A Study on the Numerical Simulation of Thermo-Mechanical Behavior of the Novel Functionally Graded Thermal Barrier Coating under Thermal Shock

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Abstract: An attempt was made to investigate the thermal and residual stress distribution in a novel three layer ($La_2Zr_2O_7$/8YSZ/NiCrAlY) during a real-like heating regime which includes heating, service time and final cooling. For achieving maximum accuracy and consistency in calculation of thermal and mechanical properties of hybrid coating system, all related and required properties were introduced to the software in temperature-dependent mode. Element modification approaches like mass scaling leads to a considerable reduction in running time while satisfying and not violating accuracy and converging criteria and constrains. Applying adaptive hybrid meshing techniques which applies both mesh–part dependency and independency during numerical iterative solution avoids element distortion and diverging in coupled problem. Heat flux and nodal temperature contours indicated that, most of damaging and harmful thermal load and residual stresses concentrate on ceramic top coats and this may lead less harm and life time reduction in the substrate.

Keywords: Finite Element Simulation, Residual Stress, Thermal Barrier Coating, Thermal Shock

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1 INTRODUCTION

In aerospace industry, achieving higher efficiency for aircraft engines working in high temperatures has always been an important case to focus [1]. Thermal barrier coatings (TBCs) are extensively used as insulation materials protecting the underlying metallic structure of a gas turbine blade [2-3].

The typical TBC is composed of double layers including the bond coat and top coat [4]. The bond coat is MCrAlY (where M = Ni and/or Co). The top-coat is often composed of yttria stabilized zirconia (YSZ) [5]. The major disadvantages of YSZ are the limited operational temperature of 1473K for long-term application due to the phase transformation, sintering induced volume shrinkages and raise the elasticity modulus [6].

To overcome these, the search for new materials has been intensified in the last decades and since then, zirconate-based TBCs are expected to be the candidate materials for the future application in aircraft, turbine and other high temperature components due to its low thermal conductivity, high stability and high sintering resistibility at high temperature[7], [8]. $La_2Zr_2O_7$ (LZ) is one of the candidate materials [9].

Functionally graded materials (FGMs) have been attracting a great deal of attention as thermal barrier coatings (TBCs) for aerospace structures working under super high temperatures and thermal gradients [10]. FGMs are ideal for applications involving severe thermal gradients because the microstructural grading of FG- TBCs could be adjusted to help reduce the mismatch in thermomechanical properties, which induce high thermal stresses in the structure [11], [12-13]. In addition, some aspects in tribological overview involving adhesion [14], corrosion [15] and oxidation [16] can be improved by using such materials. So far, little investigation has been focused on the thermal shock behavior of the double-ceramic-layer (DCL) TBCs [16].

In this study, an attempt was made to investigate the thermal and residual stress distribution in a novel three layer ($La_2Zr_2O_7$/8YSZ/NiCrAlY) during a real-like heating regime which includes heating, service time and final cooling. The application of functionally grading strategy was common in surface engineering, but, it is quietly rare in the literature to investigate the numerical aspects of functionally graded thermal barrier coatings with novel Zirconate composition as duplex ceramic layer TBCs. In addition, the concept of mass scaling was utilized in intelligent time reduction in numerical solution without losing accuracy.

2 NUMERICAL PROCEDURE

Finite element numerical method was used in this study to investigate residual stress in the double layer ceramic layer (DCL) thermal barrier coating shown in Fig. 1. The selected functionally graded TBC system used in this research possess the following layers with thickness of 100 mm for each: an Inconel 738 substrate, a NiCoCrAlY bond-coat (BC), 50% BC + 50% YSZ, Yttria Stabilized Zirconia (YSZ) top-coat as first ceramic layer, 50% YSZ + 50% LZ and Lanthanum zirconate (LZ) as second ceramic layer (Fig. 2).

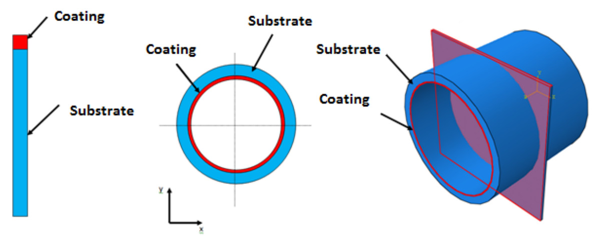

Fig. 1 TBC calculation domain

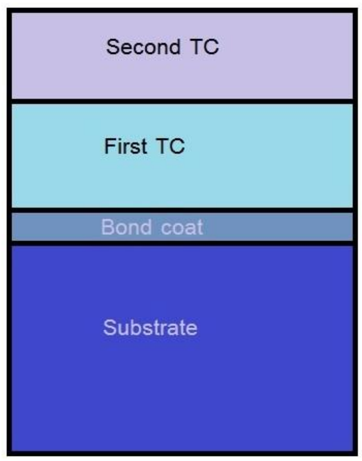

Fig. 2 Modern double layer ceramic layer

In the current research, three initial assumptions were made during modeling in commercial package. Firstly, perfect bonding between layers, second, the effect of porosity is neglected and no thermal resistance is present between layers. In order to satisfy the last mentioned constraint, a tie technique in the package was utilized that keeps the links between interface nodes during thermal loads. For modelling, material behaviour is mdscribed with temperature- dependent isotropic homogenous mode.

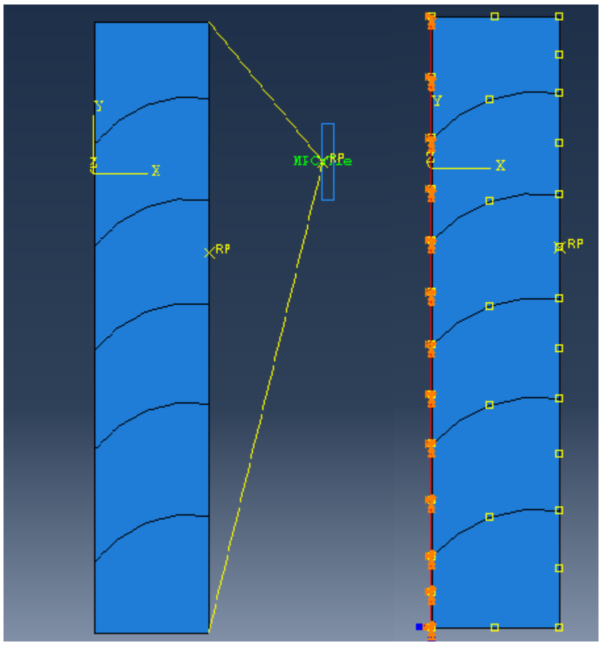

Fig. 3 Assigning symmetry and periodic boundary condition

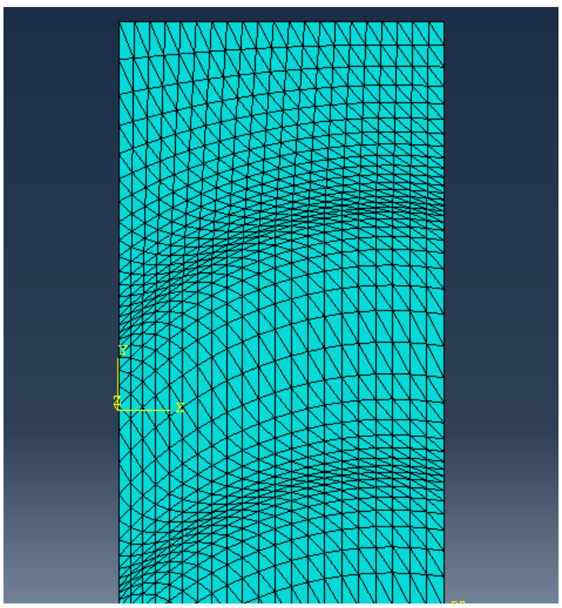

Fig. 4 Biased mesh generation in the interfaces

It should be noted that, all interfaces are modeled using sinus–like interface with a specific wavelength. For time reduction, the calculation domain assumed to be a half of original wavelength. In addition, having considered real world configuration, two useful boundary condition of symmetrical and Multi-Point Constraint (MPC) was assigned to the left and right sides of domain, respectively. MPC allow all nodes to vibrate just with each other in a specific way. Fig. 3 shows this strategy for finite element meshing geometry; mesh type is quadratic six nodes triangular elements with plane strain mode with reduced integration. To extract calculated values in interfaces, the interface regions have been meshed with a reelativly smaller element size using biased mesh technique in one direction (Fig. 4).

Thermal cycle on the top-coat surface consists of three stages which are shown in Fig. 5, i.e. the heating stage from 25°C to 1400°C in 300 s, followed by a service at 1300°C and finally, a cooling stage from1300°C to 25°C in 300s. In opposite side, convective transfer by the surrounding air is utilized with a coefficient of convection equal to18 W/m^2 K.

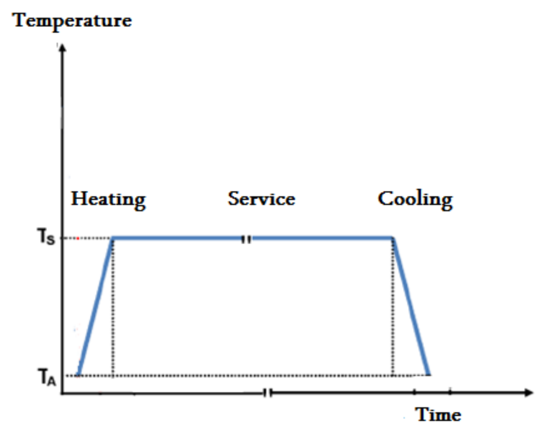

Fig. 5 Thermal cycle strategy loaded to the top ceramic coating

3 RESULTS & DISCUSSION

3.1. Optimization of numerical simulation

For solving a quasi-static problem, the values of internal and kinetic energy should be compared. In this regard, the fraction of kinetic energy to internal energy should stay approximately less than 5 to 10 percent all over process. History output for internal and kinetic energy was plotted and subsequently, combined in one graph and is compared. Fig. 6 indicates both energies with respect to each other.

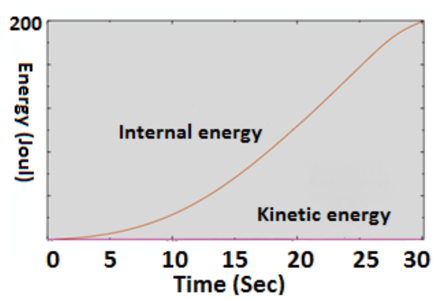

Fig. 6 Evaluation of kinetic and internal energy

Comparing the process internal and kinetic energy, it is obvious that in all steps of forming, internal energy is quite higher than kinetic energy where kinetic energy is only tiny fraction of total consumed energy. Therefore, it can be concluded that, performed analysis can be taken into account as a quasi-static type and a mass scaling method reduce solving time without any problem error. Furthermore, kinetic graph reaches its Maximum at the process middle stage where this indicates that consumed energy at these times was used for accelerating the process.

During high amount of distortion, large strain values are induced into the model meshing domain during stress induction and this can cause the solution procedure to stop after a specific solution attempt in numerical iterative solution. For doing this, ALE adaptive meshing is used as an efficient and effective method for avoiding excessive distortion of element and reaching the element mass to zero which leads to stop solution tracing. In this useful technique, distortion is independent of model deformation and because of that, the quality of elements stay in good conditions. When strain is induced to the model, only the node coordinates of elements moves and the geometry and topological feature of elements experience no change. By avoiding excessive distortion, a meaningful and appropriate frequency and sweeping factor have to be considered while implementing elements adaptively in order to impose large destructive elements. The former identifies the number of increments after that, re-meshing takes place and the later parameter gives the number of orientation change in each re-meshing attempt. A set of (10,3) was decided to be used for frequency and sweep setting for analysis [17].

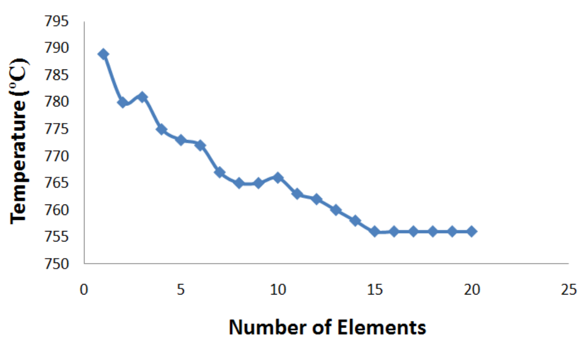

Fig. 7 Mesh sensitivity analysis for BC coating analysis

3.2. Stress analysis

Before doing the main analysis, a mesh sensitivity analysis is required to ensure that, extracted results are independent of mesh size and element configuration prior to main analysis. Small size leads to unnecessary increase in solving time and consequently in numerical errors and in contrast, large meshing size causes some error in problem solving. Having this in mind, an edge of coating was selected for this purpose and a range of element number (interpreted as element size) was tested and an optimum mesh size was selected. The optimum size can be assigned to the smallest mesh size, in which the trend of a meaningful parameter (temperature in this study) in graph starts to become plateau. Fig. 7 shows the temperature change with element size in this research which gives a proper sensitivity analysis [17].

As can be seen in Fig. 8, in thermal load time to the double layer thermal barrier coating, concentration of heat is located in the upper section of the coating system where this means that, all lower part especially substrate are away from thermal damages which is in agreement with the results achieved by similar studies [8], [14]. In this matter, utilizing this coating, heat transfer is limited to the heat resistive ceramic parts and bond coat and substrate experience lower temperatures and because of this, higher working temperatures can be experienced especially in aerospace turbine applications.

Having protected the substrate from thermal load and keeping in relatively lower temperatures cause in better fatigue life and also, increasing lifetime and decreasing maintenance cost. Improved fatigue life was also mentioned in many researches as a consequence of using functionally graded coatings in turbine hot section [16]. Fig. 9 shows the heat flux dissipation in thermal barrier coating assembled in functionally graded mode. Just like the temperature distribution, existences of double ceramic layer keep thermal load and thermal energy on itself and as a consequence, thermal equilibrium of upper hot parts with hot air of outside achieve in shorter time. The equilibrium between ceramic coats and outer air avoids thermal diffusion to the bond coat and more important, nickel-base substrate. As a definition, a thermal barrier was established when thermal equilibrium is gained in the two ceramic layers on top of the coating and this has good effects on maximum temperature.

Figs. 10 and 11 show the stress distribution contours in TBC system after cooling step considering sinusoidal interface of MCrAlY/50% McrAlY + 50% YSZ. Because of higher value of thermal expansion in bond coat with respect to the ceramic layer, compressive strength is induced in peak regions and tensile strength in valley and a slow transition is seen while approaching from peak to valley. In FGM coating, LZ constituent present in YSZ marix compensate the metallurgical flaws of this layer and just like YSZ section in McrAlY do the same and this cause a better isolation function and less downward thermal diffusion. Additionally, more similarities in thermal expansion of FGM layers lead to better adhesion between layers and less stress concentration in interfaces which are feeble regions of coating. This may cause delay of crack initiation and fatigue crack growth rate in the interface [15].

As a fabulous point in FGM material, it can be mentioned that, the utmost stress in the structure is just about half of conventional TBC structure and for that; it can be recommended as an innovative proposition of elevated temperature material. As a comparison of this work with related studies mentioned in the references, the usage of FG- TBC has been mentioned as a factor for improving corrosion and environmental damages. Also in some of them, the formation of thermally grown oxide layer was considered as a deteriorating parameter that reduces the life time of coating. However, in FGM, this oxide layer was not formed in a specific concentrated place and improve life time. Some investigations focus on the crack growth and fracture mechanism of the interfaces that influence the stress relaxation and also spallation. In this study, the zones with the maximum stress values take account as crack initiation places both in low cycle fatigue and first and second fracture modes. In addition, in a research by Jha et al. [15], the effect of ceramic layer porosity on trans-layer fracture of coating was studied and the effect of process technology and also heat treatment after fabrication was explained.

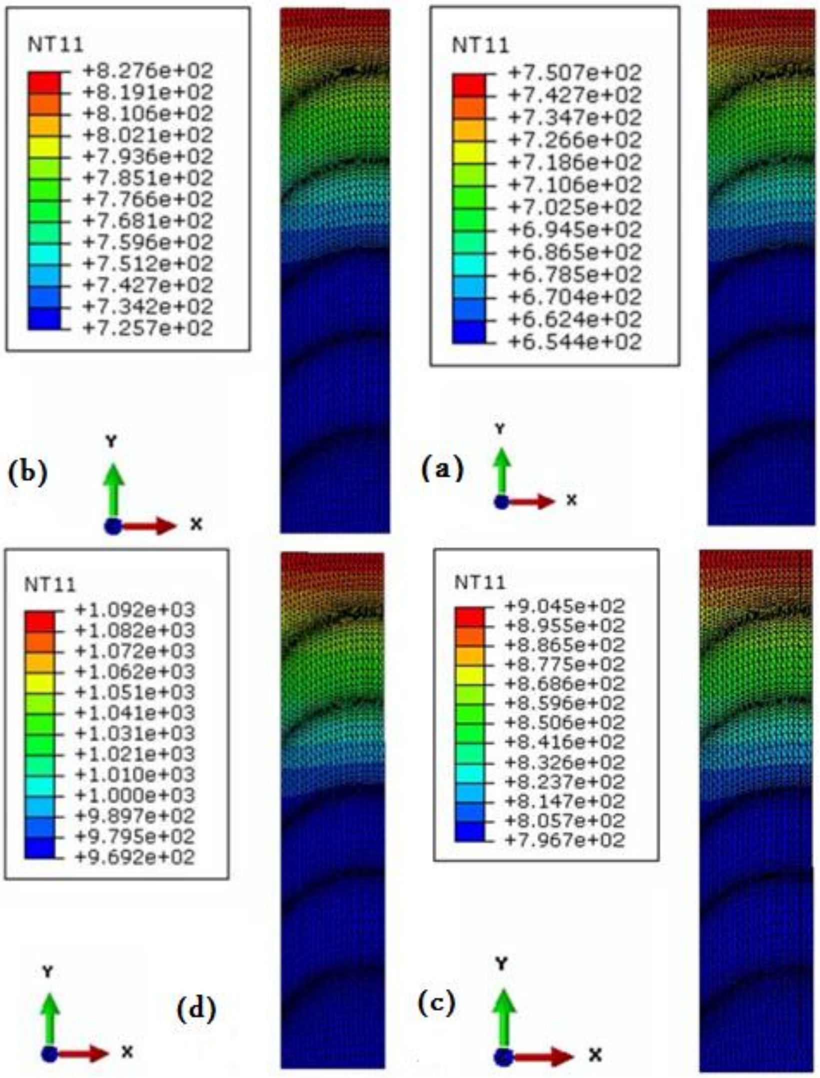

Fig. 8 Temperature distribution in TBC in (a) t = 150 s, (b) t = 175 s, (c) t = 200 s, (d) t = 225 s

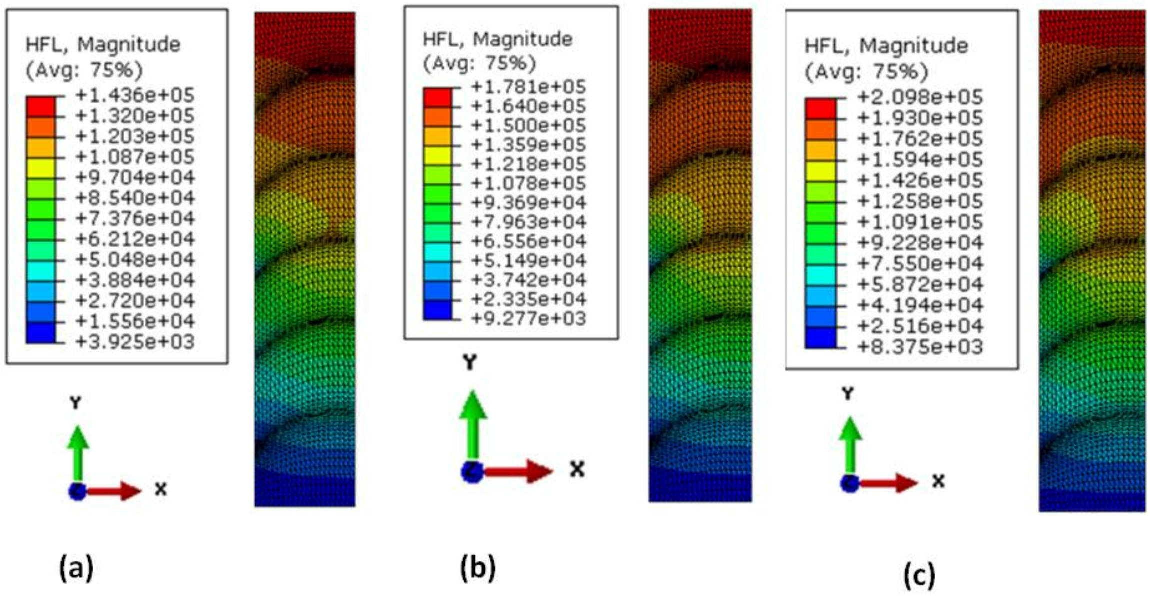

Fig. 9 Heat flux in TBC in (a) t = 150 s, (b) t = 175 s, (c) t = 200 s, (d) t = 225 s

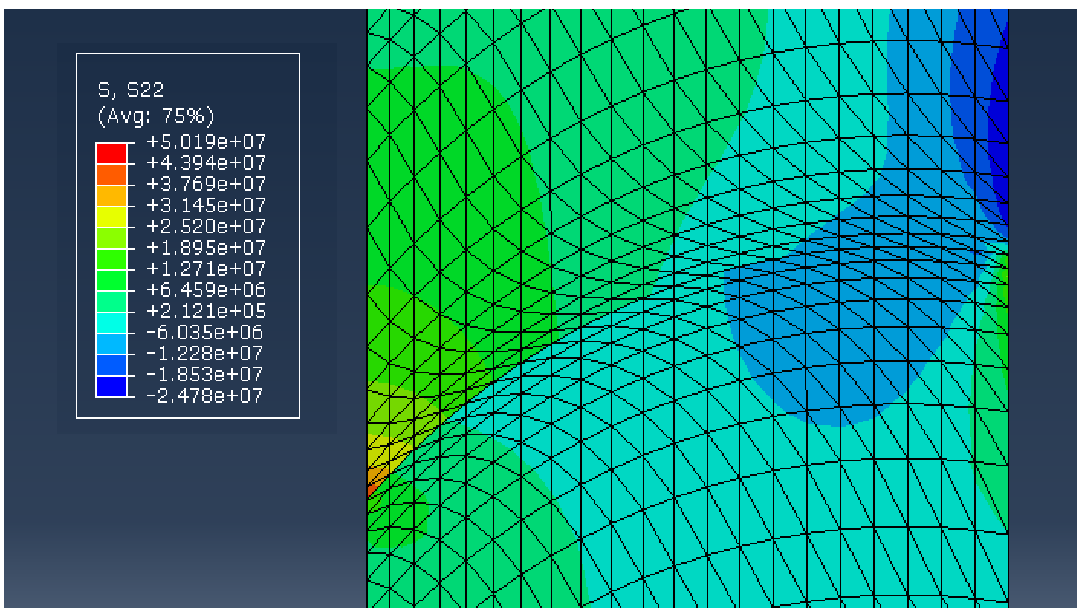

Fig. 10 Heat Stress in sinusoidal interface of MCrAlY/YSZ

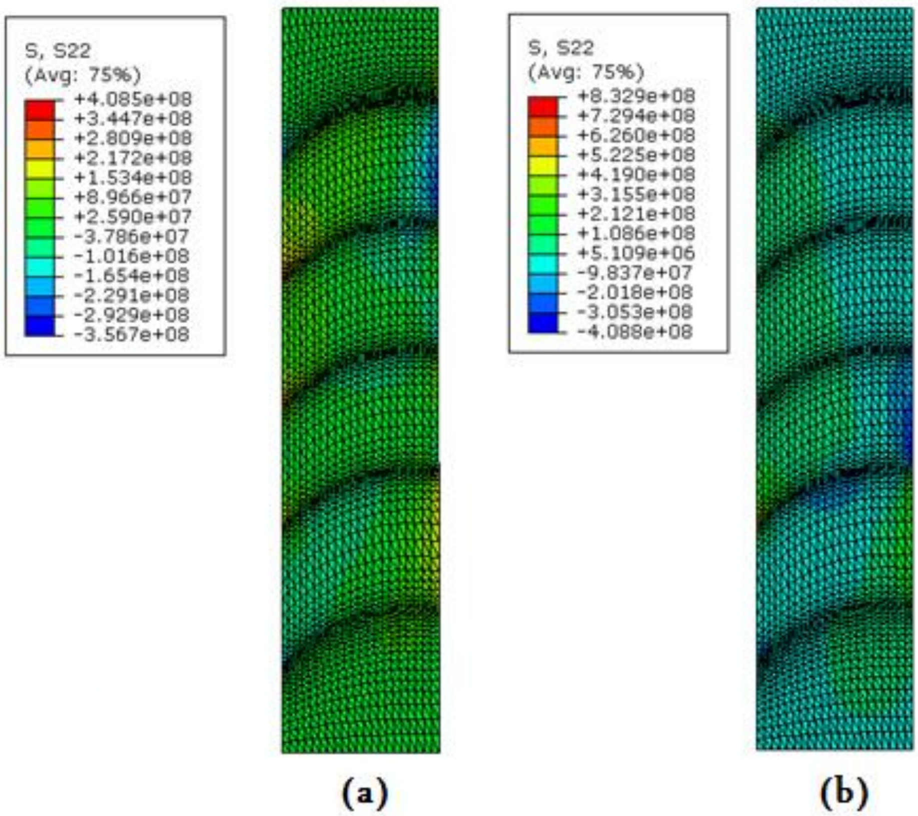

Fig. 11 Stress distribution in (a) GGM –TBC, (b) conventional TBC

4 CONCLUSION

The temperature and stress distribution in a novel three layer (La2Zr2O7/8YSZ/NiCrAlY) during an actual heating regime was studied. Results revealed that, most of damaging and harmful thermal load and residual stresses concentrate on ceramic top coats and this lead to less harm and life improvement in substrate. FGM strategy reduced the stress values in the coating to half of its value in conventional coating. Less difference in thermal expansion improve the adhesive bonding between different ceramic/ceramic and ceramic/metal interfaces and also decrease the risk for crack initiation and propagation. Mass scaling method reduce the running time while satisfying convergence and accuracy criteria and the approval of using such method was tested by comparing internal and kinetic energy during process.

REFERENCES

[1] Saeedi, B., Sabour, A., Ebadi, A., and Khoddami, A. M., “Influence of the Thermal Barrier Coatings Design on the Oxidation Behavior”, J. Mater. Sci. Technol., Vol.25, No.4, 2009, pp. 499-507.

[2] Di Girolamo, G., Blasi, C., Brentari, A., and Schioppa, M., “Microstructure and thermal properties of plasma-sprayed ceramic thermal barrier coatings”, Studi & ricerche, Research papers, 2013.

[3] Khor, K. A., “Thermal properties of plasma-sprayed functionally graded thermal barrier coatings”, Thin Solid Films, Vol. 372, No.1-2, 2000, pp. 104-113.

[4] Wang, L., Wang, Y., Sun, X. G., He, J. Q., Pan, Z. Y., and Wang, C.H., “Microstructure and indentation mechanical properties of plasma sprayed nano-bimodal and conventional ZrO_2-8wt%Y_2O_3 thermal barrier coatings”, Vacuum, Vol. 86, No. 8, 2012, pp. 1174-1185.

[5] Vaßen, R., Ophelia Jarligo, M., Steinke, T., Emil Mack, D., and Stöver, D., “Overview on advanced

thermal barrier coatings", Surface & Coatings Technology, Vol. 205, No.4, 2010, pp. 938-942.

[6] Baig, M. N.,.Khalid, F. A,.Khan, F. N, and Rehman, K., "Properties and residual stress distribution of plasma sprayed magnesia stabilized zirconia thermal barrier coatings", Ceramics International, Vol. 40, No. 3, 2014, pp. 4853-4868.

[7] Wang, L., Wang, Y., Sun, X. G, He, .J. Q., Pan, Z.Y., and Wang, C. H., "Thermal shock behavior of 8YSZ and double-ceramic-layer $La_2Zr_2O_7$/8YSZ thermal barrier coatings fabricated by atmospheric plasma spraying", Ceramics International, Vol. 38, No.5, 2012, pp. 3595-3606. .

[8] Wang, L., Wang, Y., Zhang, W. Q., Sun, X. G., He, Z. Y. Pan, and Wang, C. H., "Finite element simulation of stress distribution and development in 8YSZ and double-ceramic-layer La2Zr2O7/8YSZ thermal barrier coatings during thermal shock", Applied Surface Science, Vol. 258, No.8, 2012, pp. 3540- 3551.

[9] Matsumoto, M., Aoyama, K., Matsubara, H., Takayama, K., Banno, T., Kagiya, Y., and Sugita, Y., "Thermal conductivity and phase stability of plasma sprayed ZrO_2–Y_2O_3–La_2O_3 coatings", Surface & Coatings Technology, Vol. 194, No. 1, 2005, pp. 31-35.

[10] NAGA, S. M., "Ceramic matrix composite thermal barrier coatings for turbine parts", In book: Advances in Ceramic Matrix Composites., Edition: 1, Chapter: 21, Publisher: Woodhead Publishing Limited, Editors: I.M. Low, pp.524-533.

[11] Khoddami, A. M., Sabour, A., Hadavi, S. M. M., "Microstructure formation in thermally-sprayed duplex and functionally graded NiCrAlY/Yttria-Stabilized Zirconia coatings", Surface & Coatings Technology, Vol. 201, No.12, 2007, pp. 6019–6024.

[12] Mahamood, R. M., Akinlabi Member, E. T., IAENG, M. Shuklav, and Pityana, S, "Functionally Graded Material: An Overview", Proceedings of the World Congress on Engineering, 2012(WCE 2012, July 4 - 6, 2012, London, U.K.).

[13] Kieback, B., Neubrand, A., and Riedel, H., "Processing techniques for functionally graded materials", Materials Science and Engineering A, Vol.362, No. 1-2, 2003, pp. 81–105.

[14] Watremetz, B., Baietto-Dubourg, M. C., and Lubrecht, A. A., "2D thermo-mechanical contact simulations in a functionally graded material: A multigrid-based approach", Tribology International, Vol. 40, 2007, pp. 754–762.

[15] Jha, D. K., Kant, T., and Singh, R. K, "A critical review of recent research on functionally graded plates", Composite Structures, Vol. 96, 2013, pp. 833-849.

[16] Lee W. Y, Stinton, D. P., "Concept of Functionally Graded Materials for Advanced Thermal Barrier Coating Applications", Journal of the American Ceramic Society, Vol. 79, No. 12, 1996, pp. 3003-3012.

[17] Helwany, S., "Applied Soil Mechanics with ABAQUS Applications", John Wiley & Sons; 1 edition, 2007.