Finite Element Simulation of Temperature Distribution and Residual Stresses in New Thermal Barrier Coating La₂Zr₂O₇/8YSZ

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1-Introduction

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

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

To overcome these drawbacks, the search for new materials has been intensified in recent years 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 their low thermal conductivity, high stability and high resistance to sintering at high temperature. La₂Zr₂O₇ (LZ) is one of the candidate materials.

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. In this study, an attempt was made to investigate the thermal and residual stress distribution in a novel three-layer (La2Zr2O7/8YSZ/NiCrAIY) TBC during a real-like heating regime which includes heating, service time and final cooling.

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2- Experimental

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).



Figure 1 TBC calculation domain

Second TC
First TC
Bond coat
Substrate

Figure 2 Modern double layer ceramic layer

The thermal cycle on the top-coat surface consists of three stages which are shown in Fig. 3, i.e. the heating stage from 25 to 1400 °C in 300 s, followed by a service at 1300 °C and finally, a cooling stage from 1300 to 25 °C in 300 s. On the opposite side, convective transfer by the surrounding air is utilized with a coefficient of convection equal to $18 \text{ W/m}^2 \text{ K}$.

3- Results and Discussion

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 throughout the process. History output for internal and kinetic energy was plotted

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and subsequently, combined in one graph and is compared. Fig. 4 indicates both energies with respect to each other.





Figure 4 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 takes up a small fraction of total consumed energy. Therefore, it can be concluded that the performed analysis can be taken into account as a quasi-static type and a mass scaling method to reduce the solving time without any problematic error. Furthermore, the kinetic graph reaches its maximum at the middle stage of the process where this indicates that the consumed energy at these times was used for accelerating the process.



As can be seen in Fig. 5a, concentration of heat is located in the upper section of the coating system where this means that all lower parts, especially the substrate, are shielded from thermal damages which is in agreement with the results achieved by similar studies. In this matter, utilizing this coating, heat transfer is limited to the heat resistive ceramic parts and the bond coat and the 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 it at relatively lower temperatures lead to superior fatigue life and also lower protection cost. Fig. 5b shows the heat flux dissipation in the thermal barrier coating. Just like the temperature distribution, the co-existences of the double ceramic layer keep thermal load and thermal energy on itself and as a consequence, thermal equilibrium of upper hot parts with hot outside air is achieved in a shorter time period.

Fig. 6 shows the stress distribution and distortion in the TBC system. Because of higher value of thermal expansion in the 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. More similarities in thermal expansion of FGM layers lead to better adhesion between layers and less stress concentration in interfaces which are weak regions of the coating. This may cause delay of crack initiation and fatigue crack growth rate in the interface.



Figure 6 a) stress distribution and b) distortion in TBC system

4. Conclusion

The temperature and stress distribution in a novel three-layer (La2Zr2O7/8YSZ/NiCrAlY) TBC during a heating regime was studied. Results revealed that most of the damaging and harmful thermal load and residual stresses concentrate on the ceramic top coats and this lead to less harm and enhanced life improvement in the substrate. FGM strategy reduced the stress values in the coating to half of its value in conventional coating. Less difference in thermal expansion improves the adhesive bonding between ceramic/ceramic and different ceramic/metal interfaces and also decreases the risk for crack initiation and propagation. Mass scaling method reduces 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 the process.