A NUMERICAL STUDY OF INFLUENCE OF INTERNAL CRACK ON THERMAL PROPERTY OF APS-TBCs

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ABSTRACT
The internal crack initiation and propagation are decisive factors that dominates the failure of thermal barrier coatings under services. In this paper, TBCs samples with different crack lengths were numerically reconstructed. The temperature distribution characteristics of the surface and internal thermal barrier coatings were studied based on the coupled flow and heat transfer model of thermal barrier coatings and cooling film by using LBM-DDF method. The results show that the existence of cracks will greatly change the temperature distribution of the coating, resulting in increased temperature inhomogeneity and local sintering of the coating. This will lead to stress concentration, which can easily cause early delamination and fracture of the coating, thus affecting the durability of the coating. The results can provide a helpful reference for better technical support for life prediction of high temperature turbine blades.

INTRODUCTION
With the development of gas turbine, the limit of high temperature resistance of turbine blades has become the primary factor restricting the improvement of gas turbine efficiency. The inlet temperatures of the state-of-the-art gas turbine can achieve 1700 °C or even higher. However, the components of gas turbine cannot work properly at such extreme high temperatures (Abdelmaksoud et al., 2020). As the core technology to solve this problem, air plasma sprayed (APS) thermal barrier coatings (TBCs) and cooling film can effectively protect blades and other key components in the normal operation of turbine at high temperature, and meet their long service life and high reliability requirements (Zhang et al., 2020; Li et al., 2019; He et al., 2019; Padture, 2016; Bison et al., 2011). However, due to long-term exposure to high temperature gas shock and other harsh service environment, TBCs often peel off prematurely and cause coating failure under unpredictable circumstances, seriously affecting the safe operation of gas turbine.

To date, scholars have conducted a lot of researches on cracking problems (Weng et al., 2020; Abubakar et al., 2020; Xiao et al., 2017). The results show that the main factors that induce crack propagation in TBCs are as follows: (1) the difference of thermal and mechanical properties for the materials difference of the mismatch of thermal expansion coefficients; (2) large temperature gradient inside the coating caused by complex service environment. This will greatly affect the coating temperature distributions and lead to local thermal stress. Stress accumulates in the coating, which leads to crack initiation and propagation, resulting in coating failure. Dong et al. (Dong et al., 2018) obtained the relationship between the size of the coin-type crack inside coatings. The results found that the size of the bright spot on the coating surface by using gradient thermal cycling test and finite element simulation. It can be found that with the increase of crack diameter (from 0.4 to 4.0 mm), the surface temperature of the coating increases and the area of the
bright spot also increases in size. This indicates that the presence of crack will alter the temperature distribution of the inner coating. In fact, the residual life fraction of the coating has reached 80% when the crack propagates to 260 μm (Ahmadian et al., 2016). However, it was still not well-known how the internal crack affects the heat transfer in TBCs. Therefore, it is of great significance for online health assessment and life prediction of high-temperature blades to study the influence of crack in TBCs on heat transfer performance during service and the results can be applied for online location and size assessment of crack in TBCs.

In this study, the typical morphologies of cracks were extracted. Six TBCs samples contains cracks with different length were reconstructed by the optimized quartet structure generation set (QSGS) method. The conjugate flow and heat transfer model of TBCs and cooling film was established and the temperature distribution characteristic of the inner coating and the coating surface was analysed by the coupled double-distribution function models (DDF-LBM).

**RECONSTRUCTION OF TBCS SAMPLES**

The actual morphology of a single crack inside the coating is shown in Fig. 1. Through a large number of scanning electron microscope (SEM) images analysis, it is found that the crack morphology in xz plane (Dong et al., 2015) is approximately a rectangular, and crack morphology in xy plane (Fu et al., 2018) is more like an elliptic. The crack feature obtained by 3D X-ray microscope and image processing technique (Ahmadian et al., 2015) is approximately an elliptical slice. Therefore, it can be seen that the internal crack of the coating can be extracted into an elliptical cylinder structure.

![200μm](Image)

**Figure 1 The Actual Crack Morphologies**

The QSGS method has been widely used in numerical modeling of porous media and can be used to characterize the pore structure of TBCs (Wang et al., 2016; Wang et al., 2007). On this basis, by introducing the crack deformation factor and adopting the integrated nesting strategy, a three-dimensional reconstruction algorithm of TBCs system with crack is proposed. The reconstructed model can not only reflect the real pore morphology in the coating, but also accurately reflect the typical crack characteristics. Then this model can be used effectively to predict the thermal physical properties of TBCs in service.

The following is the reconstruction process.

1. Set the size of reconstruction area.
2. Set the solid phase as the first growth phase and set its content as \(P_{YSZ}\). Place the nucleation centre of the solid phase according to the nucleation centre formation probability \(P_i\) randomly. So the pores content \(P_{pure}\) is \((1 - P_{YSZ})\).
3. Set the directional growth probabilities \(P_i\) and regenerate adjoining nodes of different \(i\)-th directions. The phase growth begins. Then distribute random numbers between 0 and 1 which presents pores and solid respectively.
4. Set the crack content as \(P_{crack}\) and the size parameters of crack. Repeat the step 3 and 4 until the volume fraction of crack and solid reach to the pre-set \(P_{crack}\) and \(P_{YSZ}\).
5. Output the reconstruction model.

The detailed reconstruction procedures can be seen in our previous studies (Long et al., 2021a; Long et al., 2021b). As shown in Fig. 2(a), the numerical reconstructed TBCs model consists of a cooling film, a top coat and a TGO layer and its crack structure in top coat is illustrated in Fig. 2(b). The crack length \(L\) represents the crack size along x axis in cartesian coordinate system. Similarly, the crack opening and crack depth represent the crack size along y axis and z axis respectively. This study mainly analyses the influence of internal crack with different lengths (100 μm – 260 μm) on the thermal property of TBCs and cracks 100 μm in length and 260 μm in length are illustrated in Fig. 2(c) and (d).
FLOW AND HEAT TRANSFER MODEL OF TBCS AND COOLING FILM BASED ON DDF-LBM

The lattice Boltzmann method based on the coupled double-distribution function models only uses two first-order partial differential equations to replace the complex macroscopic second-order convective heat transfer equations. With advantages of simple calculation logic and good parallelism, DDF-LBM has great advantages in dealing with the flow and heat transfer problems about the porous media and has been widely used (Dai et al., 2013). Its application in TBCs calculation for the prediction of effective thermal properties has been validated in our previous studies well (Long et al., 2021b). In the DDF-LBM model, the two evolution equations are as follows.

\[
\begin{align*}
\frac{f_i(r + e_i \delta_t, t + \delta t) - f_i(r, t)}{\delta t} &= -\tau_f \frac{[f_i(r, t) - f_i^{eq}(r, t)]}{c_s^2} \\
\frac{T_i(r + e_i \delta_t, t + \delta t) - T_i(r, t)}{\delta t} &= -\tau_f \frac{[T_i(r, t) - T_i^{eq}(r, t)]}{c_s^2} 
\end{align*}
\]  

(1)

(2)

Where \( f_i \) and \( f_i^{eq} \) are the density distribution function and its equilibrium state respectively. \( e_i \) is the discrete velocities. \( r \) is the coordinate vector. \( t \) is the time and \( \delta t \) is the momentum relaxation time. \( \tau_f \) and \( \tau_s \) are the dimensionless relaxation time for fluid and temperature respectively. \( T_i \) and \( T_i^{eq} \) are the temperature distribution function and its equilibrium state.

In 3D cases, D3Q19 model for discrete speed \( e_i \) is applied.

\[
e_i = \begin{cases} 
(0,0,0), & i = 0, \\
(\pm1,0,0),(0,\pm1,0),(0,0,\pm1), & i = 1 \sim 6, \\
(\pm1,\pm0,0),(\pm0,\pm1,0),(\pm1,0,\pm1), & i = 7 \sim 18.
\end{cases}
\]  

(3)

Under the incompressible condition, the two evolution equations can be simplified as:

\[
f_i^{eq} = \rho \omega \left[ \frac{e_i \cdot u}{c_i^2} + \frac{(e_i \cdot u)^2}{2c_i^4} - \frac{u_i^2}{2c_i^2} \right] 
\]  

(4)
\[ T^m_i = \alpha_i T \left( 1 + \frac{c_s \cdot u}{c_s} \right) \]  

(5)

Where \( \alpha_i \) is the weighting coefficient (in D3Q19 model, there are \( \alpha_b = 1/3 \), \( \alpha_{a.18} = 1/18 \) and \( \alpha_{a.18} = 1/36 \)). \( c_s \) is the lattice sound speed and \( c_s = 1/\sqrt{3} \).

Therefore, the temperature \( T \) in TBCs is:

\[ T = \sum_{i} T_i \]  

(6)

**SELECTION OF WORKING CONDITIONS**

**Calculation parameters**

Six TBCs samples are obtained in this study. Five of them are cracked TBCs with a length range from 100 \( \mu \text{m} \) to 260 \( \mu \text{m} \). The rest sample is a non-cracked TBCs for comparison. All the samples are cubes of \( N = N_x \times N_y \times N_z = 300 \mu \text{m} \times 160 \mu \text{m} \times 300 \mu \text{m} \), which consists of a cooling film layer with a thickness of 90 \( \mu \text{m} \), a top coat layer with a thickness of 200 \( \mu \text{m} \) and a thermally grown oxide (TGO) layer with a thickness of 10 \( \mu \text{m} \). All the pre-set cracks are positioned in the top coat with a vertical distance of 25 \( \mu \text{m} \) away from TGO layer. The depth of the crack is taken as 18 \( \mu \text{m} \) and the crack opening is keep as 48 \( \mu \text{m} \). The crack deformation factor is set to be 0.1. The porosity of the top coat is set to be 15\%. The thermal conductivity of dense 8YSZ is selected as 2.43 \text{ W m}^{-1}\text{ K}^{-1}, while the air trapped in the defects is selected as 0.0807 \text{ W m}^{-1}\text{ K}^{-1} (Wang et al., 2017). Meanwhile, the temperatures of the top of the cooling film and the bottom of the TGO are chosen as 1212 \( ^\circ \text{C} \) and 844 \( ^\circ \text{C} \), respectively. The horizontal velocity of the gas flow is 23 \text{ m/s} according to the actual service codition of MITSUBISHI M701F gas turbine (Wang et al., 2016).

**Boundary conditions**

In the simulation of velocity field, the upper boundary adopts the non-equilibrium extrapolation format. The remaining boundaries in the flow region are set as periodic boundary conditions. At the same time, the solid boundary adopts the standard bounce-back scheme. In the simulation of temperature field, the upper boundary and the lower boundary all adopt the non-equilibrium extrapolation scheme, and the remaining boundaries are set as adiabatic boundary conditions.

**RESULTS AND DISCUSSION**

**Effect of crack on temperature distribution characteristics of the surface of the coating**

The temperature distribution of the coating surface is shown in Fig. 3. It is obvious that the temperature of the surface of the coating with crack is higher than that of the coating without crack.

![Figure 3 The temperature distributions of the coating surfaces](image_url)
Effect of crack on temperature distribution characteristics of the internal coating

The internal crack not only causes a sudden change in temperature on the surface of the coating, but also affects the temperature of its surrounding areas. Fig. 5(a) and (c) shows the microstructure and temperature distribution in the $xz$ ($y=80 \mu m$) plane of the non-cracked coating. For the APS-TBCs, pores of various shapes are randomly distributed. Because of the existence of these irregular pores, the isotherms are non-linear and have a certain degree of tortuosity. When there is no crack inside the coating, the temperature distribution is more uniform at the inner coating, and the average temperature gradient along the $z$ direction changes very little. However, when the coating is cracked (as shown in Fig. 5(b) and (d)), the isotherms in the cracked area are dense and concave. The temperature difference $\Delta T_{BB}$ at the center of the upper surface and the lower surface of crack is about 12 °C, while the temperature difference of the non-cracked coating $\Delta T_{AA}$ at the same position is smaller, only about 4 °C. At the same time, it is found that a large temperature gradient is also generated in the area near the crack (such as the area in the red dotted frame). The thermal conductivity of the dense material SYSZ is thirty times more than that of the air in crack. The static air plays a major role in hindering the heat flow. This results in an increase in the temperature gradient along the thickness of the coating. Compared with the coating without crack, the larger size of crack will increase the anisotropy of the coating’s microstructures, which will influence the local heat transfer characteristics in and around the crack and then intensify the temperature inhomogeneity in the coating.
The temperature nonuniformity coefficient $\hat{T}_{\text{non}}$ was used to quantitatively analyze and evaluate the nonuniformity of temperature distribution in the coating-cooling film system.

$$SDT_{\text{non}}(T_{z=k}) = \sqrt{\frac{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} (T(i,j,k) - \bar{T}_z(k))^2}{N_x \cdot N_y}}$$  \hspace{1cm} (7)

$$\hat{T}_{\text{non}}(z=k) = \frac{SDT_{\text{non}}(T_{z=k})}{\bar{T}_z(k)}$$  \hspace{1cm} (8)

Where $SDT_{\text{non}}$ represents the standard deviation of temperature in $xy$-plane of TBCs. $\bar{T}_z(k)$ is the mean value over $xy$-plane of the temperature when $z=k$.

The temperature nonuniformity distribution characteristic curves in the part of TBCs system are shown in Fig. 6. As can be seen from the figure, at the interface between the top coat and the cooling film ($z=220$ $\mu$m), the temperature nonuniformity coefficient increases sharply and appears a peak value. This is because the surface of the coating is rough, and there are tiny bumps or pits, which affect the heat transfer performance of the cross section of coatings. Moreover, there is interface thermal resistance between the rough surface and the cooling film, which will lead to the difference in the temperature distribution of the cross section, resulting in the increase of the temperature nonuniformity coefficient on the cross section and the distribution of wave peaks. While inside the coating (areas in $z < 200$ $\mu$m), the temperature distribution inside the coating of non-cracked sample is relatively uniform, and the range of each $xy$ plane along the thickness direction is $4.03 \times 10^{-4} \sim 5.14 \times 10^{-4}$ (black dotted line).

For coatings with cracks of different lengths, there are two obvious peaks in each temperature nonuniformity coefficient curve at $z=44$ $\mu$m and $z=62$ $\mu$m. It can be seen that the interval between the two peaks is 18 $\mu$m, which is exactly the crack depth. The results show that the temperature nonuniformity coefficient of the plane between the upper and lower surface of the crack is the highest, which can reach 40 times that of the average temperature nonuniformity coefficient of the coating. The characteristic pore size is much smaller than the characteristic crack size. This means that, the crack will greatly change the thermal properties (such as thermal conductivity) and temperature distribution (increase of temperature inhomogeneity and local sintering) of the coating, resulting in stress concentration. This can easily lead to early delamination and fracture of the coating, thus affecting the durability of the coating.

Figure 5 Comparison of Temperature Distribution in Non-cracked and Cracked TBCs
CONCLUSIONS

In this study, the TBCs samples with different crack lengths are obtained by numerical reconstruction method. Based on the coupled flow and heat transfer model of DDF-LBM, the temperature distribution characteristics inside and on the surface of the TBCs are studied. The main conclusions are as follows:

(1) The size of crack in TBCs has a significant effect on the thermal property of the coating-film cooling system.

(2) The existence of crack affects the temperature distribution on the coating surface. Compared with the non-cracked coating, with the lengthening of the crack, the maximum/average/minimum temperature of the coating surface increases by 5.2/4.6/4.9 °C.

(3) The existence of crack further strengthens the anisotropy of the coating structures and changes the temperature distributions near the crack, then intensifies the temperature inhomogeneity of the coating. The temperature difference at the center points between the upper surface and lower surface of the crack increases by 8 °C compared with that of the non-cracked coating at the same position. The temperature nonuniformity coefficients in xy planes on the two faces of the crack are 40 times higher than that of the coating without crack at the same position.

NOMENCLATURE

APS atmosphere plasma sprayed
DDF double-distribution function
LBM lattice Boltzmann method
QSGS quartet structure generation set
SEM scanning electron microscope
TBCs thermal barrier coatings
TGO thermally grown oxide
\( \epsilon_i \) discrete velocity
\( f_i \) density distribution function
\( f_i^{eq} \) equilibrium density distribution function
\( L \) crack length, m
\( \mathbf{r} \) coordinate vector
\( SDT_{xy} \) standard deviation of temperature in \( xy \)-planes of TBCs
\( t \) time, s
\( T \) temperature, °C
\( T_i \) temperature distribution function
\( T_i^{eq} \) equilibrium temperature distribution function
\( \hat{T} \) temperature non-uniformity coefficient
velocity vector

momentum relaxation time

energy relaxation time for fluid

energy relaxation time for temperature

weighting coefficient

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