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Thermal-mechanical response of microscale functional film for infrared window

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Abstract: Infrared window in hypersonic missile usually suffers complex aerodynamic force/heat during high-speed flight. A finite element method was adopted to simulate the thermal and stress response of microscale functional film for infrared window under different aerodynamic heats/forces conditions. Temperature and stress distribution were obtained with different heat fluxes. There is almost constant stress distribution along the film thickness except a sudden decrease near the substrate. The maximum stresses are located at the points which are 0.5 mm away from the edges. Different film materials result in different stress values. The temperature and stress in ZrN are larger than those in Y_2O_3. Besides the numerical simulation, an oxygen propane flame jet impingement test was performed to investigate thermal shock failure of the infrared window. Some place of the window surface has spots damage and some place has line crack damage after thermal shock.

Key words: infrared window; thin films; finite element method; thermal stress; aerodynamic heating

1 Introduction

Infrared window is a key component of a hypersonic missile's integration of structure and function. There is no doubt that infrared window has great effects on transferring the targets' infrared signal, maintaining the aerodynamic shape and protecting imaging systems. Hypersonic missile usually suffers strong aerodynamic forces and serious aerodynamic heating, which will cause coupling effects of heat, force and light on the infrared window. This will lead the whole infrared detection system paralysis. Infrared window is composed of substrate materials and functional films. Polycrystalline ZnS is a common infrared substrate material, but it still has some drawbacks, such as soft texture, low mechanical strength and big brittleness [1]. Because of those drawbacks, polycrystalline ZnS cannot resist natural condition of the erosion of the raindrops and sandstone in the atmospheric environment. Moreover, it cannot resist the intensity aerodynamic heat/force. [2] Due to its high refractive index, it has large reflecting loss. Therefore, it is badly in need of an antireflective and protective film. Commonly used film materials include diamond-like carbon (DLC) [3−5], carbon germanium (Ge_xC_{1-x}), zirconium nitride (ZrN), yttria (Y_2O_3), yttrium fluoride (YF_3) and boron phosphide (BP) [6−10].

It is very important to do research on failure of infrared window, so many organizations and scholars have studied it for a long period [11−15]. Because of the aerodynamic heats/forces, infrared window materials suffer complex three-dimensional heat/stress conditions. Window' rupture, film delamination, light distortion and other failure phenomenon carry out when the macro/micro structure and thermodynamic state of materials have tremendous changes. RUSSELL et al [16] used the ATAC3D aerothermal analysis code to provide convective and pressure boundary conditions coupled with the ANSYS finite element analysis code to solve the three dimensional finite element problem to analyze the thermal shock on infrared windows. KARAKSINA et al [17] studied the effect of hot isostatic pressing conditions on the microstructure of CVD ZnS and analyzed the mechanisms of zinc sulfide recrystallization at high temperatures and pressures. TOMBA and CAVALIERI [18] developed an elasto-dynamic solution for thermal shock due to heat convection at a constant temperature in a thick orthotropic cylindrical shell and presented the complete dynamic response of thermal shock stresses.

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LIU and HUANG [19] established a model of coupled heat transfer of radiation and condition on infrared window and investigated the effects of material properties and thermal boundary condition on temperature distribution.

In order to study the mechanisms of function film delamination in infrared window materials, obtaining the thermal stress distribution of thin films is the primary work. A finite element analysis method is carried out to simulate the thermal response of microscale functional film for infrared window under the conditions with different aerodynamic heats/forces. Two kinds of films (Y_2O_3 and ZrN) were investigated as comparison. Thermal stress distributions of the films are obtained. Additionally, oxygen propane flame jet impingement test is performed to investigate the thermal shock failure of the infrared window. Microscope pictures are taken to evaluate the damage on the infrared window.

2 Models

2.1 Heat transfer model

According to energy balance principle, the wall temperature can be described by using the thermal conduction differential equation. For three-dimensional unsteady problem in Cartesian coordinate system, heat conduction differential equation is

$$\rho c_p \frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(\lambda_x \frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial y}\left(\lambda_y \frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda_z \frac{\partial T}{\partial y}\right) \qquad (1)$$

where ρ is the density; c_p is the specific heat capacity; T is the temperature; t is the time; λ_x, λ_y, and λ_z are the thermal conductivities in x-, y- and z-direction, respectively. Additionally, the inner heat source is ignored.

Boundary conditions are as follows.

Inner surface of the solid wall is natural convection:

$$k_n \left.\frac{\partial T}{\partial n}\right|_{\tau_c} = h(T_e - T_s) \qquad (2)$$

Thermal flux of the outside surface is given by flow field calculation:

$$k_n \left.\frac{\partial T}{\partial n}\right|_{\Gamma_a} = q\Gamma_a \qquad (3)$$

where n means the outer normal of the surface; h is the convective heat transfer coefficient; T_e and T_s represent the gas temperature and surface temperature, respectively; k is the thermal conductivity in outer normal of the surface; q is the heat flux; Γ is the area of the surface.

Meanwhile, the solid wall is also transferred by radiation. When the Mach number is small, the impact of radiation heat transfer can be ignored.

2.2 Thermal stress model

The stress and strain must satisfy the following equations.

The balance equation is

$$\begin{cases}\dfrac{\partial \sigma_x}{\partial x}+\dfrac{\partial \tau_{yx}}{\partial y}+\dfrac{\partial \sigma_{zx}}{\partial z}+F_x=\rho\dfrac{\partial^2 u_x}{\partial t}\\ \dfrac{\partial \sigma_y}{\partial y}+\dfrac{\partial \tau_{xy}}{\partial x}+\dfrac{\partial \sigma_{zy}}{\partial z}+F_y=\rho\dfrac{\partial^2 u_y}{\partial t}\\ \dfrac{\partial \sigma_z}{\partial z}+\dfrac{\partial \tau_{yx}}{\partial y}+\dfrac{\partial \sigma_{xz}}{\partial x}+F_z=\rho\dfrac{\partial^2 u_z}{\partial t}\end{cases} \qquad (4)$$

where σ is the normal stress; τ is the shearing stress; F_x, F_y, F_z are the body forces of x-, y-, z-coordinate component, respectively; $\rho\frac{\partial^2 u_x}{\partial t}$, $\rho\frac{\partial^2 u_y}{\partial t}$, $\rho\frac{\partial^2 u_z}{\partial t}$ are dynamic terms.

The physical equation is given as follows:

$$\begin{Bmatrix}\sigma_x\\ \sigma_y\\ \sigma_z\\ \tau_{xy}\\ \tau_{yz}\\ \tau_{zx}\end{Bmatrix}=\frac{E(1-\mu)}{(1+\mu)(1-2\mu)}\cdot$$

$$\left(\begin{bmatrix}1 & A_1 & A_1 & 0 & 0 & 0\\ A_1 & 1 & A_1 & 0 & 0 & 0\\ A_1 & A_1 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & A_2 & 0 & 0\\ 0 & 0 & 0 & 0 & A_2 & 0\\ 0 & 0 & 0 & 0 & 0 & A_2\end{bmatrix}\begin{bmatrix}\varepsilon_x\\ \varepsilon_y\\ \varepsilon_z\\ \gamma_{xy}\\ \gamma_{yz}\\ \gamma_{zx}\end{bmatrix}-\begin{bmatrix}(1+\mu)\alpha_x\Delta T\\ (1+\mu)\alpha_y\Delta T\\ (1+\mu)\alpha_z\Delta T\\ 0\\ 0\\ 0\end{bmatrix}\right) \qquad (5)$$

where ε is the extension strain; γ is the shear strain; $A_1=\mu/(1-\mu)$; $A_2=(1-2\mu)/[2(1-\mu)]$; E is the elastic modulus; μ is the Poisson ratio; α is the thermal expansion coefficient; ΔT is the variation of temperature.

2.3 Calculation model and mesh

The material parameters in the simulation are listed in Table 1. Taking the actual computing capability of the

Table 1 Thermal and mechanical properties

Material	Density/ $(kg \cdot m^{-3})$	Thermal conductivity/ $(W \cdot m^{-1} \cdot K^{-1})$	Specific heat capacity/ $(kJ \cdot kg^{-1} \cdot K^{-1})$	Thermal expansion coefficient/$10^{-6}K^{-1}$	Elastic modulus/ GPa	Poisson ratio
CVDZnS	4090	27.2	515	6.5	74.5	0.28
Y_2O_3	5010	27	451.87	7.1	164	0.29
ZrN	7320	16.73	505.58	7.2	510	0.16