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Multi-Scale Modeling and Numerical Simulation for CVI Process

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Abstract. We consider the multi-scale modeling of the isothermal chemical vapor infiltration (CVI) process for the fabrication of C/SiC composites. We first present a microscopic model in which the preform is regarded as a two-phase porous media described by a dynamic pore-scale node-bond network during the fabrication process. We then develop a macroscopic model by a upscaling procedure based on the homogenization theory.

AMS subject classifications: 65M60

Key words: Multiscale modeling, composite materials, two-phase porous media, node-bond network, homogenization.

1 Introduction

1.1 Background

The CVI process is the chemical vapor infiltration process which is widely used in fabrication of ceramic matrix composite materials (CMCs). One important kind of CMCs is the carbon fiber reinforced silicon carbide (C/SiC) composites. The principal of CVI process is that let the agent gases pass through the reactor, and when the agent gases reach the surface of the carbon fiber, surface reaction happens and SiC solid is generated and deposited. When almost all the pores in the preform are occluded, we derive the material of carbon fiber reinforced SiC. One point to be noted is the multi-scale structure

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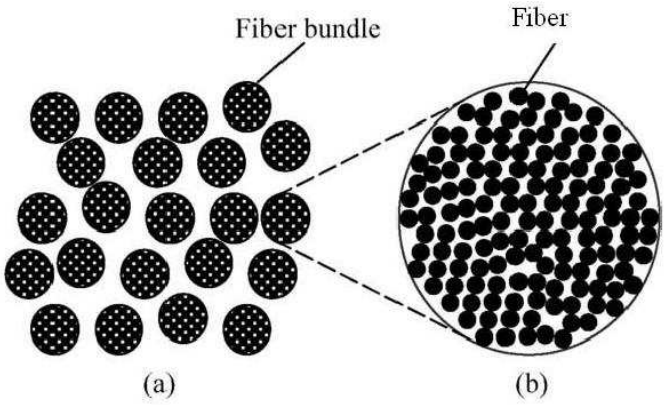

Figure 1: (a) Cross section perpendicular to randomly positioned bundles; (b) Cross section perpendicular to randomly positioned fibers inside a fiber bundle.

of the preform. A preform can have hundreds of fiber bundles or more woven together. A fiber bundle has several thousands of fibers inside. There are two kinds of pores in the preform: macro pores among bundles and micro pores among fibers inside the bundles as in Fig. 1 [16]. In the cross section of a preform, the diameter of the micro pores is in the magnitude order of μm, the diameter of the macro pores is in the magnitude order of mm and the size of a preform can be several centimeters or larger. During the numerical simulation, if we simply use the traditional numerical tools like Finite Element Method or Finite Difference Method on this multi-scale structure, a huge amount of computer memory and CPU time are required, which can easily beyond the limit of the computing resources. Some macroscale models have been developed to simulate this process, see, e.g., [9, 10, 16, 17, 19]. However, there are problems remained in these models which will be presented in Section 1.2. So a new multiscale model is proposed in this paper.

1.2 Classical model

In the last twenty years, many works are related to the modeling of the CVI process. The main model used in those works, e.g., in [13–17], will be described below.

Assume the chemical reaction in the preform is the following:

$$\mathrm{MTS}(\mathrm{CH_3SiCl_{3(v)}}) \xrightarrow{\text{excess } H_2} \mathrm{SiC_{(s)}} + 3\mathrm{HCl_{(v)}}. \tag{1.1}$$

1.2.1 Concentration equation

Assume the mass transfer in the CVI process is quasi-steady, i.e.,

$$\frac{dC}{dt} = 0.$$