The mesoscopic damage analysis of composite solid propellant under different temperature

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Abstract: HTPB composite solid propellant is a kind of multi-particle filled energetic material, and its damage process is complex. In order to analysis the mesoscopic damage behavior of composite solid propellant, the molecular dynamics method is adopted to establish packing model. According to the experiment and simulation analysis under different temperature conditions, the result show that high or low ambient temperature makes debonding of the particle/matrix interface more likely to occur. The debonding of the particle/matrix interface reduces the modulus and results in nonlinear mechanical behavior of composite solid propellant.

1. Introduction

The solid rocket engine is the main source of power for rocket weapons and the core part to ensure the operation and stability of the entire combat system. Moreover, the mechanical properties of composite solid propellants play an important role in the structural integrity of solid rocket motors "[1]. In order to meet the solid propellant’s mechanical index in each working state, the damage stating point of the solid propellant must be analyzed. In the past 30 years, domestic and foreign scholars have conducted a lot of research on the constitutive of composite solid propellant. Most of the proposed models are constitutive relations of composite solid propellants based on phenomenological theory from the perspective of continuum mechanics [2]. However, most of these theories study the composite solid propellant as a continuous uniform medium, and the influence on the mesostructured of the material is rarely involved.

The composite solid propellant is composed of the continuous phase of the matrix and the solid particles of the oxidant. The interface between matrix and particle are clear, and it has the characteristics of heterogeneity at the microscopic level. The interface dewetting between matrix and particle of propellant is observed by using scanning electron microscopy [3]. The results show that the interface dewetting is the main reason for the nonlinearity of the mechanical properties of the propellant. However, due to the limitations of test methods, it is necessary to use numerical tools to conduct an intensive study on the mesoscopic damage and evolution of composite solid propellants. Han [4] established an exponential rate-dependent cohesive zone model and obtained the cohesive zone model parameters through experimental inversion identification methods. The crack propagation process of HTPB propellant is simulate. Han [5] found that the mechanical properties of the propellant are related to the relaxation behavior of the matrix, and independent of the random distribution of particles. The surface-based cohesive method is applied to simulate mesoscopic damage of propellant.

In present work, the exponential cohesive zone model is used simulate matrix/particle interface dewetting and analyze the mechanical properties of the meso damage model.

1. Model

1.1. Material of composite solid propellant

In this paper, HTPB composite propellant with a filled particle volume fraction of 63.8% is selected. The particle size distribution follows the normal distribution, as shown in Fig. 1.
molecular dynamics method is used to generate a packing model, as shown in Fig. 2.

![Fig. 1 Particle size distribution](image1.png)

![Fig. 2 Packing model](image2.png)

As shown in Fig. 3, prony series is used to perform relaxation experiment on the matrix material of HTPB composite propellant, and the fitting expression is:

$$E(t) = E_\infty + \sum_{i=1}^{n} E_i \exp\left( -\frac{t}{\tau_i} \right)$$

(1)

![Fig. 3 Stress relaxation curve of HTPB propellant matrix](image3.png)

### 1.1 Cohesive zone model

Cohesive element is a new element embedded in two solid elements to define the damage model. In the two-dimensional model, the element type of the cohesive element is COH2D4, which has 4 nodes. The damage law of the cohesive element follows the traction-displacement relationship of the exponential cohesive zone model.

In the traction-displacement of the exponential cohesive zone model, the stress change is continuous, and the stress gradually decreases to zero in the process of decreasing. The exponential cohesive zone model selects fracture energy as the condition for judging unit damage:
\[
\phi(\Delta) = \phi_n + \phi_t \cdot \exp\left(-\frac{\Delta_n}{\delta_n}\right) \left[1 - r + \frac{\Delta_n}{\delta_n}\right]^2 \left[1 - q + \frac{r - q}{r - 1}\right] \left[\frac{\Delta_n}{\delta_n}\right] \exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)
\]

(2)

where \(\Delta_n\) and \(\Delta_t\) represent the normal and tangential displacement values of the interface, respectively. The normal characteristic displacement value and the tangential characteristic displacement value are \(\delta_n\) and \(\delta_t\) respectively.

The exponential cohesive zone model needs to determine two parameters, namely the cohesive strength \(\sigma_{\text{max}}\) and the failure displacement \(\delta_f\). Inversion recognition optimization algorithm is used to obtain the cohesive zone model parameters of the particle/matrix interface under different temperatures, as shown in Table 1.

<table>
<thead>
<tr>
<th>Temperature T/℃</th>
<th>-40℃</th>
<th>20℃</th>
<th>50℃</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma_{\text{max}})/MPa</td>
<td>0.81</td>
<td>0.22</td>
<td>0.17</td>
</tr>
<tr>
<td>(\delta_f)/mm</td>
<td>0.076</td>
<td>0.035</td>
<td>0.024</td>
</tr>
</tbody>
</table>

### 2 Result and discussion

Through the numerical simulation of the packing model, the initial modulus at different temperatures is obtained, as shown in Fig. 4. As the temperature increases, the initial modulus of the HTPB solid propellant decreases. The initial modulus at low temperature is significantly higher than that at high temperature and normal temperature. The initial modulus of the material dose not change much under high temperature and normal temperature.

Fig. 5 shows the dewetting point modulus at different temperatures. Similar to the results of the initial modulus, the dehumidification point modulus at low temperature is higher than that at high temperature and normal temperature. In order to further analyze the impact of modulus changes on damage, the rate of decrease in modulus at different temperatures will be given below, as shown in Fig. 6. The lower the temperature, the greater the rate of decrease of the modulus of the particles/matrix interface, and the greater the change in the slope of the curve. Under the condition of high temperature and normal temperature, the rate of decrease of modulus is lower than that of the condition of low temperature, which shows that temperature is one of the reasons that affect the nonlinear change of the curve. In order to ensure the mechanical properties of the propellant in the working state, the next step should be to explore how to delay the damage of the propellant under different temperature load conditions.

![Fig. 4 Initial modulus](image-url)
3 Conclusion

The dewetting of the particle/matrix interface is one of the reasons that affect the emergency nonlinear mechanical behavior of the composite solid by numerical simulation. By comparing the test and numerical simulation results at different temperatures, it can be found that the mechanical behavior of the composite solid propellant is greatly affected by the temperature. If the temperature is too high or too low, the degree of dewetting of the propellant will increase, making the propellant more vulnerable to damage.

References