New contributions to the free energy in the phase-field modeling of CVI

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Chemical vapor infiltration (CVI) is the most popular commercial method to produce the ceramic-matrix composite. In the CVI process for the production of silicon carbide (SiC), the SiC matrix is chemically deposited around the fibers during the complex pyrolysis of methyltrichlorosilane (MTS) [1]. The uniform densification and low residual porosity are two critical ascepts to get the high-performance ceramic-martix composites. The prediction of the blockage of the premature pore plays an important role in process optimisation. Thereforce we need a mathematical model to predict the evolution of the gas-solid-interface of this phase tranisition process. The sharp interface method has been used to describe the evolution of the gas-solid interface for a 1D-model [2]. However, for higher dimensions, the phase field approach seems more attractive and has been widely used [3].

The evolution of the gas-solid interface is implictly described by the evolution of the phase-field parameter ϕ. A Landau-Ginzburg type equation for the evolution of ϕ is deduced based on the free energy $\mathcal{F}(\phi)$. Here we propose new contributions to the free energy: first, to more realistically model the physical processes in the diffuse domain, we introduce the scalar-valued phase-field-dependent process intensities for the homogenous and heterogeneous process in the CVI process. Moreover, the potential energy part of the free energy is constructed by the restrictions on its local minima in the pure gas and in the pure solid phase. The whole phase-field system couples the nonlinear evolution equation for with the balance equation of the physical processes in CVI. Simulations of a 2D isothermal CVI process of SiC have been performed using the finite element method [4]. The new structure of the potential energy part has additionally been found to improve the numerical stability of the solution.

References:

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