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Numerical simulation of relation between interface topography and residual stress in thermal barrier coatings

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Abstract. With respect to thermal barrier coating, the analysis of interface cohesion and residual stress is important to the life of TBC from mechanical view point. Up to now, there is not a model of describing interface cohesion. In the paper, we give a simple model of computing residual stress and study the residual stress of TBC with ANSYS. The distribution of the residual stress in different interface topography and the relationship between the residual stress and the interface topography dimension are presented.

Keywords: thermal barrier coatings; numerical simulation; residual stress; interface topography.

1. Introduction

Based on the requirement of improving the cost and reliability of gas engine, the application and research of ceramic materials in the firebox components of gas engine were considered widely in recent years, the technology of thermal barrier coatings (TBC) has become a developing direction of high temperature proof in engine thermal components. During either the thermal cycles or the plasma-spray deposition, the thermal stress that was generated in the coating system due to big thermal expansion differences in the interface can induce the ceramic coating fracture and even spall along the interface (Taylor 1998, Ma *et al*. 2003). So how to strengthen the bonding of the coatings is a key problem about the life of TBC (Freborg 1998, Persson 2001). In the practical application, roughening surface of substrate is an effective method (Hsueh 1999, 2000, Ahrens 2002, Kawamura 2004), but this method can induce tensile stress normal to the interface in the ceramic coating during thermal cycles and the plasma-spray deposition, and high tensile stress is thought as one of major factor of spallation. It means roughening of surface that strengthens the bonding of the coatings may

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introduce the negative factor on the life of TBC system simultaneously (Sfar 2002). So it is necessary to investigate the mechanical performance of interface topography on the stress in TBC. As we know, there are two main factors to induce TBC unavailable. One is oxidization of interface between TBC and substrate; the other is strain misfit between different materials. Hsueh *et al.* (2000) studied the effect of oxide scale to residual stresses in TBC. They concerned the oxide layer. We mainly study the effect of interface topology to residual stresses in TBC from mechanical viewpoint.

2. The developing principle of residual stress during the plasma-spray deposition

In the present paper, we mainly study the thermal barrier coatings made by Plasma-Spraying. We simulate the relation between the residual stresses that generate in the coating system during the plasma-spray deposition and the interface topography (Nair 2000, Nusair 2003).

In general, the developing process of the top coating during deposition can be divided into two phases: The first phase is the solidification of the coating. The second phase is the course of cooling to room temperature of the whole coating system. After the end of spraying, thawy dope has been solidified. In the first phase, the substrate absorbs heat and expands during the solidification of the thawy dope. Because the substrate had been heated to the same high temperature, the thermal expansion should not be very big. At the same time, the solid coating has not formed completely, and we can think the whole coating system has not been constrained during the course of thermal expansion. It can be thought that there is not any thermal stress in the substrate or the coating during this phase. The structure is stress free. In the second phase, because the thermal expansion coefficient (CTE) of the substrate is much bigger than that of the coating, the contract rate of the substrate is much bigger than the contract rate of the coating, which will result in the residual stress in the coatings finally. So the development of the residual stress is due to the thermal expansion misfit between the coating that was become into solid and substrate from the state of stress free (the temperature of stress free is the controlled temperature of the heated substrate during the spray) of high temperature to the room temperature. It is reasonable to regard the temperature change of initial temperature (the temperature of stress free) and ultimate temperature (room temperature) as the thermal load of models.

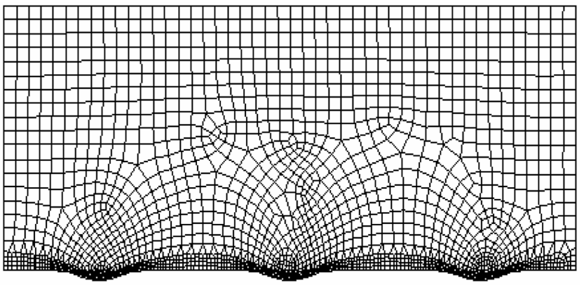
3. Numerical simulations

A typical plasma-sprayed thermal barrier coating structure of two layers is adopted (Wang 2001). The top coating is the ceramic coating, its main component is ZrO_2, preventing the substrate from working under the high temperature. Between the ceramic coating and the substrate is McrAlY bond coating, which improves the physical harmony between the substrate and the ceramic coating, and prevent the substrate from oxidation. During the thermal cycle, the fracture in the ceramic coating that result in the failure of plasma-sprayed thermal barrier coating is parallel to and near the interface of bond coating. So it is important to analysis the stress in the coating at the interface or near the interface. An issue regarding the effect of the interface topography on the residual stresses in the ceramic coating of the plasma-sprayed thermal barrier coating is hence raised. If the stress normal to the interface in the ceramic coating is tensile stress, it may result in the fracture and spallation of the ceramic coating. The interface topography can have various dimensions. Another issue regarding the effect of interface topography dimension on the tensile stress normal to the interface in the ceramic coating is hence raised. For the sake of simplicity, we select the substrate as length is far great than width, and study the cross section being perpendicular to length direction. So it is approximately considered as plane strain case.

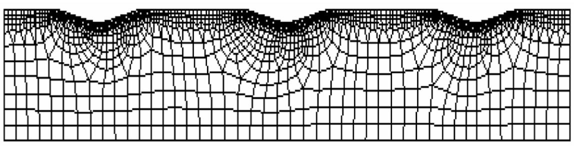
The purpose of the present study was to answer the above two issues. To achieve it, The ANSYS of finite element analysis software is utilized for numerical simulation. First, a flat interface is simulated; second, in order to study the effect of the interface topography on residual stress, numerical simulations are performed on the following several models: (1) A periodic sinusoidal curve is adopted to simulate the interface topography. (2) The sinusoid interface removed valley portion is simulated. (3) The sinusoid interface removed peak portion is simulated; third, numerical simulations are performed on several special models to determine the effects of the interface topography dimension on the tensile stress σ_y normal to the interface. The effect of the curvature of interface topography is examined by simulating two sets of periodic sinusoidal curve models with different period length, same amplitude and different amplitude, same period length, respectively. The effect of the sharp corner in interface is examined by comparing the tensile stresses σ_y normal to the interface in the ceramic coating in the topographies of the sinusoidal interface removed peak portion, the sinusoidal interface removed peak portion and smoothen and the smooth sinusoid interface with no sharp corner. The effect of the interface topography height is examined by simulating a set of semicircular topography on top with different height. The effect of the interval of convexes or concaves (or the interaction of topography) is examined by simulating a set of semicircular top convexes and a set of smooth sinusoid interface with no sharp corner which have the same height and different intervals, respectively.

3.1 Model description

As the research object in the paper, the plasma-sprayed thermal barrier coatings system consists of a ZrO_2 ceramic coating and Ni-22Cr-10Al-1Y bond coating. Thickness of the ceramic coating and the bond coating are 250 μm and 100 μm, respectively. The substrate is René N5, a single-crystal



(a)



(b)

Fig. 1 free meshing (a) the ceramic coating (b) the bond coating

Table 1 Material constant

	The ceramic coating	The bond coating	The substrate
Young modulus, E (Gpa)	50	200	213
Poisson's ratio v	0.1	0.3	0.25
CTE ($\times 10^{-6}$/°C)	10	15.2	14.5

Ni-based super alloy. The substrate is much thicker than the ceramic coating and the bond coating, so the thermal strain of the substrate is used as the boundary condition at the right and the left edges of the plots in Figs. 1(a) and (b) to constrain its deformation in the x-direction and the analysis object used in calculation is the ceramic coating and the bond coating.

For simplifying, we assume the thermal/mechanical properties used in calculation are constant. They are listed in the Table 1.

Because the dimension in the direction normal to the cross section is much bigger than that in the direction of the cross section, this question is considered as a plain strain question. In the present study, 1150°C (the controlled temperature of the heated substrate during the spray) is the temperature of stress free (i.e., the initial state) of TBC system. The residual stress is calculated from 1150°C to room temperature (25°C). The temperature change (i.e., the thermal load exerted on models) used in calculating the thermal strain is −1125°C (25°C-1150°C). In the present study, a large-scale finite element analysis software ANSYS is utilized for numerical simulation. The model consists of two parts; each one is made of polygonal structure. The top coating is ceramic coating, its thickness is 250 μm. The bottom coating is bond coating, its thickness is 100 μm. The interface in the middle is simulated by the topography mentioned above. Because the shape of the structure is special, the preprocessing module PREP7 of ANSYS is utilized to mesh the structure with freedom mode; the grid is thicker at the interface. For instance, the mesh of the sinusoidal interface removed peak portion is shown in Fig. 1.

After calculation, utilize the post processing module POST1 of ANSYS, x-axis is parallel to the interface, y-axis is normal to the interface, to plot the contour drawing in the ceramic coating with various topography in the x-direction and y-direction.

3.2 The effect of the interface topography on the residual stresses

Corresponding to various interface topography, the residual stress parallel to the interface, σ_x, in the ceramic coating is compressive stress, the residual stress normal to the interface, σ_y, in the ceramic coating is tensile stress or compressive stress. For a flat interface, the residual stress is parallel to the interface; the stress normal to the interface is almost zero. When the interface has the required topology, the local stress has significant variation along the irregular interface. (1) Corresponding to the interface simulated by a periodic sinusoidal curve, the tensile and compressive stress normal to the interface, σ_y, occur in regions of the peak and valley of topography, respectively. The maximal tensile stress occurs at the peak tip and the maximal compressive stress occurs at the valley tip. (2) To the sinusoid interface removed valley portion, the compressive stress of σ_y concentrating in the valley region spreads out to the flat interface region, the maximal compressive stress shifts to the zygomorphic location of peak region and the maximal compressive stress does not decrease with removing of valley. The tensile stress still occurs at the peak. (3) To the sinusoid interface removed peak portion, the tensile stress of σ_y concentrating in the peak region spreads out to the flat interface region, the maximal tensile stress shifts to the zygomorphic location of valley region and the maximal tensile stress does not decrease with removing of the peak. The compressive stress still occurs at the valley. The shift of tensile and compressive stress is because there is no force applied in y-direction. The compressive stress somewhere requires the tensile stress elsewhere to achieve mechanical equilibrium. Consequently, the tensile stress requires the compressive stress elsewhere. To the sinusoid and the sinusoid removed valley portion interface topography, the maximal compressive stress parallel to the interface, σ_x, occurs at the peak tip. To the sinusoidal interface topographies removed peak portion, the maximal compressive stress of σ_x occurring at the peak tip shifts to the zygomorphic location of valley topography region. According to above analysis we can get a conclusion: To remove the peak or the valley portions of topography simply may not be in favor of decreasing the stress normal to the interface in the ceramic coating. The high tensile stress is thought as a major factor of spallation of the ceramic coating. So an issue is hence raised whether the surface topography of a bond coating can be better designed to decrease the tensile stresses of σ_y normal to the interface in the ceramic coating. Numerical simulations are performed on model with several special interface topographies to examine the effect of interface topography dimension on the tensile stress of σ_y normal to the interface in the ceramic coating.

3.3 Effect of interface topography dimension on the tensile stress of σ_y normal to the interface in the ceramic coating

3.3.1 Effect of curvature of interface topography

The effect of interface curvature is examined by simulating two sets of periodic sinusoidal microstructure topography with different period lengths, same amplitude and different amplitudes, same period length, respectively. First, by simulating a set of periodic sinusoids with different amplitudes and same period length as the interface topography, It can be seen in Fig. 2 that the maximal tensile stress of σ_y normal to the interface increases with the amplitude under the condition of same period length; Second, by simulating a set of periodic sinusoids with different period lengths and same amplitude as the interface topography, It can be seen in Fig. 3 that the maximal tensile stress of σ_y normal to the interface decreases with the period lengths under the condition of same amplitude.

We know both the reduction of period length with the constant amplitude and the augmentation of amplitude with the same period length will result in the increase of topography curvature. So we come to a conclusion, i.e., the maximum of the tensile stress normal to the interface increases with the curvature of the topography.

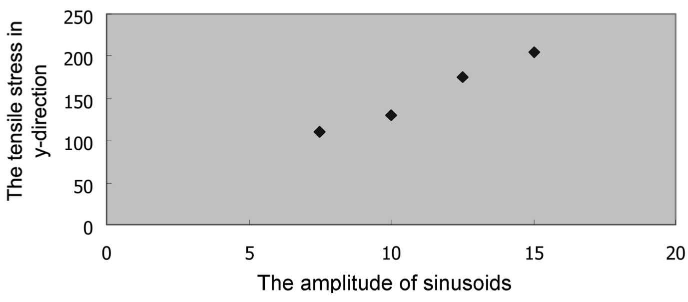


Fig. 2 Effect of amplitude to the tensile stress (x: μm, y: Mpa)

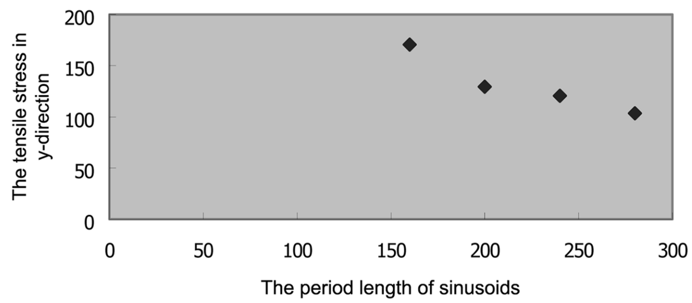


Fig. 3 Effect of period length to the tensile stress (x: μm, y: Mpa)

3.3.2 Effect of sharp corner of interface topography

To determine the effect of sharp corner, we compare the tensile stress normal to interface, σ_y, in the ceramic coating with interface topography simulated by the sinusoid removed peak portion, the sinusoid removed peak portion and smoothen and the smooth sinusoid with no sharp corner. The maximum of tensile stresses normal to the interface, σ_y, in the ceramic coating in above three models all occur at the zygomorphic location of valley regions. They are 144.878 Mpa, 106.131 Mpa and 84.29 Mpa, respectively. The reason of the distinct difference of above data is that there are sharp corners which can result in singularity at the zygomorphic location of valley portions in the interface topography of the sinusoid removed peak portion; The tensile stress normal to the interface in the ceramic coating is decreased distinctly in the interface topography of the sinusoid removed peak portion and smoothen at the zygomorphic location of valley portions; In the topography simulated by the smooth sinusoid with no sharp corner the tensile stress normal to the interface is decreased obviously. It can be seen that the sharp corner affects the tensile stress markedly.

3.3.3 Effect of height of interface topography

A set of interface topographies with the same curvature and different heights are used in the present study to examine the effect of the height of interface topography. The top of the topography is a semicircular, and the height of topography is controlled by adding a rectangular block at the base of the semicircle. Using the rectangular block induces the sharp corners that will result in the singularities, so the zygomorphic locations of rectangular block bottom are smoothen. It can be seen in Fig. 4 in the case of the same curvature the maximal tensile stress normal to the interface in the

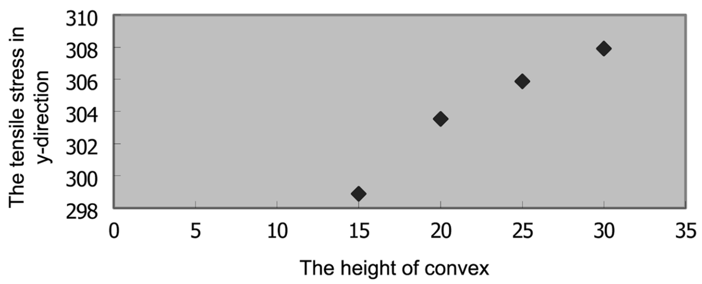


Fig. 4 Effect of the height of topography on the tensile stress (x: μm, y: Mpa)

ceramic coating at the tip of the semicircular topography increase with the height of interface topography. But the effect of the height of interface topography on the tensile stress normal to the interface in the ceramic coating is not distinct.

3.3.4 Effect of interval of interface topography (or effect of interaction of topographies)

Two sets of interface topography are used in the present study to examine the effect of the interval of the interface topography. In the first set, a set of semicircular peaks with the same height and different interval, a single semicircular peak is representative of convex topography, are simulated to determine the effect of interval of convex topography on the tensile stress in the ceramic coating. The simulated results of σ_y in the ceramic coating at the tip of the semicircular topography are shown in Fig. 5. It can be seen that the tensile stress increase with the interval of peaks in the convex topography. So the tensile is maximal in a single semicircular top.

In the second set, a set of smooth sinusoid interface with no sharp corner, the same depth and different interval, and a single valley is representative of concave topography, are simulated to determine the effect of interval of concave topography on the tensile stress in the ceramic coating. The simulated results of σ_y in the ceramic coating at the tip of the smooth sinusoidal interface with no sharp corner are shown in Fig. 6. It can be seen that the tensile stress decrease with the interval of valley in the concave topography. So the tensile is maximal in the topography whose interval is minimal.

Based on above analysis we come to a conclusion: In the convex topography, the interaction of topographies decreases the tensile stress normal to the interface in the ceramic coating, that means the tensile stresses increase with the interval of peaks in the convex topography; In the concave topography, the interaction of topographies increases the tensile stress normal to the interface in the ceramic coating, that means the tensile stresses decrease with the interval of valleys in the concave topography.

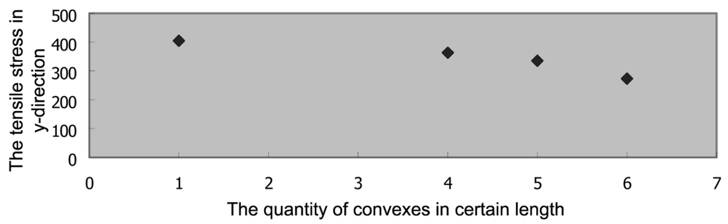


Fig. 5 Effect of the interval of convexes on the tensile stress (y: Mpa)

Fig. 6 Effect of the interval of concave topography on the tensile stress (y: Mpa)

4. Conclusions

In a plasma-sprayed TBC system, for a flat interface, the residual stress in the ceramic coating is parallel to the interface; the stress normal to the interface is almost zero. However, when the interface has rough topography required in strengthening the bonding of the coatings, the stress normal to the interface is not zero. The local stress has significant variation along the irregular interface. In section 3.2 of numerical simulation, we know the effect of interface topography on the distribution of stress. The tensile and compressive stress normal to the interface, σ_y, occur in regions of the peak and valley, respectively. Remove peak portion of topography, the stress concentrating in the peak region is spread out to the flat interface region; remove valley portion of topography, the stress concentrating in the valley region is spread out to the flat interface region, But the maximal tensile stress normal to the interface in the ceramic coating does not decrease with the shift of stress , that means removing the peak or the valley portions simply may not be in favor of decreasing the stress normal to the interface in the ceramic coating. In section 3.3 of numerical simulation, the interfaces with several special topographies are simulated to examine the effect of interface topography dimension on the tensile stress of σ_y normal to the interface in the ceramic coating. We come to conclusions (1) The tensile stress normal to the interface in the ceramic coating increases with the curvature of interface topography; (2) The tensile stress normal to the interface in the ceramic coating is affected by the sharp corner markedly, so the sharp corner that will result in the singularities should be avoided in interface topography; (3) The tensile stress normal to the interface in the ceramic coating increases with the height of interface topography. But the effect of the height of interface topography on the tensile stress is not distinct; (4) The tensile stress normal to the interface in the ceramic coating is affected by the interaction of topographies, In the convex topography, the maximal tensile stress increase with the interval of peaks; in the concave topography, the maximal tensile stress decrease with the interval of valleys.

The problem is that for a flat interface the stress normal to the interface is almost zero. Practically it should not be zero. Maybe this is the problem of the model we selected, but the other conclusions are coincident with other researcher's conclusions and the real behavior of TBC. Next step we will build space model to substitute the plane model. It would solve the above problem. Although the space model is far complicated, we will try to do it.

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