Anisotropic Constitutive Model and its Application in Simulation of Thermal Shock Wave Propagation for Cylinder Shell Composite

Xia Huang, Wenhui Tang, Banghai Jiang, and Xianwen Ran

Abstract—In this paper, a plane-strain orthotropic elasto-plastic dynamic constitutive model is established, and with this constitutive model, the thermal shock wave induced by intense pulsed X-ray radiation in cylinder shell composite is simulated by the finite element code, then the properties of thermal shock wave propagation are discussed. The results show that the thermal shock wave exhibit different shapes under the radiation of soft and hard X-ray, and while the composite is radiated along different principal axes, great differences exist in some aspects, such as attenuation of the peak stress value, spallation and so on.

Keywords—anisotropic constitutive model, thermal shock wave, X-ray, cylinder shell composite.

I. INTRODUCTION

While a material is radiated by intense pulsed X-ray, a great deal of energy rapidly deposits in the material surface, and huge temperature and pressure gradients are formed due to the fast attenuation of deposited energy from surface to inner. Simultaneously, the adiabatic expansion occurs with the quick increase of specific internal energy, and if the incident energy fluence is high enough to exceed the sublimation energy of material., the radiated material surface will sublimate to gas immediately, then the blow-off effect on the material takes place due to the forth ejection of gas. Thus a thermal shock wave is formed by these factors [1]. When the thermal shock wave propagates to the interface with low resistance or the free surface, a reflected release wave will be generated for the release of thermal shock wave. With the interaction between the reflected release wave and the rarefaction part of incident thermal shock wave, an intense tensile effect occurs which results in the material spallation.

II. PLANE-STRAIN CONSTITUTIVE MODEL FOR ELASTIC RESPONSE

For orthotropic composite material, there are three principal axis directions (use \(1, 2, 3\) denotation), and invoking the condition of plane strain (1-2 plane for example), we get 
\[
\sigma_{13} = \sigma_{13} = \sigma_{23} = 0 \quad \text{and} \quad \sigma_{13} = \sigma_{23} = 0.
\]

In the elastic deformation phase, the stress-strain relation is described by Hooke law:

\[
\begin{align*}
\sigma_{11} &= c_{11}\varepsilon_{11} + c_{12}\varepsilon_{22} \\
\sigma_{22} &= c_{12}\varepsilon_{11} + c_{22}\varepsilon_{22} \\
\sigma_{33} &= c_{13}\varepsilon_{11} + c_{23}\varepsilon_{22} \\
\sigma_{12} &= c_{44}\varepsilon_{12}
\end{align*}
\]

Where...
\[ c_{11} = E_1 \left( 1 - v_{23}^2 \right) \frac{E_3}{E_2} / \alpha \cdot \frac{c_{22} = E_2 \left( 1 - v_{13}^2 \right) \frac{E_3}{E_1}}{\alpha}, \]
\[ c_{13} = E_3 \left( 1 - u_{12}^2 \right) \frac{E_2}{E_1} / \alpha \cdot \frac{c_{12} = E_2 \left( u_{13} + v_{13}u_{23} \right) \frac{E_3}{E_2}}{\alpha} \cdot \frac{c_{23} = E_3 \left( u_{13} + v_{13}u_{23} \right) \frac{E_2}{E_1}}{\alpha}, \]
\[ c_{44} = 2G_{12} \cdot \alpha = 1 - u_{12}^2 \frac{E_2}{E_1} - v_{13}^2 \frac{E_3}{E_1} - u_{23}^2 \frac{E_3}{E_2} - 2u_{12}u_{13}u_{23} \frac{E_3}{E_1}, \]

\[ E_i \] are the Young’s moduli, \( G_{ij} \)’s are the shear moduli, and \( \nu_{ij} \)’s are the Poisson ratios.

To separate thermodynamic (equation of state) response from the ability of material to carry shear loads (strength), it is convenient to partition the strains into volumetric and deviatoric components. For plane-strain problem, under the condition of small strain, the volumetric strain \( \varepsilon_{11} = \varepsilon_{22} \), and the deviatoric strains are expressed as the difference between total strain and volumetric strain:
\[ \varepsilon_d = \varepsilon - \theta \delta / 3 \]

Equation (2) is the deviatoric stress component and \( \delta \) is the Kronecker delta function.

The total stress tensor is also decomposed into pressure and deviatoric stress component:
\[ \sigma = -p\delta + s \]

where pressure \( p \) is defined as the negative of mean stress which is the average of the three normal stress components, and \( s \) is the deviatoric stress component.

Therefore, the pressure is:
\[ p = -\left( \sigma_{11} + \sigma_{22} + \sigma_{33} \right) / 3 \]
\[ = -\left( c_{11} + 3c_{12} + c_{13} + 2c_{22} + 2c_{23} \right) \theta / 9 \]
\[ = -\left( c_{11} + c_{13} - c_{22} - c_{23} \right) \varepsilon_d / 3 \]

It is clear that, for the anisotropic material, in addition to the volumetric strain, the pressure also depends on the deviatoric strain component. That is to say the pressure can result in shape deformation, and in the limit of isotropic material, (4) reduces to \( p = -k\theta = -E\theta / \left[ 3 \left( 1 - 2\nu \right) \right] \), where \( k \) is the bulk modulus, \( E \) is the Young’s modulus, and \( \nu \) is the Poisson ratio of isotropic material. The deviatoric stress components can be written as:
\[ s_{11} = \left( 2c_{11} + 3c_{12} - c_{13} - 2c_{22} - 2c_{23} \right) \theta / 9 \]
\[ + \left( 2c_{11} - 3c_{12} + c_{13} + 2c_{22} + c_{23} \right) \varepsilon_d^2 / 3 \]
\[ s_{22} = \left( c_{11} - c_{13} + 4c_{22} - 2c_{23} \right) \theta / 9 \]
\[ + \left( -c_{11} + 3c_{12} - c_{13} - 2c_{22} + c_{23} \right) \varepsilon_d^2 / 3 \]
\[ s_{33} = \left( -c_{11} - 3c_{12} + 2c_{13} - 2c_{22} + 4c_{23} \right) \theta / 9 \]
\[ + \left( -c_{11} + 2c_{13} + c_{22} - 2c_{23} \right) \varepsilon_d^2 / 3 \]
\[ s_{12} = c_{44} \varepsilon_d^2 = c_{44} \varepsilon_d^2 \]

But the linear relation in (4) is satisfied only at very low pressure. To calculate the nonlinear behaviour of volume change, the equation of state is introduced. Under background of intense X-ray radiation, the material state is very complex, and PUFF equation of state is often used to depict both the compressive shock state with relatively low temperature and the coupling state of energy deposition and fluid dynamics movement [3], which is written as:

**compression region:**
\[ p = p_h (\gamma) + \rho \gamma (e - e_h) \] (6)

**expansion region:**
\[ p = \rho \left[ \gamma - 1 + \left( \Gamma_0 - \gamma + 1 \right) \sqrt{\rho / \rho_0} \right] \left[ e - e_s \left( 1 - \exp \left[ N \rho_0 \left( 1 - \rho / \rho_0 \right) / \rho \right] \right) \right] \] (7)

where \( p_h \) is Hugoniot pressure, \( \gamma \) is specific internal energy, \( \Gamma_0 \) is Grüneisen parameter, \( \gamma \) is adiabatic exponent, \( N=c\gamma/G \), and \( e_s \) is sublimation energy. Equation (6) and (7) are continuous at \( p=p_h \), and (7) can transit from solid state to gas state very well.

Equation (8) and (9) are the traditional PUFF equation of state, and they can be rewritten as a Taylor’s series expansion of \( \mu \), where \( \mu = \rho / \rho_0 - 1 = -\theta \), so the following equations are gotten:

**compression region:**
\[ p = -A_1 \theta + \left( A_2 - A_1 \Gamma_0 / 2 \right) \theta^2 \]
\[ -\left( A_3 - A_1 \Gamma_0 / 2 \right) \theta^3 + \left( \rho_0 \Gamma_0 - \rho_0 \Gamma_0 \theta \right) e \] (8)

**dilation region:**
\[ p = -B_1 \theta + B_2 \theta^2 - B_3 \theta^3 \]
\[ + \left[ \rho_0 \Gamma_0 - 3 \rho_0 \Gamma_0 \theta / 2 + \rho_0 \left( \gamma - 1 \right) \theta / 2 \right] e \] (9)

where \( A_i = \rho_0 c_s^2 \), \( A_2 = A_1 \left( 2s - 1 \right) \), \( A_3 = A_1 \left( 3 - 4s + 1 \right) \),
\( B_1 = \rho_0 c_s^2 \), \( B_2 = -B_1 / 2 - B_1 \left( \gamma - 1 \right) / 2 \Gamma_0 + B_1 \Gamma_0 / 2 \),
\( B_3 = \frac{5B_1}{24} + \frac{5}{8} \left( \frac{\gamma - 1}{\Gamma_0} - \frac{5}{4} \right) B_1 \Gamma_0 + \frac{1}{6} B_1 \Gamma_0^2 \). \( c_0 \) and \( s \) are the parameters gained from dynamic experiment. Equation (8) and (9) are the series forms of PUFF equation of state which are only suitable for isotropic materials without reflecting any anisotropic characteristics. In the elastic deformation phase,
according to (4), the modified PUFF equation of state which considers both nonlinear volume change and anisotropic property is obtained [4 - 6]:

**compression region:**

\[
p = -A\varepsilon \theta^3 + (A_2 - A_1\varepsilon \Gamma_0 / 2)\varepsilon \theta^2 - (A_1 - A_1\varepsilon \Gamma_0 / 2)\varepsilon \theta - (\rho_0\varepsilon \Gamma_0 - \rho_0\varepsilon \Gamma_0 \theta)\varepsilon - (c_{11} + c_{13} - c_{22} - c_{23})\varepsilon^p_{ij} / 3 \tag{10}
\]

**expansion region:**

\[
p = -B\varepsilon \theta^3 + B_1\varepsilon \theta^3 + \left[ \rho_0\varepsilon \Gamma_0 - 3\rho_0\varepsilon \Gamma_0 \theta / 2 + \rho_0(\gamma - 1)\theta / 2 \right] \varepsilon - (c_{11} + c_{13} - c_{22} - c_{23})\varepsilon^p_{ij} / 3 \tag{11}
\]

where \( A' = B' = (c_{11} + 3c_{12} + c_{13} + 2c_{22} + 2c_{23}) / 9 \). \( A' \) ( \( B' \)) reflects the anisotropic property and is called as effective bulk modulus.

Thus, for elastic response, the pressure can be gained from (10) and (11), and the deviatoric stresses are calculated by (5), then the total stresses gotten fro \( \varepsilon_{ij} = -\rho_0\varepsilon_{ij} + s_0 \) can account for both nonlinear behaviour of volume change and anisotropic property.

### III. Plane-strain Constitutive model for Plastic Response

#### A. Plastic Constitutive Model

In the plastic deformation phase, the Hooke law is satisfied between stress increment and strain increment, so the constitutive relation can be depicted by increment form:

\[
\begin{bmatrix}
\frac{d\sigma_{11}}{d\varepsilon_{11}} \\
\frac{d\sigma_{22}}{d\varepsilon_{22}} \\
\frac{d\sigma_{33}}{d\varepsilon_{33}} \\
\frac{d\sigma_{12}}{d\varepsilon_{12}}
\end{bmatrix} = \begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 \\
c_{21} & c_{22} & c_{23} & 0 \\
c_{31} & c_{32} & c_{33} & 0 \\
0 & 0 & 0 & c_{44}
\end{bmatrix} \begin{bmatrix}
\frac{d\varepsilon_{11}}{d\varepsilon_{11}} \\
\frac{d\varepsilon_{22}}{d\varepsilon_{22}} \\
\frac{d\varepsilon_{33}}{d\varepsilon_{33}} \\
\frac{d\varepsilon_{12}}{d\varepsilon_{12}}
\end{bmatrix}
\]

**\( \sigma_{ij} \)** represents elastic strain increment, and \( \varepsilon^p_{ij} \) is plastic strain increment calculated by yield criterion which will be discussed later.

Also the stress increment is decomposed to pressure increment and deviatoric stress increment, then the pressure increment in plastic region can be written as:

\[
dp = -(d\sigma_{11} + d\sigma_{22} + d\sigma_{33}) = -\left( c_{11} + c_{13} - c_{22} - c_{23} \right) d\varepsilon_{11} / 3 - \left( c_{11} + c_{13} - c_{22} - c_{23} \right) d\varepsilon_{11} / 3 + \left( c_{12} + c_{22} + c_{23} \right) d\varepsilon_{22}^p / 3 + \left( c_{12} + c_{22} + c_{23} \right) d\varepsilon_{22}^p / 3
\]

From (13), it is clear to find that, for the anisotropic material, the pressure increment depends on not only volumetric strain increment, but also the deviatoric strain and plastic strain increment. In the limit of isotropic material, (13) reduces to

\[
dp = -\kappa d\theta = -\frac{E}{3(1-2\nu)} d\theta
\]

**The deviatoric stress increment components are:**

\[
\begin{align*}
d_{11} & = \left( 2c_{22} - c_{12} - c_{22} - 2c_{33} \right) d\varepsilon_{11} / 9 + \left( c_{11} + c_{13} - c_{22} - c_{23} \right) d\varepsilon_{11} / 3 - \left( 2c_{11} - c_{12} - c_{13} \right) d\varepsilon_{11}^p / 3 - \left( c_{12} - c_{12} - c_{23} \right) d\varepsilon_{22}^p / 3 - \left( 2c_{13} - c_{23} - c_{23} \right) d\varepsilon_{33}^p / 3
\end{align*}
\]

\[
\begin{align*}
d_{22} & = \left( -c_{11} + 4c_{12} - c_{22} - 2c_{33} \right) d\varepsilon_{22} / 9 + \left( -c_{11} + 3c_{12} + c_{13} + 2c_{22} + 2c_{23} \right) d\varepsilon_{11} / 3 - \left( 2c_{11} - c_{12} - c_{13} \right) d\varepsilon_{11}^p / 3 - \left( c_{12} - c_{22} - c_{23} \right) d\varepsilon_{22}^p / 3 - \left( c_{13} - c_{23} - c_{33} \right) d\varepsilon_{33}^p / 3
\end{align*}
\]

\[
\begin{align*}
d_{33} & = \left( -c_{11} - 3c_{12} + 2c_{22} + c_{23} - 4c_{33} \right) d\varepsilon_{33} / 9 + \left( -c_{11} + 3c_{12} + c_{13} + 2c_{22} + 2c_{23} \right) d\varepsilon_{11} / 3 - \left( 2c_{13} - c_{12} - c_{13} \right) d\varepsilon_{11}^p / 3 - \left( 2c_{23} - c_{23} - c_{33} \right) d\varepsilon_{22}^p / 3 - \left( 2c_{33} - c_{33} - c_{33} \right) d\varepsilon_{33}^p / 3
\end{align*}
\]

Like Eq. (4), to consider both nonlinear behaviour of volume change and anisotropic property, the modified PUFF equation of state is introduced, and Eq. (13) is rewritten as:

**compression region:**

\[
dp = -A'd\theta + 2\left(A_2 - A_1\varepsilon \Gamma_0 / 2\right)d\theta \times \theta
- 3\left(A_1 - A_1\varepsilon \Gamma_0 / 2\right)d\theta + \left(\rho_0\varepsilon \Gamma_0 - \rho_0\varepsilon \Gamma_0 \theta\right)d\varepsilon
- \rho_0\varepsilon \Gamma_0 d\theta - \left(c_{11} + c_{13} - c_{22} - c_{23}\right)d\varepsilon^p_{ij} / 3 + \left(c_{11} + c_{13} - c_{22} - c_{23}\right)d\varepsilon^p_{ij} / 3 + \left(c_{12} + c_{22} + c_{23}\right)d\varepsilon^p_{22} / 3 + \left(c_{12} + c_{22} + c_{23}\right)d\varepsilon^p_{22} / 3
\]

\[
\]

\[

\]

\[

\]

\[

\]
After the deviatoric stress increment components and pressure increment are calculated from (14) – (16), the stress increment components can be obtained by \( d\sigma_{ij} = -dp\delta_{ij} + da_{ij} \). But the plastic strain increment must be gotten first, then the anisotropic yield criterion is discussed.

B. Rate-related Tsai-Hill Yield Criterion

For anisotropic materials, the Tsai-Hill yield criterion is used to judge whether the material has enter the plastic deformation state, and under condition of plane strain, the basic form is:

\[
F = \frac{\sigma_{11}^2}{Y_{11}^2} + \frac{\sigma_{22}^2}{Y_{22}^2} + \frac{\sigma_{33}^2}{Y_{33}^2} + \frac{\sigma_{12}^2}{Y_{12}^2} + \frac{\sigma_{13}^2}{Y_{13}^2} + \frac{\sigma_{23}^2}{Y_{23}^2} - 1 = 0
\]  

(17)

where \( Y_{ii} = 1/Y_{11}^2 - 1/Y_{22}^2 - 1/Y_{33}^2 \), \( Y_{ij} = 1/Y_{22} - 1/Y_{11} - 1/Y_{33} \), \( Y_{ij} = 1/Y_{33} - 1/Y_{ij} \), \( Y_{11}, Y_{22}, Y_{33} \) are the yield strengths in three principal directions and \( Y_{ij} \) is shear yield strength in 1-2 plane without considering strain rate effect, but they are related with strain hardening effect and equivalent plastic strain, i.e. \( Y_{ij} = Y_{ij0} \left[ 1 + a_{ij} \left( \overline{e} \right)^n \right] \). \( Y_{ij0} \) are the initial yield strengths from quasi static experiments, \( a_{ij}, n_{ij} \) are the parameters reflecting the strain hardening property, and \( \overline{e} \) is the equivalent plastic strain defined as \( \overline{e} = \sqrt{2e_{pl}^0 e_{pl}^0} / 3 \).

Considering the strain rate sensitivity [7, 8], use \( Y_{ij} \left[ 1 + \beta_0 \ln \dot{e} / \dot{e}_0 \right] \) to represent the yield strengths at different strain rate, where \( \beta_0 \) is the parameter reflecting strain rate sensitivity from dynamic experiment, \( \dot{e}_0 \) is the reference strain rate, and consider strain rate \( \dot{e} \) as effective plastic strain rate \( \overline{\dot{e}} = \sqrt{2e_{pl}^0 e_{pl}^0} / 3 \). For convenience of numerical simulation, we set \( \beta \) as the average value of \( \beta_0 \), and strain rate factor is \( R(\dot{e}) = 1 + \beta \ln \dot{e} / \dot{e}_0 \). Then the rate-related Tsai-Hill yield criterion is:

\[
(F + 1) / R^2 - 1 = 0
\]

(18)

Equation (18) can be rewritten as the rate separated yield criterion form:

\[
f = \dot{e}_0 \exp \left[ \frac{1}{\beta} \left( \sqrt{F + 1} - 1 \right) \right] - \dot{e} = 0
\]

where \( d\lambda = 2\beta \sqrt{F + 1} / \sqrt{3 D_0} \) is plastic flow factor, and \( D_0 = \partial F / \partial \dot{e}_0 \).

According to \( d\overline{\dot{e}} = \sqrt{2e_{pl}^0 e_{pl}^0} / 3 \) and (20), we get:

\[
d\lambda = d\overline{\dot{e}} / \sqrt{\frac{2}{3} \partial F / \partial \dot{e}_0} \]

(21)

From (20) and (21), the plastic strain increments are obtained, then the pressure and deviatoric stress increments are easily gotten by using (14) – (16).

IV. NUMERICAL SIMULATION AND DISCUSSIONS

A. Problem Simplification and Material Model

Assume that with enough distance from the nuclear explosion center, the approximately parallel X-ray radiates the cylinder shell surface along the vertical direction of axial line, thus a series of cirque profiles are formed (see Fig. 1). If the axial dimension is much larger than the radial direction, this problem can be simplified as plane-strain problem, and the thermal shock wave propagation property can be discussed within an arbitrary cirque (see Fig. 2).

TF composite material has three principal axes (use 1, 2, 3 denotation) respectively called as thickness, warp, and fill directions, and the system axes are denoted by (x, y, z). We make numerical simulations based on three model cases. At the beginning of radiation, for the first model called TF1, the material thickness direction is along the radial direction of cylinder shell, the warp is along circumferential direction, and the fill is along axial (z axis) direction. For the second model called TF2, the material warp is along the radial direction of cylinder shell, the fill is along circumferential direction, and the thickness is along axial (z axis) direction. For the third model
called TF3, the material fill is along the radial direction of cylinder shell, the thickness is along circumferential direction, and the warp is along axial (z axis) direction. The X-ray blackbody spectra are set as $kT=1$ keV and 3 keV, initial energy flux density is 200 J/cm², and the rectangular pulse width is 0.1 ms. The outer radius of cirque is 1 cm, the inner radius is 0.8 cm, and the main material parameters are shown in Table I - III [9].

### Table I
**EOS PARAMETERS OF TF MATERIAL**

<table>
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<th>Parameters</th>
<th>Values</th>
<th>Parameters</th>
<th>Values</th>
</tr>
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<tbody>
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<td>$\rho_0$ (g/cm³)</td>
<td>1.38</td>
<td>$F_0$</td>
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<tr>
<td>$c_0$ (km/s)</td>
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<td>$\gamma$</td>
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<td>$\alpha$</td>
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### Table II
**ELASTIC PARAMETERS OF TF MATERIAL**

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<td>$E_1$ (GPa)</td>
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<td>$E_2$ (GPa)</td>
<td>6.96</td>
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### Table III
**PLASTIC PARAMETERS OF TF MATERIAL**

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**B. Numerical Simulation Results and Discussions**

Using the orthotropic elasto-plastic dynamic constitutive model, a 2-D finite element program is made to simulate the thermal shock wave propagation in TF material. The Profiles of $\sigma_{xx}$ versus radius along the direction of 0° under radiation of 1 keV and 3 keV X-ray are given in Fig. 3-6 (positive values represent compression). The contours of $\sigma_{xx}$ are shown in Fig.7-10, and for the symmetry, only half of the cirque is displayed.
speed and attenuation of stress values, attenuation speed, and so on. The propagation are obvious differences in stress wave propagation speed, peak value is much lower, and a rarefaction wave is followed by the compression wave. From Figure 4 - Figure 6, we find that while the warp and fill axes are dominated by fibre whose fracture strengths are much lager.

V. Conclusion

A plane-strain orthotropic dynamic constitutive model which considers elasto-plastic deformation, strain rate sensitivity, strain hardening effect, and nonlinear property of volume change in both compression and expansion states is proposed in this paper. Taking the carbon fiber-reinforced phenolic composite composite for example, a 2-D finite element program is made to simulate the thermal shock wave propagation in cylinder shell under radiation of 1 keV and 3 keV X-ray, and the thermal shock wave propagation properties are discussed and obtained ultimately. The results show that the thermal shock wave exhibit different shapes under the radiation of soft and hard X-ray, especially for the sublimation phenomenon, and while the composite material is radiated along different principal axes, great differences exist in some aspects, such as wave propagation speed, attenuation of thermal shock wave peak value, spallation and so on.

REFERENCES