Deposition in a Rotating Disk CVD Reactor

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Summary

This application note presents a model for the CVD of silicon from silane in a steady-state rotating disk reactor.

Project Description

This is a fixed-surface temperature simulation that represents the experimental rotating-disk reactor used by Ho, Coltrin and Breiland,[1] with the conditions corresponding to *Figure 4* in that paper. The inlet gas is a dilute mixture of silane in helium. The use of a helium carrier gas, rather than hydrogen, favors the gas-phase decomposition reactions of silane. For this case, a surface temperature of 923 K (650° C) is used. This example has two continuations, where the silane partial pressure is increased.

The chemistry set used in this application is CVD of silicon from silane. This CVD system has been the subject of numerous studies, facilitated by the simplicity of the precursor molecule. This reaction mechanism was published by Coltrin and coworkers at Sandia National Laboratories in the last[2] of a series of papers. This mechanism has been validated with a variety of optical diagnostic measurements and deposition rate data in a variety of experimental reactor geometries.

The chemistry input file, *chem.inp*, includes 3 elements (helium is used as a carrier gas), 9 gas-phase species, and 10 reversible gas-phase reactions. Many of the reactions are unimolecular decomposition reactions with explicit treatment of pressure dependent rate parameters. The most important reaction is the decomposition of SiH_4 to SiH_2 and H_2. The other reactions include the reaction of SiH_2 with SiH_4 to form Si_2H_6, which can then react again to form Si_3H_8, or decompose to H_3SiSiH and H_2. Other reactions involve interconversion between various silicon-hydride species, plus the formation of atomic silicon, which was one of the experimentally measured species. This mechanism was originally much larger, but over time, it was substantially reduced by the elimination of species and reactions deemed to be unimportant.

The surface input file, *surf.inp*, includes two surface species, open Si sites and hydrogen covered silicon sites, plus solid silicon as a bulk species. There are eight surface reactions, all written as irreversible reactions with placeholders for the thermodynamic data of the surface species. These reactions include the two-site dissociative adsorption of silane, disilane and trisilane, which form

[1] "Laser-Induced Fluorescence Measurements and Kinetic Analysis of Si Atom Formation in a Rotating Disk Chemical Deposition Reactor", P. Ho, M. E. Coltrin, W. G. Breiland, *J. Phys. Chem.* **98**: 10138 (1994), and references therein.
[2] Ibid.

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hydrogenated silicon sites, deposited bulk silicon, and H_2. Collisions of Si atoms, SiH_2, H_3SiSiH and H_2SiSiH_2 species with the surface result in deposition of bulk silicon and formation of gas-phase H_2 with unit probability. Adsorbed hydrogen is removed from the surface by the associative desorption of H_2, where a coverage dependence parameter has been used to alter the default second-order dependence to the experimentally observed first order.

Project Setup

This reactor diagram contains only one inlet and one rotating-disk CVD reactor. The properties of the inlet gas are described on the C1_Inlet panel. The inlet gas temperature is input on the Stream Property Data tab. You do not need to enter an inlet gas velocity for a steady-state rotating disk simulation, as it is calculated from the spin rate, pressure, and gas-properties, but you may override this value on the Reactor Physical Property tab's Basic sub-tab, if you wish. Enter the composition of the inlet gas on the Species-specific Property tab of the C1_Inlet panel. Use the Continuations panel to input the new compositions of the reactant gas mixture for the second and third simulations in this sample project.

Enter the parameters describing the reactor conditions on the Reactor Physical Property tab, Basic sub-tab of the C1_Rotating Disk panel. The choice of a steady-state simulation solving the gas energy equation is also entered here, as well as the use of multicomponent diffusion and thermal diffusion (the Soret effect). The temperature for the deposition surface (923 K), pressure (200 Torr), and disk rotation rate (450 rpm) are input on this tab. The Initial Grid Property tab of the Reactor Physical Property tab allows you to specify the locations of the deposition surface ($x = 0$, default) and the end axial location where the gas enters (6.2 cm). You also use this tab to specify grid parameters on this tab. This reactor model includes adaptive gridding, and the use of a relatively-low value for the initial number of grid points is recommended. The Species-specific Data tab allows you to specify initial guesses for the gas composition at the inlet, adjacent to the surface, or maximum mole fractions for intermediate species, none of which are used in this example. However, estimated values for the surface site fractions and bulk activity are provided. A good initial guess for these values can be very helpful in attaining convergence.

Project Results

Figure 1 shows the axial, radial and circumferential velocity components for the rotating disk reactor as a function of height above the surface. The deposition surface is at the origin, and the gas enters at $x = 6.2$ cm with an axial velocity of -12.4 cm/sec and zero radial and circumferential velocity components. As the gas approaches the rotating surface, the axial velocity initially increases slightly then decreases while the radial and circumferential velocity components increase. At the surface, the axial and radial velocity components are zero, and the circumferential velocity matches that of the disk (in radians/sec), as expected.

Figure 1 Deposition in a Rotating Disk—Gas Velocity Components

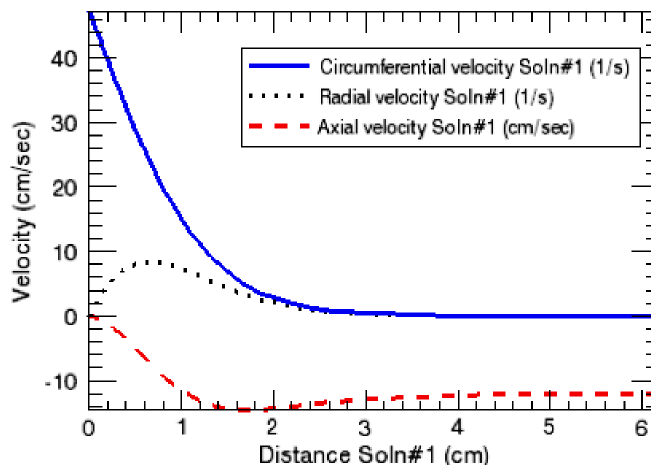


Figure 2 shows predicted mole fractions for the various silicon hydrogen species as a function of distance above the surface (the helium carrier gas is not included), again for the first simulation in the project. The composition at the grid point with largest x value is constrained to that of the inlet gas (silane and helium only). The other grid points show varying amounts of product and reactive intermediate species that are formed by gas-phase and surface reactions. Si atoms are present in very low amounts (mole fractions ~10^{-12}), but can easily be detected by laser-induced fluorescence techniques, so they are kept in the mechanism. You can choose concentration units for species composition in the Species/Variables tab of the Select Results to Load panel when the Post-Processor is first launched. This yields the results shown in *Figure 3*, illustrating that Si atom concentrations increase with increasing silane concentration, as expected. The profiles of the Si atom concentrations are shown as a function of distance above the surface for different starting silane partial pressures: #1 = 0.11 Torr, #2 = 0.34 Torr, #3 = 0.67 Torr. The curves in this figure suggest that the profiles might also be changing shape. This is confirmed in *Figure 4*, which was made by exporting the simulation results, normalizing and plotting experimental results from Ho, Coltrin and Breiland (see *Figure 4* of the referenced paper) in third-party software. It shows that: a) Si atom profiles are experimentally observed to be narrower for higher silane concentrations, and b) this reaction mechanism reproduces this observation. Comparisons between the model and this experimental data set show that the original reaction proposed for Si atom formation, the collisionally-induced decomposition of SiH_2, could not account for the experimental observations. Two other reactions, $H_3SiSiH \leftrightarrow Si + SiH_4$ and $Si + Si_2H_6 \leftrightarrow H_3SiSiH + SiH_2$, are instead the primary reactions involving Si atoms.

Figure 2 Deposition in a Rotating Disk—Mole Fractions

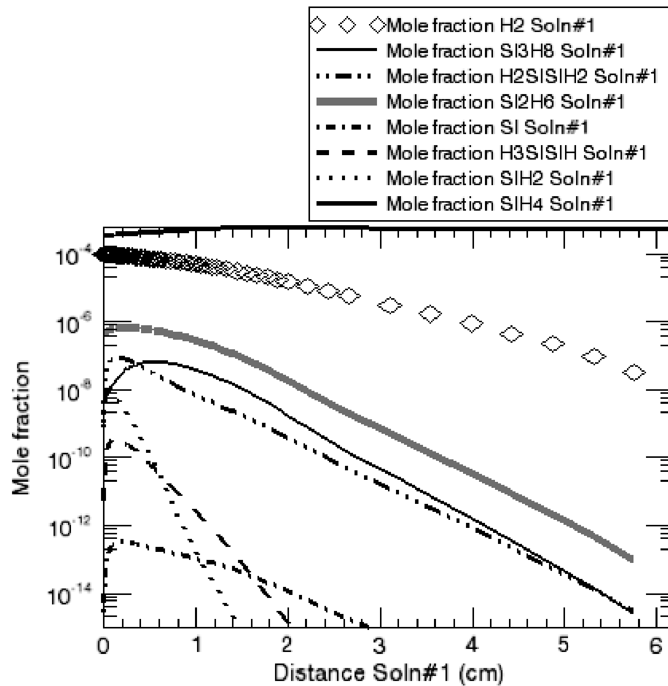


Figure 3 Deposition in a Rotating Disk—Si Atom Concentrations

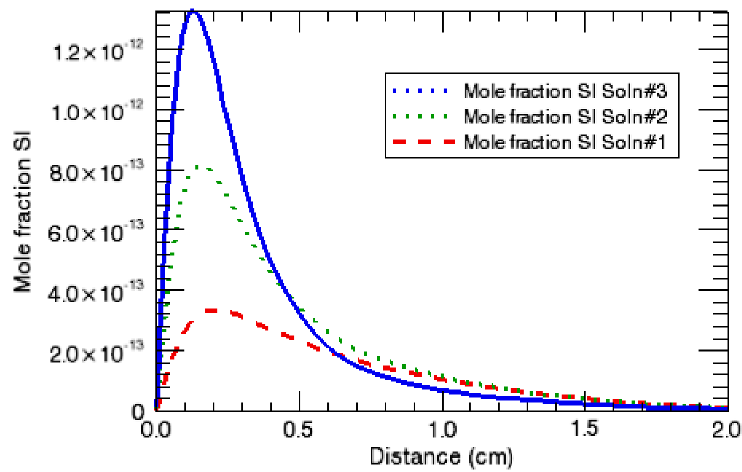
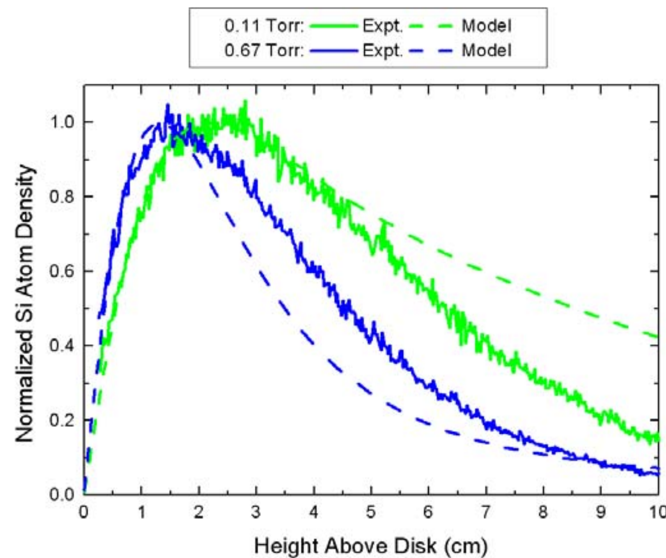


Figure 4 Deposition in a Rotating Disk—Experimental Data



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