Meso - damage of composite solid propellant and its numerical simulation

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Abstract

The experimental research progress of meso-mechanical properties of composite solid propellants is summarized. At the same time, the progress of the numerical simulation of meso-damage of composite solid propellants is reviewed from the establishment of the meso-scale solid propellant model and the finite element calculation. On this basis, it points out the deficiencies in current research and the direction for further research.

Keywords

Solid propellant, numerical simulation, review.

1. Introduction

Solid rocket motor in the production, transportation, storage and use of the process, to withstand thermal stress, impact, acceleration, vibration and ignition pressure and other load. These loads will cause the stress and strain inside the column. If it exceeds the allowable range of mechanical properties, the column will crack, deform and even de-bond the shell lining, eventually losing the efficiency of use and causing the mission to fail. Thus, the reliability of solid rocket motors depends largely on the structural integrity of the grain. Composite solid propellants are energetic composites with a high solid-to-high particle-fill ratio and their macroscopic mechanical behavior strongly depends on their meso-structure. Therefore, in recent years, the meso-damage of composite solid propellant and its numerical simulation have become the research hotspot of scholars at home and abroad. At present, there are generally three steps in the study of meso-damage and numerical simulation of composite solid propellants at home and abroad: (1) Perform mechanical tensile or compression tests on composite solid propellants to obtain experimental data, depict stress-strain curves, and analyze The mechanical properties of the composite solid propellant under tension or compression; (2) Establish a constitutive model of the composite solid propellant that meets the requirements, and fit the constitutive model curve through the stress-strain curve obtained from the test to obtain the constitutive model established. (3) Establish a meso-structure model of the propellant, combine it with the constitutive model established in the previous period, and compare it with the experimental results to verify the correctness of the simulation results. This article will also review the above three aspects.

2. Experimental Research and Summary on Meso-Mechanical Properties of Composite Solid Propellants

2.1 Experimental study on meso - mechanical properties of composite solid propellant

The composite solid propellants have the characteristics of multi-scale internal, divided according to their research object and feature size, mechanical studies are generally divided into macroscopic mechanics, meso-mechanics, micro-mechanics. On the mesoscale, composite solid propellants are
generally considered to be three-phase structures consisting of oxidized particles, polymeric binders, and the interface between particles and binders. At present, for the study of meso-mechanical properties of composite solid propellants, the composite solid propellants are mainly subjected to tensile or compressive destruction at home and abroad. The fracture of propellants is observed by optical microscope, electron microscope scanning and micro-CT. The situation then analyzes the experimental data to investigate the correlation between the mesoscopic damage and the macroscopic mechanical properties of the propellant.

Zeng Jiaya et al. [1] The fracture behavior of the specimen under the tension state through the fracture morphology and scanning electron microscopy of the butyrolactam results in qualitatively predicting the change of macroscopic mechanical properties through the variation of the dehumidification behavior of the meso-structure of the propellant.

Field [2] scanning electron microscopy of quasi-static tensile fracture of PBX explosives showed that there is no obvious fracture of the HMX transgranular fracture, the specimen damage is mainly intergranular fracture between solid particles, macroscopic cracks mainly along the explosive crystal Interface extension.

Cheng Pengwan [3] Brazil experiment (indirect tensile test or splitting experiment) on the PBX explosives were studied by experiments found that the size and location of the initial damage with randomness, so the fracture location of the specimen is also random. But the crack is usually first generated in the large grain boundary, and the fracture occurs mainly in the particle and matrix bonding interface (Figure 1).

Luo Jingrun [4] performed a tensile fracture test on a three-point bending polymer bonded explosive test piece, and found that the fracture toughness of the polymer bonded explosive has a large correlation with the time crack length, and the crack follows the increase in fracture toughness, maximum load, and critical load drastically decreased.

Chen Yu [5] using in situ tensile scanning electron microscopy (SEM) NEPE propellant was uniaxial tensile test to study the damage process. Scanning electron microscopy showed that the propellant firstly fractured at the interface between the matrix and the particles to produce microcracks. The microcracks were continuously expanded and merged, resulting in the deformation of the adhesive. Macroscopic cracks or voids eventually appeared, which led to the rupture of the propellants.

Chang Wujun [6] carried out a uniaxial tensile test on HTPB propellants, using a CCD microanalysis technique to synchronously photograph mesoscopic images. Through the analysis of experimental results, it is found that the macro-stress-strain curve can be roughly divided into four stages: linear elastic zone, dehumidification zone, stress platform zone and tending to fracture zone. The relationship between dehumidification and strain rate was analyzed. It was found that with the increase of strain rate, the dehumidification of matrix / particle interface became less and less obvious. Under high strain rate stretching, the damage of propellant showed more obvious Matrix rupture.

In addition to the uniaxial tensile test of composite solid propellants under normal temperature and non-aging conditions, domestic and foreign scholars observed the mechanical properties and fracture morphology, in order to reflect the mechanical properties of solid propellants under long-term storage conditions, and also carried out aging conditions. Under the tensile test.

Zhang Xudong [7] used a nitrogen-enclosed system of high-temperature and high-humidity aging environments to simulate the storage environment of naval solid rockets. Through experiments, it was found that the tensile strength of composite solid propellants gradually decreased with the aging time. The oxidative crosslinking and hydrolysis chain scission exist at the same time, resulting in no significant change in the maximum elongation. It is also believed that the aging of the propellant is mainly caused by the oxidative crosslinking of the binder, the hydrolysis and scission of the binding agent, and the dehumidification.

According to the experimental data, Cao Liang [8] conducted an accelerated aging test. According to the experimental data, the maximum tensile strength decreases, increases, decreases, increases and
decreases with the aging time. During the process, the rate of change of the maximum tensile strength is basically positive, the effect of oxidative crosslinking is stronger than the effect of degradation and chain scission (as shown in Fig. 2), and the electron microscope scanning observation of the propeller section shows that some of the matrix \( \text{Dewetting of particle interface.} \)

Figure 1 PBX Brazil experiment  
Figure 2 Changes in maximum elongation with aging time

### 2.2 Experimental study on meso - mechanical properties of composite solid propellant

Based on the previous studies, it is found that the mechanical properties and fracture morphology of composite solid propellants show the following three main characteristics: (1) In the low-speed quasi-static tensile process, the composite solid propellant damage is mainly concentrated near the large particles, the bigger the particles are, the more severe the dehumidification damage is. The small particles, the initial microcracks and the micropores have little effect on the damage of the propellant. (3) The fracture of the composite propellant mainly extends along the particle / matrix interface. Under the aging conditions, the tensile strength of the composite propellants decreases with the aging time due to the oxidative crosslinking of the adhesive, the hydrolysis and scission of the bonding agent and the dehumidification.

### 3. Research and Summary of Constitutive Model of Composite Solid Propellant

#### 3.1. Study on Constitutive Model of Composite Solid Propellant

The constitutive model of the material reflects the mechanical behavior of the material under external factors (temperature, pressure, loading rate, etc.). Through the constitutive model of the material, the mechanical behavior of the material under external load can be accurately predicted. Material design provides the theoretical basis. Domestic and foreign scholars have done a lot of research on the constitutive model of composite solid propellant.

Peng et al. [9] used the equivalent inclusion theory of Eshelby to analyze the influence of slender ellipsoidal particles on the viscoelastic constitutive equation of slender ellipsoid-particle reinforced composite solid propulsion line. It was found that the reinforcing effect of slender particles on the matrix was mainly concentrated in the vertical direction, the enhancement effect of disordered orientation of slender particles on the substrate and the enhancement effect of the uniaxial orientation of the particles on the longitudinal direction of the substrate have a quantitative relationship.

Based on the theory of linear elastic fracture, Peng Wei [10] constructed a nonlinear viscoelastic constitutive model of composite solid propellants that includes the matrix viscoelasticity effect, the particle reinforcement effect and the "dehumidification" microcrack damage at the particle / matrix bonding interface model. The parameters of the constitutive model were determined by dynamic tensile tests on HTPB propellants.

Xu [11] proposed a nonlinear viscoelastic constitutive model with damage based on the homogenization theory of composite materials. The relaxation experiment and uniaxial pulling of the solid propellant under quasi-static loading were proposed. Stretching experiments confirmed the parameters of the constitutive model.
HAN Long et al. [12] combined the characteristics of macro and micro studies and proposed a research approach that can consider macro-mechanical behaviors of micro-factors. He took NEPE propellant as the research object, combined with the viscoelastic dehumidification criteria, the quantitative changes of the mesoscopic structure were introduced into the macroscopic viscoelastic constitutive relationship, and a new method was proposed to effectively consider the "dehumidification" of the mesoporous particles of the NEPE composite solid propellant. The nonlinear viscoelastic constitutive model.

3.2. Research Summary of Constitutive Model of Composite Solid Propellants
In the study of composite solid propellant containing damage, high strain rate, low strain rate and other constitutive models, a large number of domestic and foreign scholars have done a lot of research and achieved a lot of achievements. With the deepening of researches, the research on the constitutive model of composite solid propellant generally goes through linear elastic constitutive model, superelastic constitutive model and viscoelastic constitutive model. The constitutive model is more in line with the actual situation of propellant. Through these constitutive models, the macroscopic mechanical behavior of propellants can be grasped more accurately, which has great application value to practical engineering applications.

4. Research and Summary of Constitutive Model of Composite Solid Propellant

4.1. Research Progress in Numerical Simulation of Mesoscopic Damage of Composite Solid Propellant
At present, the finite element method is the most widely used and most technologically sophisticated numerical analysis method, which can save a lot of experimental time and experimental cost when solving scientific and engineering problems. Compared with other numerical methods, the finite element method has the advantages of being suitable for any set shape and material, boundary conditions and geometric nonlinear problems, easy to program, mature and large commercial software and more. Scholars at home and abroad have conducted a large number of numerical simulations on the meso-damage process of composite solid propellants using the finite element method. At present, for the study of composite solid propellants, the finite element method mainly focuses on the process of "dehumidification" at the particle / matrix interface of composite solid propellants.
Xu [13] constructed a cohesive region constitutive equation composed of a rate-independent cohesive region model and Maxwell. Through experimental and numerical calculations, the strain rate effect and interface debonding failure behavior of adhesively bonded cantilever beams were analyzed.
Wang Guang [14] conducted a micro-CT scan of the bonded interface of the composite solid propellant and the propellant / lining, expanded the particle filling algorithm, established the meso-particle filling model of propellant and introduced the bonding interface unit, and in the process of meshing, the "balance of force method" is adopted. Through the simulation results, it is found that the interface element can describe the mechanical behavior of the interface under different aging time accurately.
Zhi Shijun [15] established a composite solid propellant filling model using molecular dynamics algorithm, using Surfaced-based cohesive method to set contact damage at the particle/matrix bonding interface, and using finite element method to the mesoscopic damage evolution of propellant. The process was numerically simulated (as shown in Figure 3).
The finite element method uses a continuous displacement approximation function. When dealing with some strong discontinuities (such as high stress areas near the crack tip), there are disadvantages such as poor solution accuracy, low efficiency, and huge workload, and when dealing with inclusion problems The boundary of the unit must be located at the interface between the inclusion and the substrate. The two-dimensional model with a higher degree of automation for the grid is not easy, and it is more complicated for the three-dimensional problem.
In order to solve the problem of large deformation and fracture in finite element method, Belytschko of Northwestern University in 1999 proposed a modified finite element method (FEM) for solving discontinuity problem based on finite element method (XFEM ). [16] Extended finite element method Based on the standard finite element method, the standard finite element method is used to solve continuous problems, and the displacement function of the finite element is modified on the problem of containing discontinuities. At the same time, the description of the discontinuous boundary is added method. Therefore, the extended finite element method once proposed has shown a strong superiority, just a dozen years time in the crack propagation is widely used.

Based on the ABAQUS platform, Liu Jian [17] simulated the crack propagation process of a flat plate with holes based on the extended finite element method. The simulation results show that the crack propagation path is first curved and then extends horizontally. The presence of holes causes the stress concentration and affects the crack propagation path. As shown in Figure 4.

![Figure 3 Simulation result based on Surfaced-based cohesive](image3.png)

![Figure 4 Fracture failure with holes in the plate](image4.png)

The extended finite element method can simulate the propagation of meso-cracks more effectively and simulate the propagation of cracks more realistically. The propagation direction of cracks can not be limited by the boundaries of elements and can even be extended through the elements. The extended finite element method does not require local encryption of the unit, which can effectively reduce the number of units, increase the speed of calculation, and save computational costs.

4.2. Summary of numerical simulation research on meso-damage of composite solid propellant

At present, the numerical simulation of meso-damage of composite solid propellants is mainly based on the fact that the bilinear bonding unit or the surfaced-based cohesive unit is inserted at the interface between the particles and the matrix. The generation of the meso-crack and the evolution of the polymerization are simulated by the finite element method process. With the extensive application of the XFEM method, some scholars began to apply this method to the numerical simulation of the macro-fracture of the composite solid propellant and achieved good results.

5. Conclusion

At present, the numerical simulations of mesoscopic damage of composite solid propellants by domestic and foreign scholars only focus on the degree of "dehumidification" at the bonding interface between the particles and the matrix, and do not fully reproduce the dewetting of the composite solid propellant microparticle interface "The whole process of matrix fracture; In addition, solid missile weapons have the characteristics of long-term storage and use. In long-term storage, the mechanical properties of propellant must change due to aging. Therefore, using XFEM method to study the evolution of meso-damage of composite solid propellants under aging condition can completely reproduce the whole process of microcracks generation, propagation and polymerization until the macro cracks occur under long-term storage conditions of propellants.
References


