Automatic application of periodic boundary conditions in meso analysis of composite solid propellant

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Abstract. In the meso numerical simulation of composite solid propellant, the periodic boundary conditions are difficult to be applied due to the complexity of the model and the number of element nodes, which makes it not widely used in the meso analysis. Therefore, based on the periodic boundary condition theory, this paper adopts ABAQUS_Python secondary development, periodic boundary conditions were applied to the meso numerical model of composite solid propellant by Python script under three working conditions of two-dimensional principal axis direction and plane shear direction. The results show that the deformation and stress distribution of the numerical model of composite solid propellant conform to the characteristics of periodic boundary conditions.

1. Introduction

With the development of data analysis methods and the progress of computer technology, it is one of the hot spots to carry out the multi-scale structure analysis of composite solid propellant in the micro structure analysis. Compared with the given macroscopic constitutive model of composite solid propellant and the analysis of composite solid propellant structure at a single macro scale, the macro mechanical behavior of composite solid propellant is given based on the results of meso analysis in multi-scale analysis, which has higher theoretical accuracy. In order to realize the connection between macro scale and micro scale in multi-scale analysis, it is usually necessary to assign a representative volume unit (RVE) to any material point on the macro scale. Then, the macro strain is transformed into the boundary conditions of the micro RVE by downscaling technology, and the meso mechanical response of RVE is obtained by meso analysis. On this basis, the meso scale results are transformed into the constitutive behavior required by macro scale calculation by ascending scale (computational homogenization)[1]. It is one of the key links to transform macro strain into meso RVE boundary conditions. At present, the commonly used micro RVE boundary conditions mainly include uniform strain boundary conditions, uniform stress boundary conditions and periodic boundary conditions. For a fixed size RVE, the macroscopic validity of materials obtained by periodic boundary conditions is more accurate than the other two boundary conditions[3]. However, most scholars did not give a detailed description of the boundary conditions applied in the research process when the composite solid propellant was studied by meso structure modeling[4]. Han long[9] studied the macro relaxation behavior of composite solid propellant based on meso structure model. In the treatment of boundary conditions, uniform displacement boundary conditions were used instead of periodic boundary conditions, but when the size of representative volume unit was small, there would be large error. Feng Tao[10] uses fixed constraints in the treatment of boundary conditions, which ensures the straight boundary of the specimen during the debonding process of composite solid propellant, but it will inevitably lead to the material being over constrained. In order to study the macro and micro structure...
changes of composite solid propellant more accurately, periodic boundary conditions must be applied. However, for composite solid propellant, the shape and size of particles inside the material are quite different, and the corresponding RVE size is also large. Therefore, there are many boundary nodes. When applying periodic boundary conditions to RVE manually, it is necessary to match the nodes on the corresponding boundary one by one and apply boundary constraints point by point, which will cause huge workload. Therefore, based on the theory of periodic boundary conditions, combined with the finite element calculation software ABAQUS platform, using Python program development, this paper puts forward the method of automatic application of periodic boundary conditions, and develops the script of automatic application of periodic boundary conditions in meso analysis of composite solid propellant based on ABAQUS. Finally, the feasibility of the script is verified by an example.

2. Basic theory of periodic boundary conditions

The expression of periodic displacement field is\(^1\)[11]

\[ u_i = \bar{\varepsilon}_{ik} x_k + u_i^* \]  

In the formula: \( \bar{\varepsilon}_{ik} \) is the cell average strain; \( x_k \) is the coordinate of any point in the cell; \( u_i^* \) is the periodic displacement correction. For composite solid propellant structures, most of the cell models have parallel and paired interfaces. On one pair of interfaces, the periodic displacement field can be written as\(^1\)[12]

\[ u_i^{(+)} = \bar{\varepsilon}_{ik} x_k^{(+)} + u_i^* \]
\[ u_i^{(-)} = \bar{\varepsilon}_{ik} x_k^{(-)} + u_i^* \]

In the formula: superscripts \( + \) and \( - \) represent the positive and negative directions along the \( X_j \)-axis respectively; \( u_i^* \) is the same on the parallel opposite plane of periodic cell. By subtracting formula (2) and formula (3), we can get

\[ u_i^{(+)} - u_i^{(-)} = \bar{\varepsilon}_{ik} (x_k^{(+)} - x_k^{(-)}) = \bar{\varepsilon}_{ik} \Delta x_k^{j/} \]  

For each group of parallel opposite faces of a square cell, \( \Delta x_k^{j/} \) is a constant. Once \( \bar{\varepsilon}_{ik} \) is given, the displacement difference on the right side of equation (4) becomes constant. Therefore, equation (4) can be rewritten as

\[ u_i^{(+)}(x, y) - u_i^{(-)}(x, y) = c_{i/}^{(j/)} \]  

\( i, j = 1, 2, 3 \)

Equation (5) does not contain periodic displacement correction \( u_i^* \), which can be easily realized by applying multi-point constraint (MPC) equation in finite element analysis.

In the homogenization theory, the boundary conditions imposed on the rve should satisfy the conditions of equal macro and micro deformation energy, i.e. the Hill-Mandel condition, as follows:

\[ \bar{\sigma}_i \varepsilon_{ij} = \int_{\partial V} \bar{\sigma}_i \varepsilon_{ij} \, ds \]  

According to the principle of virtual work, the work done by the external force on the allowable displacement is equal to the work done by the stress on the allowable strain. Huang Yefei\(^1\)[13]obtained a simplified Hill-Mandel formula without considering physical strength

\[ \frac{1}{V} \int_{\partial V} t_i \nabla \bar{u} \, ds = 0 \]  

In the formula, \( t_i \) is the stress vector and \( \nabla \bar{u} \) is the displacement. It can be seen that when the
displacements of the corresponding sides are equal, the stress vectors are equal in size and opposite in direction (i.e. the displacement continuity and stress continuity conditions are satisfied), and the Hill-Mandel condition is satisfied. Xia et al[14] further proved that equation (4) satisfies the condition of stress continuity. Therefore, equation (5) can be used to impose periodic displacement boundary conditions on composite solid propellant.

3. **Automatic application and verification of periodic boundary**

3.1. **Automatic application of periodic boundary conditions**

For RVE model, the boundary conditions are determined by the macro strain field converted to the displacement of the boundary node on the meso scale[15], so the macro strain is transformed into the displacement of the boundary node on the meso scale for constraint. The automatic application of periodic boundary conditions is based on the meso structure finite element model of composite solid propellant. Firstly, it is necessary to mesh the meso structure model of composite solid propellant and ensure that the grid density on the boundary is the same. Due to the high filling ratio and large size difference of composite solid propellant particles, it is necessary to refine the mesh of RVE model, which will lead to more grid nodes. Therefore, through ABAQUS_Python secondary development, the python script is written. Through Python script, the node number and other information are automatically read, and the position of the nearest node on the opposite side is calculated automatically, and the node pair is established. Through equation (4), the node pair is constrained by Python script.

3.2. **Example verification**

According to the mesostructure of composite solid propellant, a two-dimensional mesostructure model of 4mm × 4mm composite solid propellant is established by random algorithm, as shown in figure 1. The model parameters are shown in Table 1. With the help of finite element software ABAQUS, the micro structure of composite solid propellant is meshed. The grid density is set as 0.4 times of the minimum particle size of aggregate, and the corresponding edge distribution is the same, which ensures one-to-one correspondence of nodes on the relative boundary.

![Figure 1. Meso structure model of composite solid propellant.](image)

| Components     | HTPB | AP  | Al   |
|----------------|------|-----|-----|
| Elastic modulus (MPa) | 0.36 | 32  | 68  |
| Poisson's ratio  | 0.49 | 0.14| 0.33|

Python script is used to establish periodic boundary conditions for the meshed model, and three different constraints are imposed on the composite solid propellant, including the tension in the principal axis direction and shear in the plane. The macroscopic strain components under these three conditions are shown in Table 2.
Table 2. Boundary conditions of RVE

| Working condition | $\varepsilon_{11}$ | $\varepsilon_{22}$ | $\gamma_{12}$ |
|-------------------|---------------------|---------------------|----------------|
| 1                 | 0.25                | 0                   | 0              |
| 2                 | 0                   | 0.25                | 0              |
| 3                 | 0                   | 0                   | 0.25           |

Figure 2, figure 3 and figure 4 show the deformation diagram and equivalent stress diagram under condition 1, 2 and 3 respectively. It can be seen that under different working conditions, the relative boundary of the specimen shows the same deformation shape and equal displacement difference, which meets the requirement of continuous displacement under periodic boundary conditions; The stress distribution of composite solid propellant is not uniform, but the corresponding region of relative boundary presents the characteristics of consistent stress, which meets the requirement of continuous stress under periodic boundary conditions.

![Deformation diagram](image1)
![Equivalent stress diagram](image2)

Figure 2. Loading result diagram of sample under condition 1.

![Deformation diagram](image3)
![Equivalent stress diagram](image4)

Figure 3. Loading result diagram of sample under condition 2.

![Deformation diagram](image5)
![Equivalent stress diagram](image6)

Figure 4. Loading result diagram of sample under condition 3.
4. Conclusion
In order to solve the problems of complicated operation and long time-consuming in the application of periodic boundary conditions in meso analysis of composite solid propellant, this paper is based on periodic boundary condition theory and combined with ABAQUS Python secondary development, the method of automatic application of periodic boundary conditions is proposed, and the correctness of the method proposed in this paper is verified by an example.

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