Transient 2D simulation of CVI of methane using multi-step deposition and hydrogen inhibition models

Aijun Li*[1], Olaf Deutschmann[1], Andreas Pfrang[2], Thomas Schimmel[2]

[1]*Institute for Chemical Technology and Polymer Chemistry, University of Karlsruhe, D- 76131 Karlsruhe, Germany*
[2]*Institute for Applied Physics, University of Karlsruhe, D- 76128 Karlsruhe, Germany*

Abstract

Based on the multi-step reaction scheme for pyrocarbon deposition and the hydrogen inhibition model of pyrocarbon growth, transient 2D simulations of chemical vapor infiltration (CVI) of methane were carried out by FEM coupling the mass transports (convection and diffusion) and the evolutive surface area per volume (S_v) with gas-phase and surface chemical reactions. Three sets of experiments were simulated with inlet flows of 20 kPa CH_4, 20 kPa CH_4 with 4 kPa H_2, and 20 kPa CH_4 with 10 kPa H_2, respectively, all at a temperature of 1368 K. The predicted density distribution agrees well with experimental data from the literature. The continuous infiltration, pyrolysis and deposition of methane and its consecutive C_xH_y products lead to continuously varying hydrogen concentration inside the carbon felt. The higher diffusion of hydrogen compared to hydrocarbon species results in a varying distribution of $[H_2]/[C_xH_y]$ mixture ratios inside the carbon felt, which significantly affects the carbon deposition rate. The densification mode (from inside to outside) seems to depend not only on the concentration ratios of $[C_2H_n]/[C_6H_m]$ but also of the $[H_2]/[C_xH_y]$ ratio. Moreover, hydrogen addition may be used as a probe to study the varying textures of the pyrolytic carbon (pyrocarbon) structure formed.

Keywords: Chemical vapor infiltration, modelling, pyrolytic carbon