Vol 18 No 11, November 2009
1674-1056/2009/18(11)/4976-05

Chinese Physics B

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Numerical study on the thermo-stress of ZrO_2 thermal barrier coatings by high-intensity pulsed ion beam irradiation*

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(Received 29 September 2008; revised manuscript received 7 April 2009)

This paper studies numerically the thermo-mechanical effects of ZrO_2 thermal barrier coatings (TBCs) irradiated by a high-intensity pulsed ion beam in consideration of the surface structure. Taking the deposited energy of ion beams in TBCs as the source term in the thermal conduction equation, the distribution of temperature in TBCs was simulated. Then, based on the distribution, the evolution of thermal stress was calculated by the finite element method. The results show that tensile radial stress formed at the valley of TBC surfaces after irradiation by HIPIB. Therefore, if cracks happen, they must be at valleys instead of peaks. As for the stress waves, no matter whether through peak or valley position, tensile and compressive stresses are present alternately inside TBCs along the depth direction, and the strength of stress decreases with time.

Keywords: high-intensity pulsed ion beam, ZrO_2 TBCs, stress field, numerical method
PACC: 6180J, 8120L, 6740K, 5265

1. Introduction

In the 1980s, a high-intensity pulsed ion beam (HIPIB) was first used to try to modify semiconductor materials for technical purposes.[1,2]

Thermal barrier coatings are complex coating systems of a ceramic top layer on a metallic layer by means of electron beam physical vapour deposition (EB-PVD). TBCs play an important role in aero and spatial land based gas turbines.[3−5] Therefore, the application in the last ten years has developed rapidly in the aero spacing, chemical and alloy fields. But there are still some problems to be solved. These mainly include high porosity, lack of denseness and failing spallation, bad anti-thermal properties etc. In recent years, for the problems mentioned above, great effort has been made to improve some properties of the coatings by the art of generation like gradient coatings[6], the hybrid spraying technique or the modification of the deposited coatings with laser or focused sun light beams.[7−11] Through the interaction between the HIPIB and TBCs, the top ceramic layer is melted and then re-solidified to form a dense modification layer, thus one can improve some characteristics of the ceramic obviously, and certainly can use them to modify the surface properties of TBCs. A numerical method was used to study the irradiation process in this paper.

2. Theoretical models

The energy of a single ion among a HIPIB is as high as several tens of keV to a few MeV. The high energy of the beam is efficiently deposited into TBC materials in the ion range 0.1–10 μm, often for less than 1 μs during a short pulse width to rapidly melt the near-surface layer. Therefore, the chemical and physical properties of surfaces can be changed because the melted surface re-solidifies due to thermal conduction. We simulate the evolution of the temperature field and further analyse the thermal stress distribution in TBCs after HIPIB irradiation.

The average accelerating voltage of ions generated by a magnetically insulated ion diode (MID) of a TEMP-type accelerator in the experiment is typically 300 kV. The ion current density with full pulse duration 120 ns has a radial distribution with a maximal value of 200 A/cm^2 in the centre of the beam spot. The ceramic specimens prepared for this study were ZrO_2 stabilized by 7%Y_2O_3 fabricated by EB-PVD on the NiCoCrAlY bond coat, and HIPIB irradiation was

*Project supported by the National Natural Science Foundation of China (Grant No 50575037) and the Doctoral Foundation of Dalian University of China (Grant No SBQ200810).

performed with one shot at room temperature under the vacuum condition of 10^{-3} Pa.

The thermal conduction equation is:

$$\rho C(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(T)\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\kappa(T)\frac{\partial T}{\partial y}\right), \quad (1)$$

where T is the temperature, and ρ, $c(T)$ and $\kappa(T)$ are the mass density, specific heat and thermal conductivity, respectively. During the process of changing phase, the latent heat of fusion is considered by enthalpy changed with temperature. The enthalpy is a function of specific heat, mass density and temperature, $H = \int \rho c(T)\mathrm{d}t$. In the calculation, we take the initial temperature included from Ref.[12] which gave the results of temperature distribution of the ceramic materials at the end of a HIPIB pulse. The boundary conditions at the exterior surface are treated to be adiabatic. The room temperature is taken as 20 °C. ANSYS was used to analyse the transient heat conduction. The thermo-physical properties of ZrO_2 are assumed to be isotropic.

The temperature of the irradiated surface changed dramatically: the temperature gradient with time along the depth direction reached the order of 10^8 or/and 10^9 K/s. While the temperature changed, the volume of the target expanded or was compressed. The expansion or compression size is different because of the temperature gradients in different zones inside the bulk; the thermal expansion of any cell of materials was confined by the surrounding cell, and therefore thermal stress formed.

According to the stress theory, the total strain of the cell consists of two parts; one is the stress and the other is the changing temperature. The general Hooke's law expressed by stress and temperature is

$$\begin{aligned}
\varepsilon_x &= \frac{1}{E}[\sigma_x - \mu(\sigma_y + \sigma_z)] + \alpha T_t,\\
\varepsilon_y &= \frac{1}{E}[\sigma_y - \mu(\sigma_x + \sigma_z)] + \alpha T_t,\\
\varepsilon_z &= \frac{1}{E}[\sigma_z - \mu(\sigma_x + \sigma_y)] + \alpha T_t,\\
\gamma_{xy} &= \frac{1}{G}\tau_{xy},\\
\gamma_{yz} &= \frac{1}{G}\tau_{yz},\\
\gamma_{zx} &= \frac{1}{G}\tau_{zx}, \qquad (2)
\end{aligned}$$

where typical terms ε_x = direct strain in the x direction, σ_x = direct stress in the x direction, τ_{xy} = shear stress on the $x-y$ plane, γ_{xy} = shear strain in the $x-y$ plane. α is the coefficient of thermal expansion, E is Young's modulus, the shear elastic modulus $G = \dfrac{E}{2(1+\mu)}$, μ is Poisson's ratio, $T_t = T - T_0$, T_0 is the reference temperature at the point where the stress is zero. Therefore, the functions related to stress and strain expressed by displacements are

$$\begin{aligned}
\sigma_x &= \lambda\Theta + 2G\frac{\partial u}{\partial x} - \beta T_t,\\
\sigma_y &= \lambda\Theta + 2G\frac{\partial v}{\partial y} - \beta T_t,\\
\sigma_z &= \lambda\Theta + 2G\frac{\partial w}{\partial z} - \beta T_t,\\
\tau_{xy} &= G\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right),\\
\tau_{yz} &= G\left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right),\\
\tau_{zx} &= G\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right), \qquad (3)
\end{aligned}$$

where

$$\beta = \alpha E/(1-2\mu), \quad \lambda = \frac{E\mu}{(1+\mu)(1-2\mu)},$$

the volumetric strain $\Theta = \varepsilon_x + \varepsilon_y + \varepsilon_z$.

Taking the displacements u, v and w as variables, we can write a suitable balance equation as

$$\begin{aligned}
G\nabla^2 u + (\lambda + G)\frac{\partial \Theta}{\partial x} - \beta\frac{\partial T_t}{\partial x} = 0,\\
G\nabla^2 v + (\lambda + G)\frac{\partial \Theta}{\partial y} - \beta\frac{\partial T_t}{\partial y} = 0,\\
G\nabla^2 w + (\lambda + G)\frac{\partial \Theta}{\partial z} - \beta\frac{\partial T_t}{\partial z} = 0. \qquad (4)
\end{aligned}$$

The temperature T can be solved from Eq.(1). Then, substituting it into Eq.(4), we can obtain the displacements *u, v and w* of the material spot suiting the boundary and initial conditions, and finally the thermal stress can be solved from Eq.(3).

3. Results and discussion

The surface of ZrO_2 TBCs fabricated by the EB-PVD method is not flat; based on the section profile of the specimen, a zigzag surface structure model shown in Fig.1 was built. Take the tip (such as point M) as the peak position and the bottom (point O) as the valley. The coordinate system is shown in Fig.1. Let the longitudinal direction be expressed on the y axis, and horizontal direction on the x axis. The impact

angle θ is 45°.

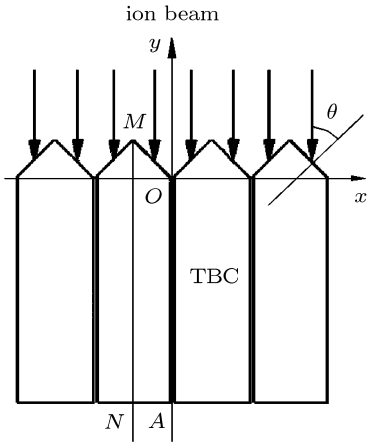


Fig.1. The surface structure of ZrO_2 TBCs.

The feather style profiles of the radial stresses in TBCs at different places are shown in Figs.2(a) and 2(b) at 100 μs after a pulse, which expresses the radial stress along the path MN and OA respectively. The radial stress is zero at the peak position all the time, but at the valley position it appears to be tensile. No matter along path MN or OA, we can see both the phenomena that the compressive stress and tensile stress appear alternately.

At time 500 μs after a pulse, the radial and axial stresses are both zero at the peaks; the alternate phenomenon of tensile and compressive stresses exists in TBCs too. The radial stress is about 70 MPa and the axial stress is approximately 30 MPa at the valley position at the time; the radial stress is larger than the axial one. The case is shown in Figs.3(a) and 3(b). Figure 4 gives a contrast profile of radial stress along the longitudinal direction at the position of peak and valley at 500 μs after a pulse. The distributions of stresses are almost the same inside the TBCs, but near the surface, the distributions show obvious differences. At the valley of the surface the radial stress is about 70 MPa, but at the peak it is zero. It means that if a crack happens it must be at the valley instead of the peak, as shown in Fig.5.

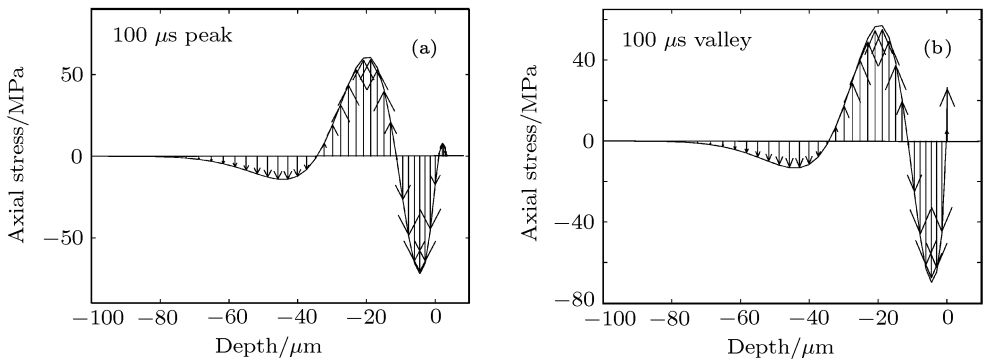


Fig.2. The feather like distribution of radial stresses in coatings through (a) peak and (b) valley at 100 μs after a pulse.

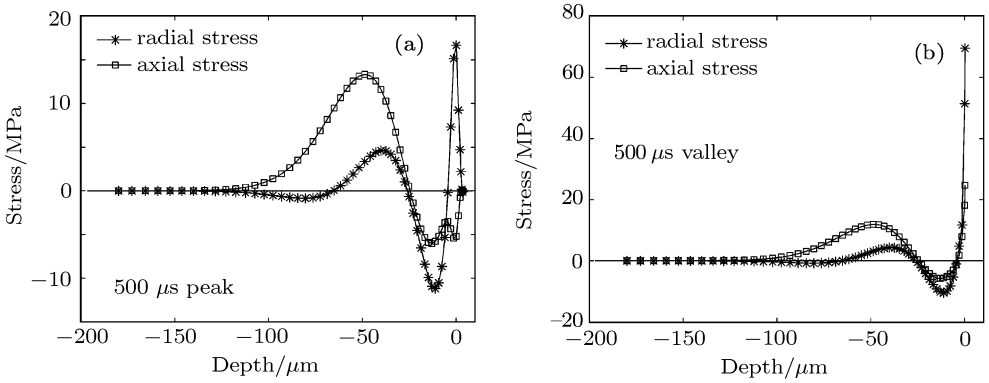


Fig.3. The contrast profiles of radial and axial stresses inside the coatings at 500 μs through (a) peak and (b) valley.

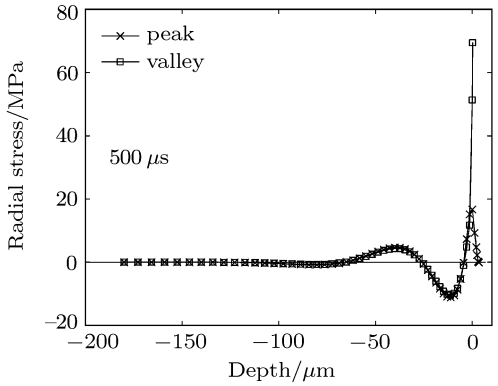


Fig.4. The contrast profile of radial stress inside the coatings through peak and valley at 500μs after a pulse.

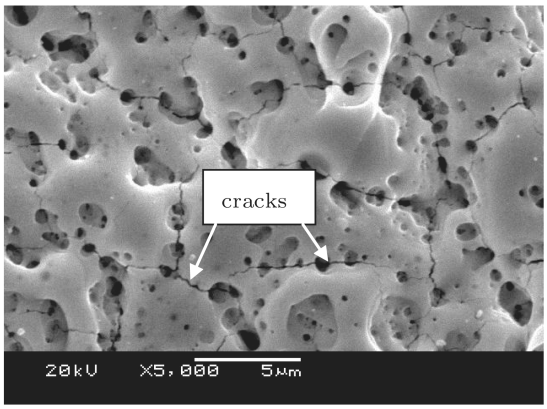


Fig.5. Cracks formed on a TBC surface irradiated by HIPIB under an ion current density of 300 A/cm^2.

The distributions of radial and axial stresses along the longitudinal direction at peak position at 100 μs, 200 μs and 500 μs are shown in Fig.6. The radial and axial stresses remain zero at peak position because of no restrain and they do not change with time. Both radial and axial stress waves propagate inside the TBCs. The amplitude and therefore the strength of the stress wave decrease during the transmission, and tensile and compressive stresses appear alternately. Finally, under the surface near the top layer axial compressive stress appears.

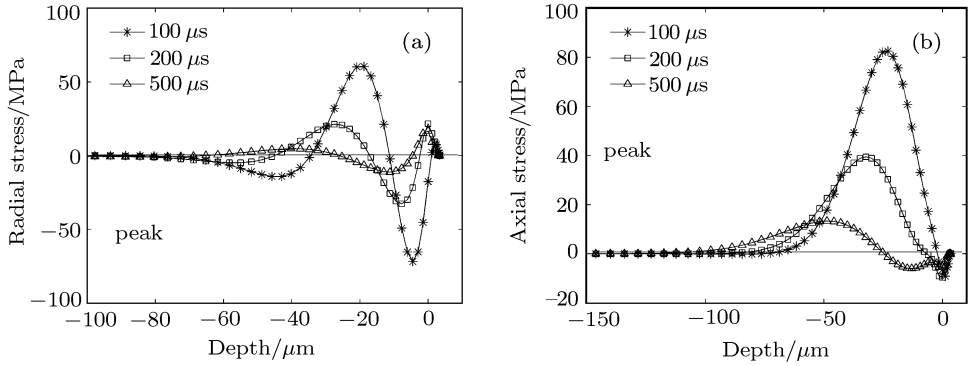


Fig.6. (a) Radial and (b) axial stresses along path MN formed by HIPIB irradiation at 100, 200 and 500 μs after a pulse.

The distribution of radial and axial stresses along the longitudinal direction at valley position at 100 μs, 200 μs and 500 μs are shown in Fig.7. It also shows radial and axial stresses propagating in TBCs. But neither the radial nor the axial stress is zero at the valley, and the radial tensile emerged at the place.

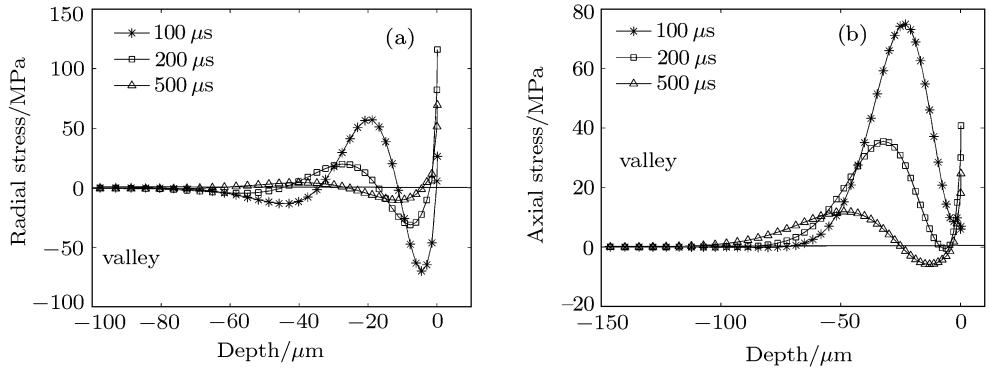


Fig.7. (a) Radial and (b) axial stresses along path OA formed by HIPIB irradiation at 100 μs, 200 μs and 500 μs after a pulse.

4. Conclusions

According to the simulation results of TBCs irradiated by a HIPIB based on thermo-mechanical models, the following conclusions are obtained:

1) Tensile radial stress is formed at the valley of a TBC surface after irradiation by a HIPIB. Therefore, if cracks happen, they must be at valleys instead of peaks;

2) Either radial or axial stresses increase first and then decrease with time at a valley position on a TBC surface;

3) Stress waves form and transfer into TBCs, compressive and tensile stresses appear alternately, and the strength decreases along the depth direction, no matter whether through peaks or valleys.

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