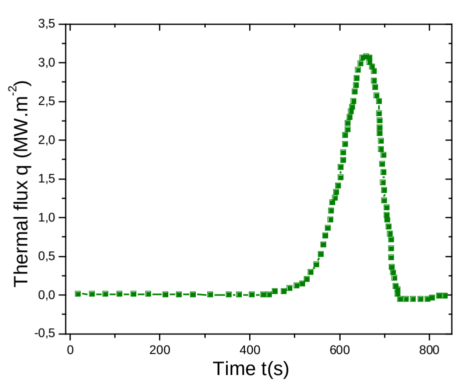


Figure 2. Thermal flux history during the atmospheric re-entry

A number of cases corresponding to varying the micro structural composition, length and position of the FGM layer are analyzed in order to assess the performance improvement when compared to barriers without transition zones between insulation and the basic structure. The bar goes through a thermal shock by applying to its left extremity the heat flux presented in Fig. 2. This flux reproduces the atmospheric heating typical of a re-entry maneuver, as the one simulated in Cotta (2003).

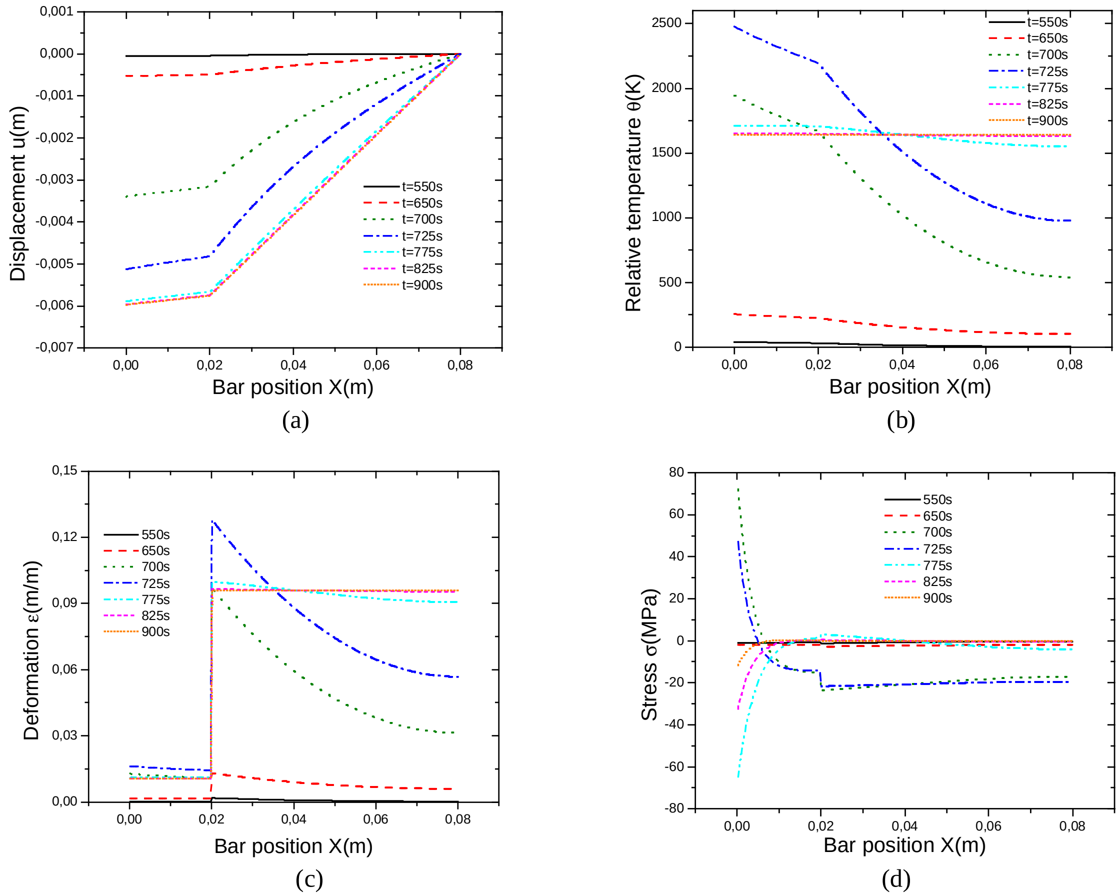


Figure 3. Displacement u (a), relative temperature θ (b), deformation ε (c) and stress σ (d) induced fields of the thermo elastic bar without FGM submitted to thermal shocks

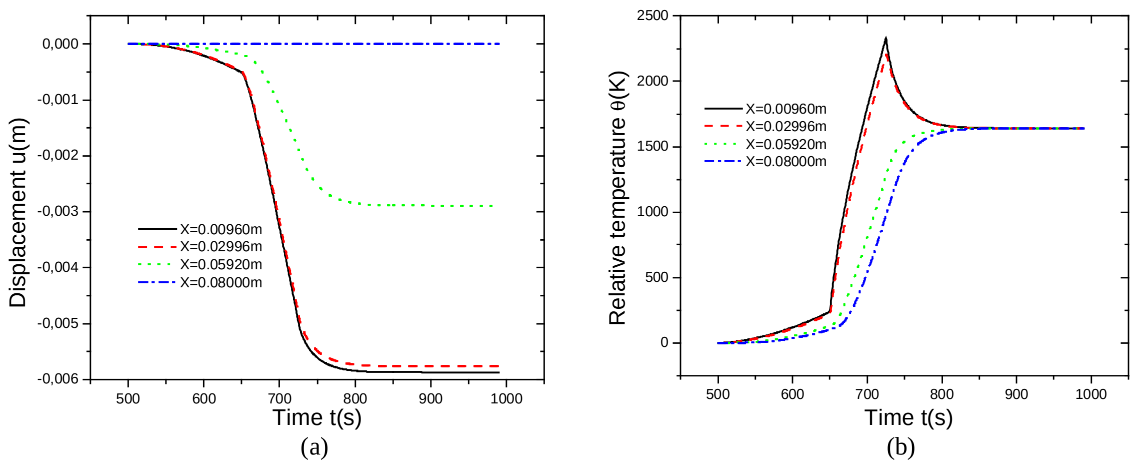
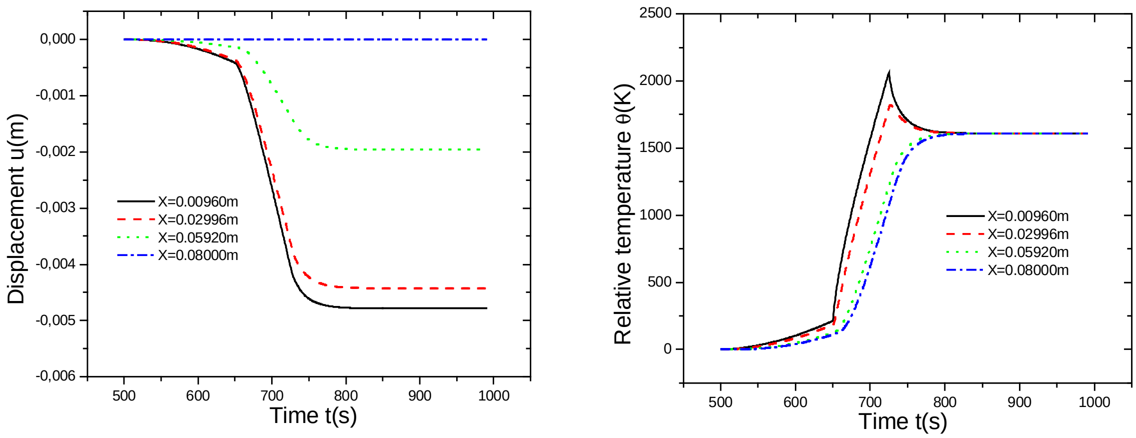


Figure 4. Displacement u (a), relative temperature θ (b) induced fields obtained in fixed points of the bar without FGM submitted to thermal shocks

The first analysis deals with a configuration in which the lengths of ceramic L_1=20 mm and of metal L= 60mm with no FGM layer, e.g., d=0. Figure 3 (a) presents the displacement field along within the bar along the re-entry maneuver. It is important to remark the deformation mismatch across the interface. Usually this sort of non-smooth response is responsible for damage nucleation that can give rise to the development of failure mechanisms. Furthermore, we can verify the decrease of the relative temperature θ and the stress σ, in the bar's domain due to action the ceramic material as insulator, protecting the mechanical structure, as shown in figures 3b and 3d, respectively. Also, it is possible note the variation of this decrease for different materials.

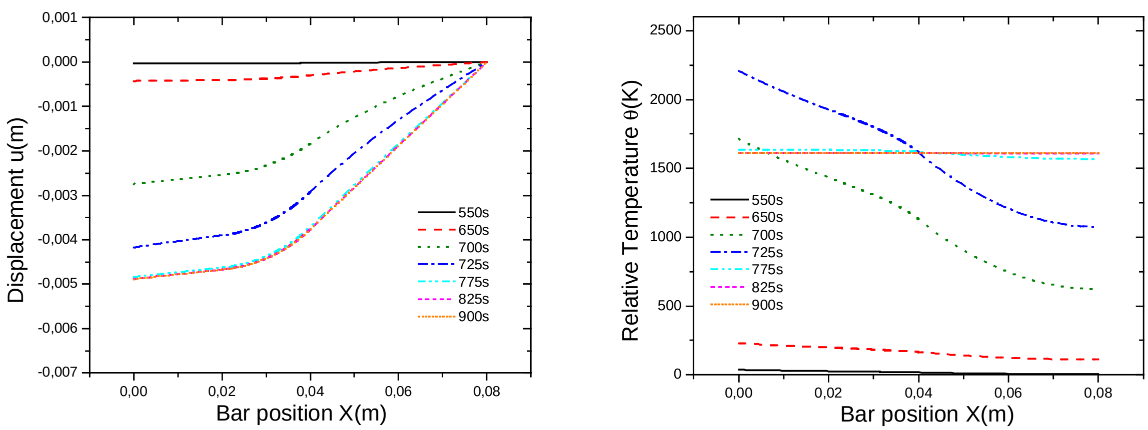


(a) (b)

Figure 5. Displacement u (a), relative temperature θ (b) induced fields obtained in fixed points of the FGM thermo elastic bar with exponent n=1 submitted to thermal shocks

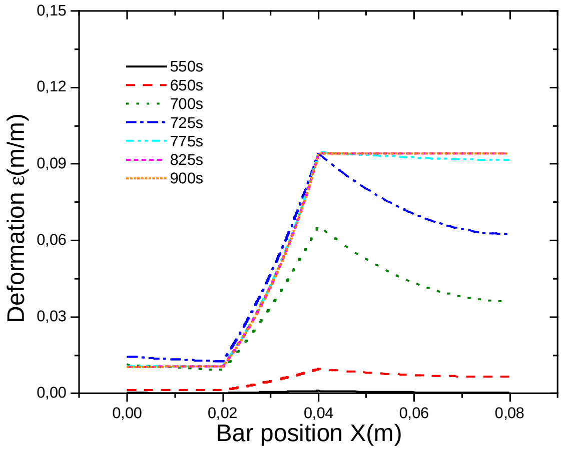
The analysis of the dynamics process is complemented by observing the state variables along the time on four representative points of the bar, which are X=0.00960m (average point of the region I contend the ceramic), 0.02996m (average point of the region of the FGM), 0.05920m (average point of the region that contains the metal) and 0,0800m (end of the bar where the contour conditions are imposed). The thermo-elastic response is summarized in Figs. 4 and 5.

Now the study comes to the analysis of thermal barriers containing a FGM layer. The first example deals with a layer of 0.02 meters that has it microstructure dictated by a metal power-law distribution with n=1. Comparing with the previous barrier configuration (no FGM layer), one can clearly verify from Figure 6 the displacement and relative temperature fields with no sharp transition across the interfaces. In addition, one can observe a decrease of magnitude of the state variables, in special, deformation ε and stress σ fields. The FGM region attenuates the induced stresses and acts to minimize the stress and deformation gradients in this FGM domain.

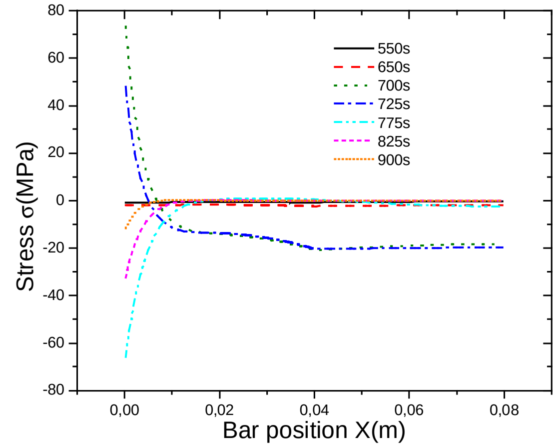


(a) (b)

Figure 6. Displacement u (a), relative temperature θ (b), deformation ε (c) and stress σ (d) induced fields of the thermo elastic FGM bar with n=1 and d=0,02m submitted to thermal shocks

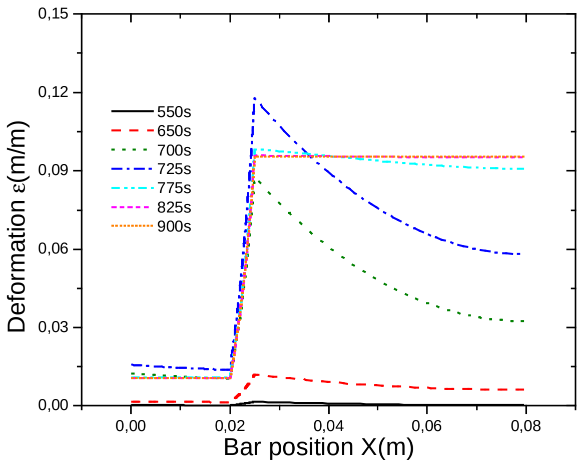


(c)

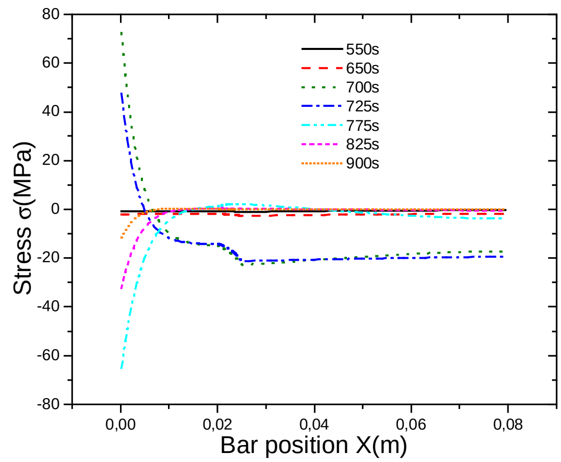


(d)

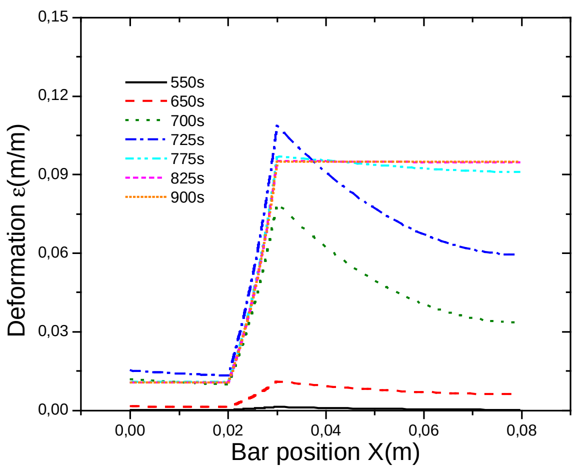
Figure 6. Displacement u (a), relative temperature θ (b), deformation ε (c) and stress σ (d) induced fields of the thermo elastic FGM bar with n=1 and d=0,02m submitted to thermal shocks



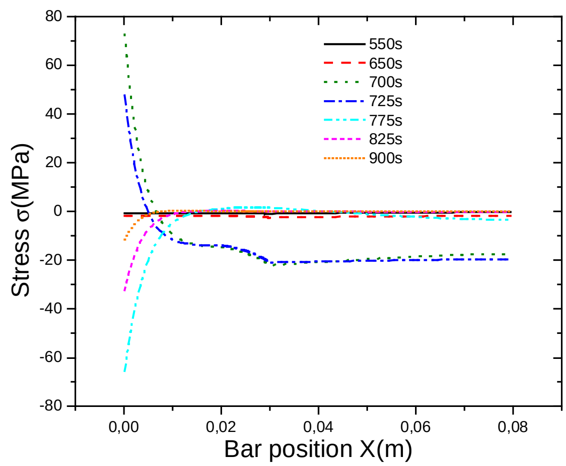
(a)



(b)



(c)



(d)

Figure 7. Deformation ε and stress σ induced fields of the thermo elastic FGM bar with variations of FGM length d=0.005m, d=0.01m and d=0.02m, respectively, when submitted to thermal shocks

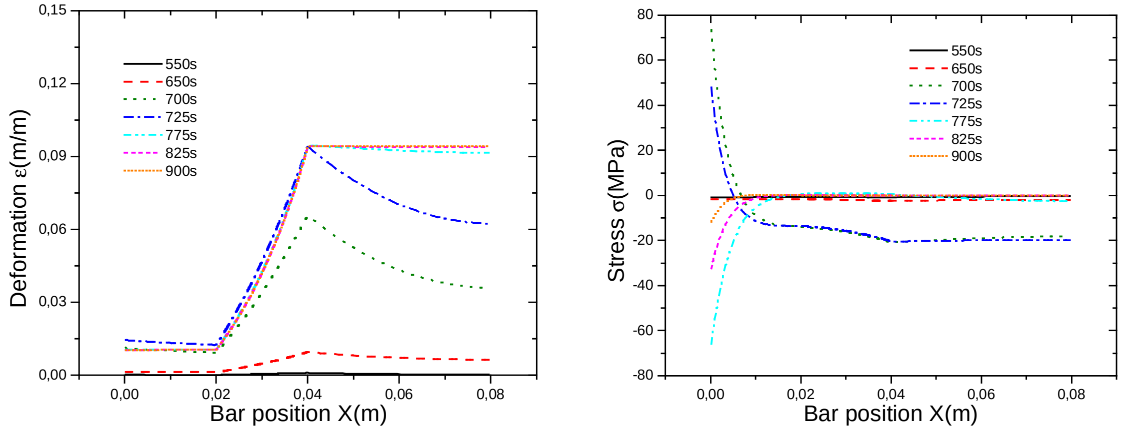


Figure 7. Deformation ε and stress σ induced fields of the thermo elastic FGM bar with variations of FGM length d=0.005m, d=0.01m and d=0.02m, respectively, when submitted to thermal shocks

A comparative analysis is accomplished for different values of the length, as shown in figure 7, keeping the initial position of FGM region at X=0.02m, comparing the deformation and stress fields obtained at bar's domain. We can observe variations in the deformation amplitude decreasing with a increase of FGM length, in the same way to deformation gradient, as illustrated figures 7a, 7c and 7e. Observing the stress distribution, we can say that the similar analysis to deformation fields to respect stress amplitude and gradient. It is noticeable that FGM actually smoothes the stress distribution in its region consequently attenuates the stress in this region.

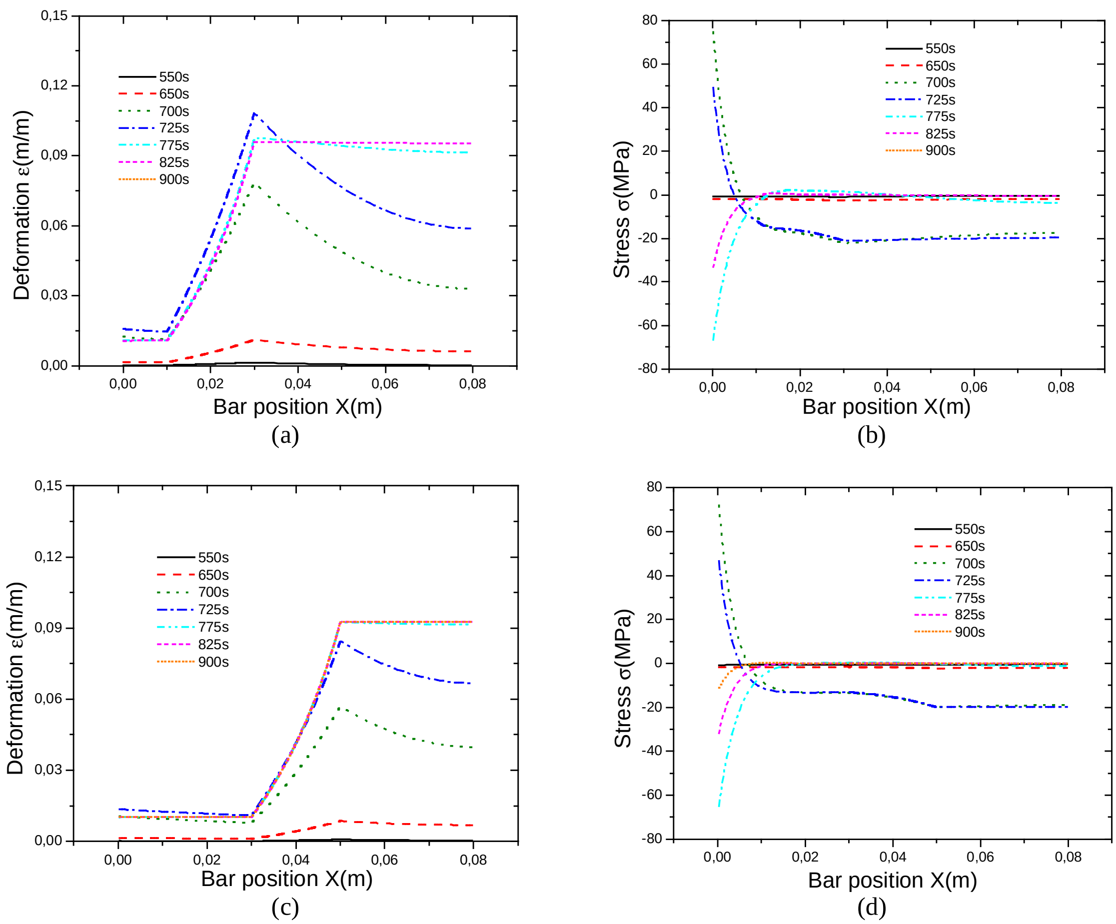


Figure 8. Deformation ε and stress σ induced fields of the thermo elastic FGM bar with variations of relative initial position L_1 of FGM region with n=1 and d=0.02m for L_1=0.01m and L_1=0.03m

Other interesting analysis involves the variation of relative position of the FGM region in the bar, maintaining its length d = 0.02m and the same micro structural composition, by using n=1. By analyzing the deformation fields it is possible to note that presents a significant reduction in its magnitude when migrate the FGM relative position in the bar when L_1 = 0.03m, as shown figure 8c and the smoothness of the stress distribution in this FGM region, as shown figure 8d, as well as the reduction the deformation gradient. This fact occurs due to major ceramic volume in the bar acting to attenuate the stress field in despite of its thermo mechanical properties.

As a first conclusion to be drawn, one can observe that the parameters L_1, d and n affect significantly the performance in thermal barriers acting to minimize the stress and deformation amplitude in these structures. An optimal choice of these parameters is necessary to establish a best configuration the FGM structure to take care of the desirable technical requirements.

5. Final remarks

With intention to apply the elaborated solution method, a sufficiently complex problem is presented that consists of the atmospheric re-entry problem. After its agreement, was possible the accomplishment of some interesting numerical simulations to describe the thermodynamic behavior of a FGM bar, in an one dimensional case, representing a thermal protection system for a space vehicle. Through the shown results in item 4, it was possible to acquire certain knowledge of the application of FGM materials in thermo elastic structures. However, for the case of the re-entry problem, the presented results show a qualitative accompaniment of the phenomenon, not representing quantitatively the evolution of the state variables that describe the presented problem.

We observe that variations the essential parameters which describe the physics properties of FGM material, we can establish the optimal configuration of this material to withstand high temperatures and thermal shocks. A significant improvement of interfacial resistance is verified with variations these parameters. An optimization process is directly associated to FGM characterization.

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7. References

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