Micromechanical modeling and numerical simulation of ablation of 3D C/C composites

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Abstract Carbon-carbon (C/C) composites, in which a carbon matrix is reinforced by carbon fibers, are mainly used as thermo-structural protections in the aerospace engineering. The ablation of C/C composites at high-temperature causes mass loss, which is dominated by coupling effect of physical, chemical and mechanical factors. This paper classified the C/C ablation into three types according to the ablation mechanism: linear-rate reaction, parabolic-rate reaction and logarithmic-rate reaction. In this work, a micromechanical model of C/C composite with high-temperature heat conduction was established. A linear heat-transfer finite element analysis was carried out for revealing the damage morphology of C/C composites at an ultra high temperature.

Keywords C/C composites, ablation, surface recession, thermal damage

1. Introduction

Thermal protection materials, which are highly required in advanced thermal protection systems and envisioned for use on future hypersonic and space craft, will inevitably be subjected to utmost high temperature and strong oxidizing environment, such as the intercontinental ballistic missile nose cap often suffer an ultra high temperature of 7000~8000K atmosphere, dozens of megawatt heat flow density, unexpected high erosion of particle cloud and nuclear radiation in reentry [1]. Ablation phenomenon is frequent occurrence on the re-entry progress of space shuttle or rocket caused by aerodynamic heating, which can heat the surface of spacecraft up to a extremely high temperature in seconds. The thermal energy may lead to solid surface melting, evaporation, sublimation or decomposition of solid surface in the ultra temperature environment. Therefore, it is important for protecting the inner structure and astronauts from high temperature thermal damage.

Carbon-carbon(C/C) composites consist of carbon matrix and reinforced carbon fibers[2] and possess a series of excellent mechanical properties, such as high temperature resistance, low density, high specific modulus, high specific strength, small coefficient of thermal expansion, high ablation resistance and high temperature resistant. Therefore, C/C composites are widely used in technological applications as excellent ablation resistance and thermal protection materials, e.g. solid rocket motor (SRM) nozzle throats, reentry rocket nose cone, missile nose-tips and leading edges [3,4]. In the ablation process, the sublimation or decomposition of C/C composites will take away lots of heat and the surface temperature of aerospace craft will be effectually lowered down. Consequently, the ablation resistance of C/C composites is directly related to the strengths of astrovehicle, determining the achievement of task scheduled. Hence, the research on the ablation of C/C composites has a great significance.

In generally, researchers investigate the ablation mechanism of C/C composites in high temperature environment from two aspects: experiment research and numerical simulation research. The experiment is an effective method to understand the ablation mechanism of C/C composites. Unfortunately, the experimental simulation is extremely expensive because of the complexity of the extreme environmental conditions. Therefore, computer-based numerical simulation, which can predict the thermo-mechanical response of these composite heat shields, have become an effective method for analyzing the ablation behavior of C/C composites. Ultimately, it will achieve the design purpose of C/C thermal protective materials based on the ablation research and simulation

In recent study, Aspa et al.[5] carried out a one-dimensional diffusion model to describe the effective surface ablation recession. Their analysis focused on the ablation of diffuse-controlled reaction. Vignoles et al.[6,7] investigated surface roughness of C/C composites by SEM. They discovered that fibers, matrices and interphase have different ablation resistance, which usually leads to typical surface roughness feature. In their work, a three-dimensional reaction-diffusion local model was set up to simulate the formation of the typical needle shape of the carbon fibers during ablation. Laborde et al.[8] established a damage model for carbon-carbon orthotropic composite materials with a special attention to the thermo-mechanical effects. They performed a numerical solution using an implicit incremental scheme implemented in ABAQUS.

The origanization of the paper is as follows. In the section 2, a brief introduction is given of ablation mechanism of C/C composites. Section 3 is devoted to classify the C/C ablation recession into three types according to the ablation mechanism. In section 4, a mesoscopic analytical model of C/C composite with high temperature heat conduction was established. The analysis used a heat-transfer finite element in ABAQUS to simulate the ablation morphology of C/C composites at ultra high temperature. The last section is the summary of the main conclusion resulted from the present work.

2. Ablation mechanism of C/C composites

There are mainly two types of carbon-oxygen (C/O) reaction for C/C composites in oxidation atmosphere: $C+O_2=CO_2$ and $2C+O_2=2CO$.
In the ablation process, the surrounding oxygen is transferred to the surface of the C/C composites. Ablation reaction primarily occurred on the surface of those materials, which resulted in mass loss with melting, sublimation and particle erosion. Then with the inward diffusion of oxygen in the surface microcracks and pores of C/C structure, further oxidation occurred. During the reaction process, fiber and matrix are oxidized simultaneously. Whereas the reaction rate of fibers is lower than the matrix. That means, along with the aggravation of ablation, the first melted interface layers separate the fibers and matrix. Ultimately, the fibers are burned into needle shape, while the around matrix are eroded into cylindrical shell. Fig.1 shows the ablation process of a C/C composite.

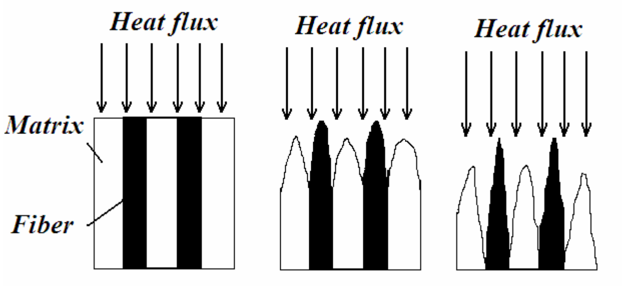


Figure 1. The ablation of the C/C composites

3. Ablation reaction rate of C/C composites

The oxidation reaction of C/C composites without high-temperature oxidation resistant coating is time-independent, and is mainly controlled by gas/solid interface reaction rate. In this case, the mass loss rate of C/C composites is linear with response time, as shown in Equation 1.

$$\frac{\Delta m}{A} = k_l t \tag{1}$$

where $\frac{\Delta m}{A}$ is the mass loss of C/C composites per unit area; k_l denotes coefficient of linearity relation, which is determined by experiment; and t is the reaction time. Fig.2 shows the recession location of the ablation surface during the ablation process.

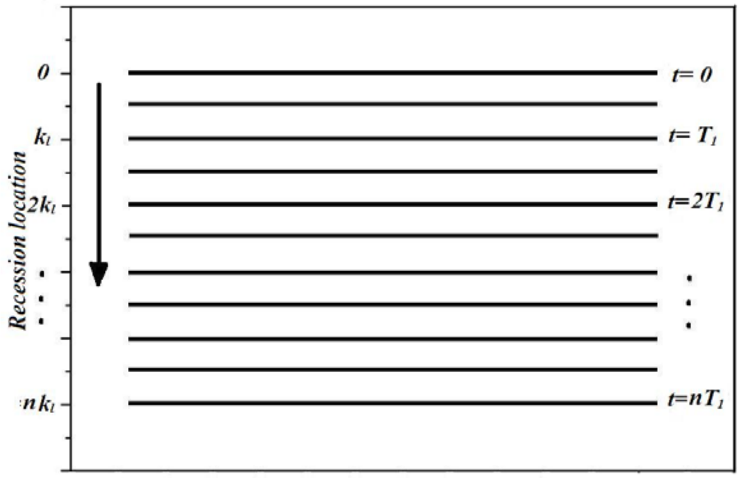


Figure 2. Recession location of the ablation surface

The ablation reaction of C/C composites with high-temperature oxidation resistant coating follows the parabolic-rate law, and the reaction rate is inversely proportional to the square root of time, which is determined by the diffusion rate of oxygen in the inner material, as shown in Equation 2.

$$\left(\frac{\Delta m}{A}\right)^2 = k_p t \tag{2}$$

where k_p is the parabolic rate constant or diffusion constant, which is derived from Arrhenius law as shown in Equation 3.

$$k_p = k_0\, exp\left(-\frac{Q}{RT}\right) \tag{3}$$

where k_0 is the constant obtained by experiment; Q is the activation energy of oxidation; and R presents gas constant; T is the reaction temperature.

Logarithmic rate reaction is suitable for C/C composites with silicon elements. Early in the reaction process of ablation, the oxidation of silicon elements is rapidly, and silicon oxide produced from the oxidation between silicon and oxygen can generate a compact oxide layer covering the surface of C/C composites. The generated SiO_2 layer will prevent further diffusion of the oxygen and then increase the ablation resistance of the C/C. With the exacerbated of oxidation, the ablation of C/C composites will become severe and accompany with mass loss. Hence, the logarithmic-rate reaction mechanism is only appropriate for representing the early reaction of the C/C composites with silicon in lower high temperature.

3. Analytical model

C/C composite is a homogeneous multi-scale material. In microstructure, the “skeleton” of the composite consists of unidirectional bundles made of several thousands of fibers which are linked together by a pitch-based matrix. The formation of the typical roughness patterns of C/C composites in ablation process depends on the unidirectional fibers perpendicular to material surface. Due to the different ablation rates between carbon matrix and carbon fibers, the unidirectional fibers perpendicular to material surface will separate from the carbon base, expose to the external oxidation environment, and take the shape of “needle clusters”. This paper focuses on the unit cell model of C/C composites in micromechanical structure, analyzing the change laws of C/C composites in high temperature thermal radiation and predicting the ablation morphology change.

There are two basic kinds of unit cell model of C/C composites. The first model, as shown in figure 3, is a hexahedron representative volume element (RVE), in which matrix and fibers are assumed homogeneous and isotropic, and the internal pores are negligible. The second model is a cylinder RVE, in which the fiber bundles are fit together into a 3D C/C structure. This meso-structure forms a network of meso-scale pores, as shown in figure 4.

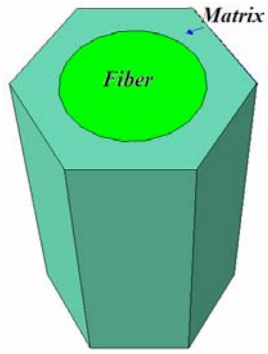


Figure 3. Hexahedron RVE of C/C

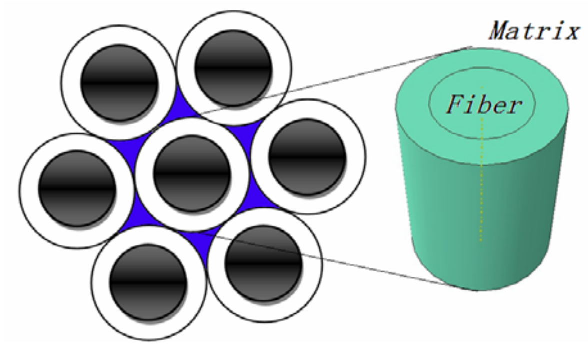


Figure 4. Cylinder RVE of C/C

In the finite element software of Abaqus, the thermal radiation analysis can be conducted according to the following steps: (ⅰ)modeling, (ⅱ) defining the materials property, (ⅲ) assembly model, (ⅳ) creating heat conduction steps and interaction, (ⅴ) applying boundary condition and load, (ⅵ) meshing and selecting element type, (ⅶ) creating analysis job, (ⅷ) results visualization.
The physical properties of C/C composite in the two models are listed in table 1. In the thermal radiation analysis, the physical constants of absolute zero temperature and Stefan-Boltzmann constants are -273.15 ℃ and 5.67E-8 W/(m^2 • k^4).

Table 1. Physical properties of C/C composites in the simulation models

Characteristic	Density	Elastic modulus	Poission’s ratio	Thermal conductivity	Specific heat
Unit	kg/m^3	GPa	--	W/(m • ℃)	J/(Kg • ℃)
Fiber	2000	230	0.22	1.15	5000
Matrix	1600	4.07	0.25	10.38	1000

Both of the two models use standard linear heat transfer element type DCC3D8 to analyze the thermal radiation. We assume the heat transfer is a transient state. It is subjected to surface radiation with ambient temperature of 2000℃ on top of the RVE and predefined temperature field of 300℃. We ignore the mass diffusion during the ablation process. The governing equation is

$$[C]\{\dot{T}\}+[K]\{T\}=\{F_q\}+\{F_r\},$$

where [C] is the element capacitance matrix, [K] is the sum conductivity matrix of heat conduction and thermal radiation. {F_q } and { F_r} are the load vectors due to applied heat flux and radiation respectively. We can obtain the temperature distribution in the C/C composite, and then calculate the heat flux by the following rule:

$$q = A((T - T^Z)^4 - (T^0 - T^Z)^4)$$

where A is the radiation constant , which was set to be one emissivity times the Stefan-Boltzmann constant; T^Z is the value of absolute zero on the temperature scale being used.

4. Numerical results

Damage analysis of hexahedron RVE in the ablation process was carried out first. The numerical example was presented to bring out for analyzing the potential ablation damage location. The finite element model was implemented in ABAQUS using a heat transfer element to analyze the ablation property of C/C composites during high temperature radiation of 2000℃. Figure 5 shows the heat flux distribution in a time of 0.13 seconds. The thermal flux magnitude of the 14 nodes along the circumscribed circle radius of the hexahedron is shown in figure 6.

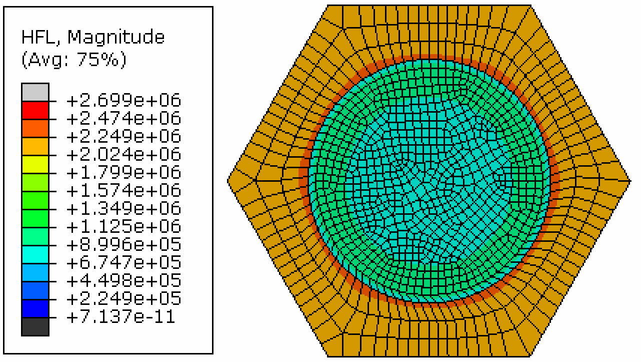


Figure 5. Heat flux distribution in micromechanical structure at 0.13seconds

The simulation result indicated that the heat flux at the interface between fiber and matrix is maximum, which make the interface damage easily, as shown in red colored area in figure 5. The result in figure 6 demonstrated that because of the mismatch between fibers and matrix, the thermal flux at the interface jumps to a higher value than the values inside the fiber, implying the debonding between fibers and matrix may happen during the ablation process.

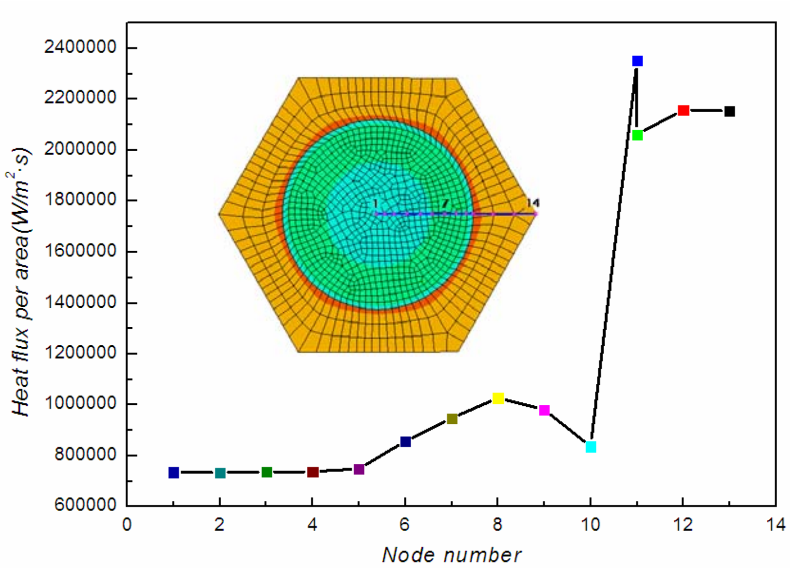


Figure 6. Variation of heat flux of selected nodes

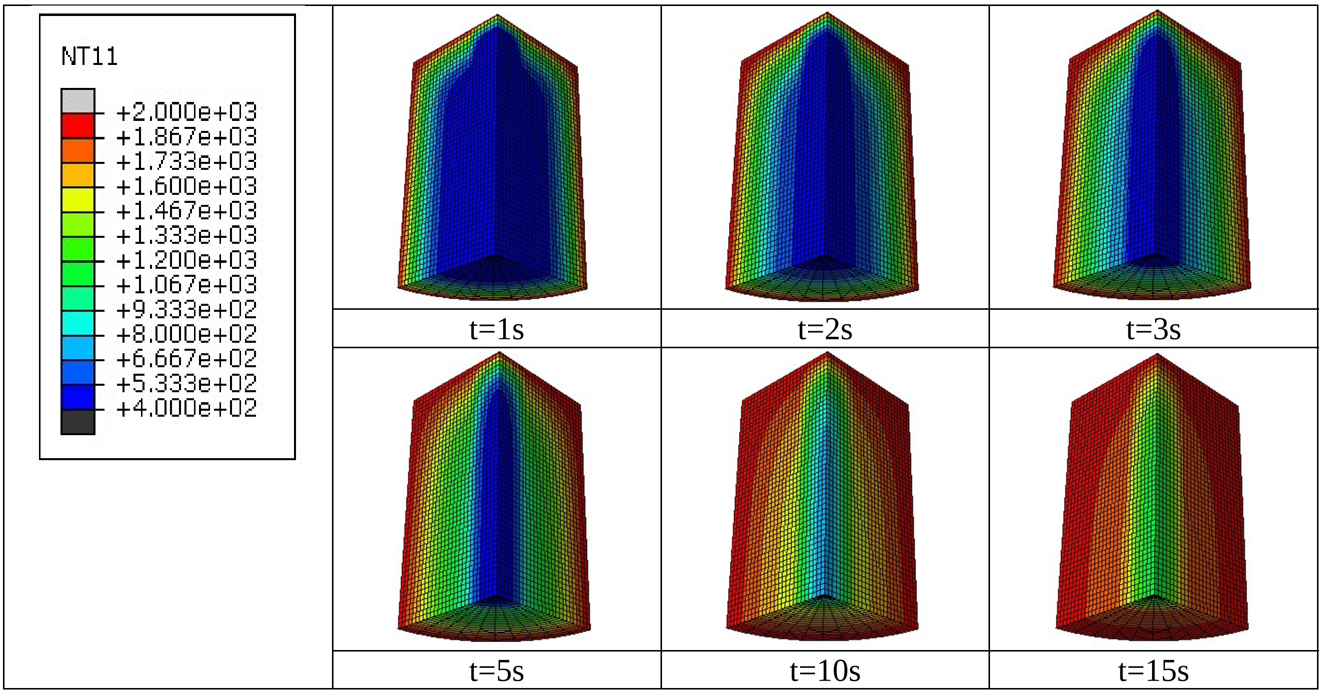
Next, the damage analysis of Cylinder RVE in the ablation process was conducted. The numerical simulation focused on the temperature rise period of cylinder RVE in ultra thermal radiation environment. According to the symmetry of the cylinder RVE of C/C composites, a 3D axisymmetric model was established in software ABAQUS. The heat-transfer element was used to simulation the progress of temperature rising up during the ultra thermal radiation. It was subjected to specified surface radiation interaction with a temperature of 2000℃on the surfaces except the bottom one. Both matrix and fibers are assumed homogeneous and isotropic. Figure 7 (a) illustrates the axisymmetric model of cylinder RVE, and the mark numbers of selected nodes are shown in meshed model in Figure 7(b).

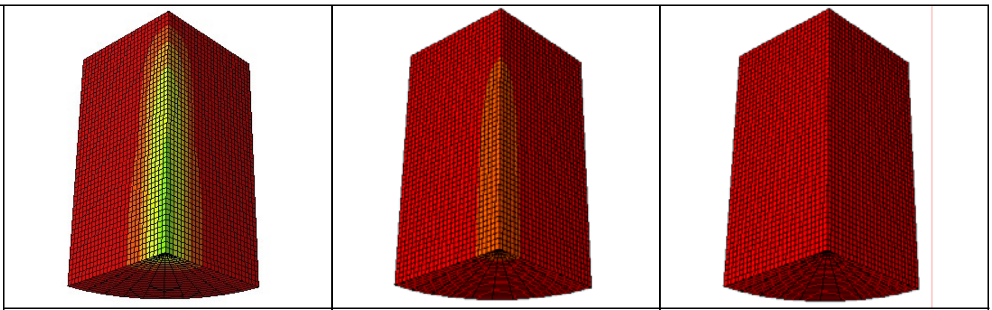
(a) (b)

Figure 7 (a) Axisymmetrical model (b) Selected node numbers

The ablation morphology of C/C composites is determined by the temperature when the oxidation is adequate. As shown in Figure 8, it was indicated that the carbon fiber presented a cone head, and the carbon fibers took the shape of needles after ablation processes. The total ablation time was about 50 seconds. In the ablation process, the temperature of the material came to balance in 40s. The results indicate that the ablation morphology of C/C takes the shape of typically “needle clusters” due to the mismatch of the thermal property of the carbon fibers and matrixes.

The analysis result is consistent with experimental results in Ref.9. Figure 9 illustrates that the temperature gradient of material surface exposed to the external environment changes greatly, which will increase the incidence of material surface damage.





	t=20s	t=30s	t=40s

Figure 8. Temperature distribution of cylinder C/C RVE during thermal radiation

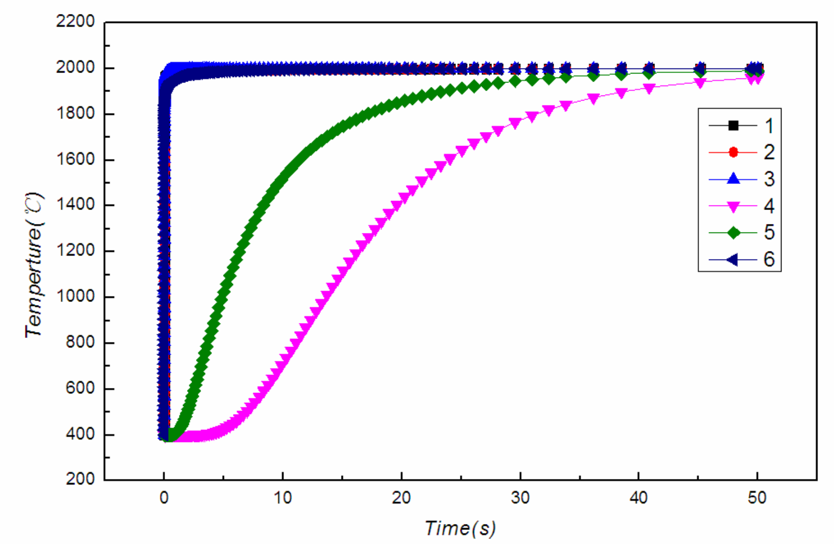


Figure 9. Temperature change process of selected nodes

5. Conclusion

In this paper, the ablation damage of C/C composites in high temperature radiation environment was investigated. The conclusions can be remarked as follows.

(1) The mismatch of ablation rate between fiber and matrix leads to a high heat flux and damage at the interface during thermal radiation.

(2) The ablation morphology of C/C composites takes the shape of typical “needle clusters” due to the mismatch of the thermal property of the carbon fibers and matrixes.

Acknowledgements

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