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Optimization Design Model of Functional Gradient Thermal Barrier Coating Material by Using Parallel Computation

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Abstract. It is important for huge ship to find the ceramic/metal functional gradient thermal barrier coating materials. A parallel computation model is built for optimization design of three-dimensional ceramic/metal functionally gradient thermal barrier coating material. According to the control equation and initial-boundary conditions, the heat transfer problem is considered, and numerical algorithms of optimization design is constructed by adapting difference method. The numerical results shows that gradient thermal barrier coating material can improve the function of material.

1 Introduction

The research of ceramic/metal functional gradient thermal barrier coating material is a hot project of ship[1]. Some parts of related with combustion engine, such as cylinder head, piston, cylinder sleeve, and valve have high thermal load reliability. Higher thermal load reliability requires that these components have higher mechanical properties, such as Impact resistance, high temperature resistance, heat insulation, anti-oxidation, anti-corrosion[2]. In theory, the gradient thermal barrier coatings and metal ceramic combination (gradient material) can meet the above requirements. This caused a large number of research [3-4], such as material heat transfer characteristics of [5], gradient material processing technology research [6], gradient material design research [7]. Due to the rapid development of scientific research, the speed of the new material is also accelerating. This esquire people to research how to design new material.

This paper will consider heat conduction problem of gradient thermal barrier coating material, and find the relationship between thermal conductivity and the temperature distribution.

2 Mathematical Model

Gradient thermal barrier coating must have good insulation effect, high temperature oxidation resistance and thermal shock resistance. According to the special requirements in corrosive medium, it must be high corrosion resistance. In this paper, we mainly consider

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the heat insulation effect, and analyze the distribution of temperature, which includes the temperature distribution of the metal bonding layer and the ceramic layer. The temperature distribution of gradient material is supposed as T (x, y, z, t), where (x, y, z) is the space coordinates and t is the time. Heat conduction coefficient is a (x, y, z, T), and the heat conduction equation is [8]

$$\frac{\partial(cT)}{\partial t} = \nabla(a\nabla T) \qquad (x,y,z)\in\Omega \qquad t>0 \tag{1.1}$$

here c is coefficient of heat capacity, or is product of heat capacity with density, Q is the calculative region with boundary $\Gamma \cup L$.

Initial condition and boundary conditions are

$$\begin{aligned} & T(x,y,z,t=0) = G(x,y,z) \qquad (x,y,z)\in\Omega \\ & T((x,y,z)\in\Gamma,t) = B(\Gamma,t) \qquad t>0 \\ & \frac{\partial T}{\partial n}((x,y,z)\in L,t) = q(L,t) \qquad t>0 \end{aligned} \tag{1.2}$$

here G(x,y,z) is initial temperature, B(t) is temperature on boundary Γ. q(L,t) is temperature change rate on the boundary L. If coefficient of heat capacity c is not relate with time, the control equation may be written as

$$c\frac{\partial T}{\partial t} = a\Delta T + \nabla a\nabla T \qquad (x,y,z)\in\Omega \qquad t>0 \tag{1.3}$$

In the case of heat conduction coefficient is constant, the control equation may be written as:

$$c\frac{\partial T}{\partial t} = a\frac{\partial^2 T}{\partial x^2} + a\frac{\partial^2 T}{\partial y^2} + a\frac{\partial^2 T}{\partial z^2} \qquad (x,y,z)\in\Omega \qquad t>0 \tag{1.4}$$

3 Parallel Design

For the positive problem, we will give the thermal conductivity coefficient a, the initial temperature G(x,y,z), temperature on boundary B(t). For low dimension, the problem is solved in parallel computing. But for the high dimension, the computation is large, and it needs to speed up the design time by using the parallel computer.

If thermal conductivity coefficient a(x,y,z,T) is not constant, or irregular boundary shape,

The parallel computation steps are:

1) P processor in a parallel computer is selected, and the computing area is divided into P sub-domain;

(2) the sub-domain are divided into grid;

(3) an implicit difference scheme is chosen to solve equation as below.

$$c_{ijk}^{(s)}\frac{T_{ijk}^{(s+1)}-T_{ijk}^{(s)}}{\tau}=\frac{1}{h^2}a_{ijk}^{(s)}DT_{ijk}^{(s+1)}-\frac{6}{h^2}a_{ijk}^{(s)}T_{ijk}^{(s+1)}+\frac{1}{4h^2}AT_{ijk}^{(s+1)} \tag{2.1}$$

here $T_{ijk}^{(s)}=T(x_i, y_j, z_k, t_s)$, $t_s=s\tau$, τ is time step length,s is subscript. DT and AT are defined as

$$\begin{aligned}
DT_{ijk}^{(s+1)} &= T_{i+1jk}^{(s+1)}+T_{i-1jk}^{(s+1)}+T_{ij+1k}^{(s+1)}+T_{ij-1k}^{(s+1)}+T_{ijk+1}^{(s+1)}+T_{ijk-1}^{(s+1)}\\
AT_{ijk}^{(s+1)} &= (a_{i+1jk}^{(s+1)}-a_{i-1jk}^{(s+1)})(T_{i+1jk}^{(s+1)}-T_{i-1jk}^{(s+1)})+(a_{ij+1k}^{(s+1)}-a_{ij-1k}^{(s+1)})(T_{ij+1k}^{(s+1)}-T_{ij-1k}^{(s+1)})+\\
&+(a_{ijk+1}^{(s+1)}-a_{ijk-1}^{(s+1)})(T_{ijk+1}^{(s+1)}-T_{ijk-1}^{(s+1)})
\end{aligned} \tag{2.2}$$

Initial and boundary condition are

$$\begin{aligned}
&T_{ijk}^{(0)}=G(x_i,y_j,z_k)\\
&T_{ijk}^{(s)}=B(\Gamma,t_s) \qquad (x_i,y_j,z_k)\in\Gamma\\
&\frac{\partial T_{ijk}^{(s)}}{\partial n}=\frac{\partial T}{\partial n}((x_i,y_j,z_k)\in L,t_s)=q(L,t_s)
\end{aligned} \tag{2.3}$$

In the case of heat conduction coefficient is constant, the above equation may be written as

$$\begin{aligned}
&DT_{ijk}^{(s+1)}=T_{i+1jk}^{(s+1)}+T_{i-1jk}^{(s+1)}+T_{ij+1k}^{(s+1)}+T_{ij-1k}^{(s+1)}+T_{ijk+1}^{(s+1)}+T_{ijk-1}^{(s+1)}\\
&AT_{ijk}^{(s+1)}=0
\end{aligned}$$

and

$$c_{ijk}^{(s)}\frac{T_{ijk}^{(s+1)}-T_{ijk}^{(s)}}{\tau}=\frac{1}{h^2}a[T_{i+1jk}^{(s+1)}+T_{i-1jk}^{(s+1)}+T_{ij+1k}^{(s+1)}+T_{ij-1k}^{(s+1)}+T_{ijk+1}^{(s+1)}+T_{ijk-1}^{(s+1)}]-\frac{6}{h^2}aT_{ijk}^{(s+1)}$$

Because above is the space and time problem, there are many variables in the equation. For more variable equation, the iterative method calculation time is less than the one of direct iteration method. When the heat transfer coefficient a(x,y,z,T) is related to temperature T, the equations are nonlinear and should be calculated by the iterative method. So the iterative method is used to solve the equations in the paper.

4 Example of Problem

Consider the NICrBSi ceramic/metal graded thermal barrier coatings, thickness 0.8mm, length 2.4mm, width 2.4mm. The surface temperature is lower than the lower surface 500 K0C. For calculation, the upper surface temperature is recorded as 0 degrees, and the lower surface temperature is recorded as 500 K0C. The length and width of the adjacent two surface insulation, the other adjacent two surface temperature is equal to the temperature of the low temperature surface. The heat transfer coefficient in the laboratory is a function of thickness (i.e., z), and the expression of the coefficient of conductivity is given[9]

$$a = a_1 a_0$$
$$a_1 = [1-(\frac{z}{Z})^2](0.1-0.01\frac{T}{T_0}+0.001(\frac{T}{T_0})^2)+(\frac{z}{Z})^2(1.0+0.1\frac{T}{T_0}+0.01(\frac{T}{T_0})^2)$$
$$a_0 = 45[J/(s.m.K)] \tag{3.1}$$

or

$$a = 45[1-(\frac{z}{Z})^2](0.1-0.01\frac{T}{T_0}+0.001(\frac{T}{T_0})^2)+(\frac{z}{Z})^2(1.0+0.1\frac{T}{T_0}+0.01(\frac{T}{T_0})^2)$$

here Z=0.8mm， is thickness of gradient material, T0=500 K0C is maximum difference temperature. Heat capacity coefficient c is calculated from the following formula

$$c = c_1 c_0$$
$$c_1 = 1+0.1308\frac{z}{Z} \tag{3.2}$$
$$c_0 = 3494.4[J/(m^3.K)]$$

or

$$c = 3494.4[1+0.1308\frac{z}{Z}]$$

take initial temperature T(0)=0，Boundary condition：on the sides of x=0 and y=0, take T=0，on the sides of x=2.4mm and y=2.4mm，The derivation of T in the normal direction is taken as zero.

$$T(t=0)=0$$
$$T(x=0)=T(y=0)=0$$
$$T(z=0)=500 \qquad T(\frac{z}{Z}=1)=0$$
$$\frac{\partial T(\frac{x}{Z}=3)}{\partial x}=\frac{\partial T(\frac{y}{Z}=3)}{\partial y}=0 \tag{3.3}$$

We take 121 points in the x,y directions, 33 points in the z direction. Total space points is 464640, Z=0.8mm, space step length h=0.0025Z。

The parallel computer of the Seaborg is used to calculate our problem. We choose 100 processors. The k=i×j processor response the calculation temperature in domain {0.3(i-1)Z ≤x≤0.3iZ, 0.3(j-1)Z ≤y≤0.3jZ, 0 ≤z≤0.8Z}, i,j=1,2,3,..,10. the speedup rate of parallel computation is 83, time step is 0.00001s. Take time t=0.3600s, X=x/Z, Y=y/Z are non dimensional coordinates. We find the change of temperature is large. The reason of the temperature change is that the gradient material has good heat insulation effect. The distance between the contour lines of temperature distribution is not constant, the distance from the corner of the origin is larger, and the distance from the corner is smaller, the temperature changes fast near the corner, which has three characteristics. The temperature varied with (x,y) in the z=0 is shows in Fig.1. From the figure, the temperature is decrease fast near boundary.

When the temperature distribution of the gradient material is obtained, the design parameters of the high temperature gradient material can be obtained according to the physical quantities of the thermal stress and the related theory.

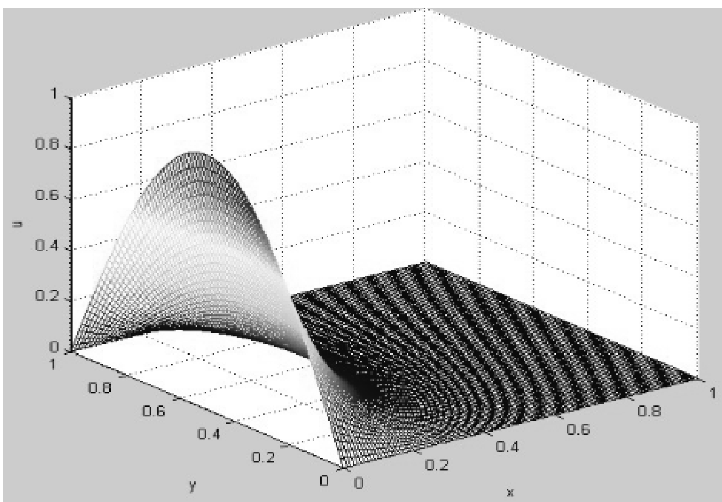

Fig.1 Temperature varied with (x,y) in z=0.

5 Conclusion

The ceramic/metal functional gradient thermal barrier coating materials is consider by using mathematical method. The parallel optimization design method of the ceramic/metal functional gradient thermal barrier coating materials is shown in the paper. By using the finite difference method, the three-dimensional numerical equation of heat transportation problem are solved.

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