reaction DESIGN

CHEMKIN-PRO

Optimizing Chemical Vapor Deposition

Chemical vapor deposition (CVD) is a chemical process used to produce high-purity, high-performance solid materials. The process is often used in the semiconductor industry to produce thin films. The groundwork for CVD and other high-dimensional simulations can be carried out with low-dimensional simulations to assess the chemistry and to help simplify a reaction. The CHEMKIN-PRO Planar Shear Flow Reactor provides a method for modeling horizontal-flow CVD systems

Simulating CVD in a Planar Channel Flow Reactor

This process for depositing trichlorosilane operates in a cross-flow horizontal reactor, with atmospheric pressure and a high temperature. In this case, upper wall temperature is held at a temperature (773 K) that is significantly lower than the deposition substrate, but higher than the inlet gas temperature (623 K). The simulation uses input definitions of:

- **Gas-phase reactions:** Reversible decomposition reactions of various chlorosilanes and chlorinated disilanes. The gas-phase reactions are reversible decomposition reactions of chlorosilanes and chlorinated disilanes and cause the conversion of some of the initial chlorosilane material to these other gas-phase species.
- **Surface reactions:** Ten surface reactions, which include the dissociative adsorption of $SiCl_3H$, $SiCl_2H_2$ and $SiCl_4$. These result in the formation of deposited silicon and hydrogenated/chlorinated silicon surface species.

Results

The simulation shows that the gas heats up substantially near the deposition surface. The hot zone expands with the axial distance, as expected. The inlet gas temperature is lower than the upper wall temperature, so the coolest gas lies in a region near to but below the top wall. This cooler gas region is reflected in the trichlorosilane mole fraction contours shown in Figure 1. Depletion as a result of chemical reaction causes the low $SiCl_3H$ mole fractions near the lower wall, but thermal diffusion causes the heavier gas to move away from the upper wall. Figure 2 shows how the deposition rate of solid silicon varies as a function of axial distance. Initially, the deposition rate is quite high, but it drops rapidly as the $SiCl_3H$ near the surface is depleted, indicating that the deposition process is transport-limited in this system.

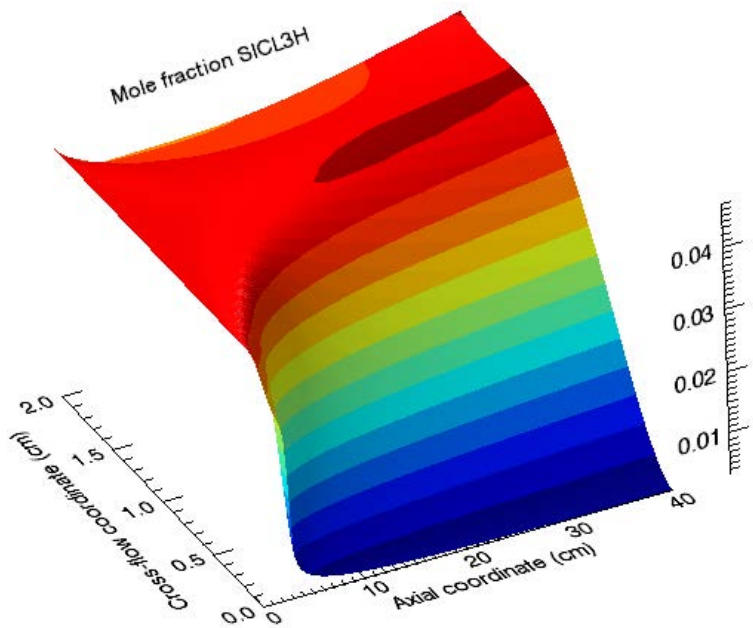

Figure 1. Trichlorosilane CVD–Trichlorosilane Mole Fraction.

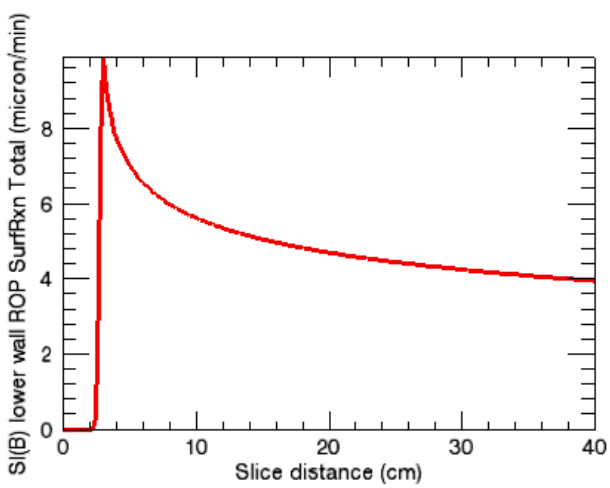

Figure 2. Trichlorosilane CVD–Silicon deposition rate reflects depletion of $SiCl_3H$ at surface.