# Chemical Vapor Deposition

Chemical vapor deposition (CVD) is a process in which chemical reactions in a gas and on the surface of an adjacent solid substrate are used to induce the growth of a thin, solid film directly onto the surface. Its most common application is in the electronic component industry, where it used to form the thin silicon wafers that comprise most semiconductor devices and integrated circuits. But it is also finding increased use as a general technique for creating high temperature ceramic coatings (Galasso, 1991).

As implemented in STORM, the chemical vapor deposition model contains two distinct components: (1) A finite-rate, multi-step gaseous phase chemistry model, and (2) a *surface reaction* model. These models must be specified individually by the user, and they must be compatible with each other. Currently, STORM includes just two gaseous phase reaction models suitable for CVD, both of which are intended for simulations of silicon deposition from a mixture of silane ($SiH_4$) and molecular hydrogen. By selecting either of these models, STORM automatically activates an additional term in the species conservation equation that simulates the effect of thermal-gradient driven mass diffusion (the *Soret term*). Kinetic and stoichiometric data for both CVD reaction models is contained in the file **react1.lib** (the finite rate chemistry input file), and the Soret term is modeled in the user-accessible Fortran file **ucvddif.f**.

| Reaction Name | Type | *Number of-* Reaction Steps | Species | Elements |
|---|---|---|---|---|
| Copper + $N_2$ | Catalytic | 1 | 2 | 1 |
| Copper + $O_2$ | Catalytic | 1 | 2 | 1 |
| Copper + Air | Catalytic | 2 | 4 | 2 |
| Carbon + $O_2$ | Fast combustion | 1 | 4 | 2 |
| Carbon + $O_2$ | Slow combustion | 1 | 2 | 2 |
| $SiH_4$ deposition | Catalytic (CVD) | 2 | 4 | 2 |

*Surface reaction library models*

STORM also contains a library of models for several types of surface reactions, each of which can be classified as being either a *catalytic* type or a *combustion* type reaction (see Table). In catalytic reactions, the solid substrate acts only to induce (catalyze) the gas phase reaction and remains chemically inert. (Such reactions are also sometimes referred to as adsorption reactions.) On the other hand, in combustion surface reactions, the substrate actually participates in reaction itself, such as in the case where an oxidizing gas passes over a solid fuel surface.

In most CVD reactors, deposition is initiated by heating the substrate—typically either by thermal conduction or by the dissipation of high frequency radio energy. Thus the types of surface reactions relevant for CVD modeling clearly fall into the catalytic category. Currently, only one CVD surface reaction model of this type is available from the STORM reaction library. This model—a two-step, four species, finite rate catalytic model—is intended for use in simulations of Si deposition from silane gas. As such, it serves as the appropriate complement to either of the two $SiH_4$+$H_2$ finite-rate, gaseous phase CVD models available from the library.

## Example Applications

Chemical vapor deposition (CVD) has emerged as an important industrial technique for the manufacture of thin solid films for applications in optoelectronic devices and high-speed digital circuits. The CVD process involves introducing metered amounts of the thin film material in a gaseous state dispersed within a carrier gas into a reactor. The reactor contains a substrate placed on a susceptor. Heating the susceptor induces the deposition of the film onto the substrate.

Although CVD reactors are widely used, efficient reactor and process design still require a better understanding of the involved chemical and physical processes. Numerical simulations of CVD processes, in particular, offer a detailed understanding of the physical and chemical processes. STORM accurately models CVD processes by calculating the flow field and temperature field inside the reactor, by modeling the gas phase and surface chemical reactions, and by modeling the diffusion of precursor species in the gas phase due to temperature and concentration gradients.

## Model Description

STORM was used to study the chemical vapor deposition of silicon from silane. The silicon/silane system offers extensive experimental and numerical results for comparison. The system is a horizontal CVD reactor. The lower plate of the reactor, the "susceptor", is heated to $T_h$ = 1300 K. The carrier gas and the reactants flow into the reactor at $T_c$ = 300 K. There is 0.1 mole % of $SiH_4$ in 1 atm of $H_2$.

Homogeneous gas-phase reaction:

$$SiH_4 \leftrightarrow SiH_2 + H_2$$
$$Si_2H_6 \leftrightarrow SiH_4 + SiH_2$$

Sticking coefficients for surface reactions:

For $SiH_4$: $\gamma_j = 5.37 \times 10^{-2} \exp[-18{,}680/RT \text{ cals/mole K}]$
For $SiH_2$ and $SiH_6$: $\gamma_j = 1$ (infinitely fast surface reaction)

It is assumed that a constant flow of a reactive gas mixture in a carrier gas flows from an isothermal section through a bottom heated plate of the same cross section.

## Results

STORM predicted the growth rate distributions for the silicon/silane system. In comparison to purely Fickian diffusion, thermal diffusion decreases the growth rate near the leading edge of the susceptor and increases the growth rate in the downstream region. This results because at the leading edge of the susceptor (where there is a strong temperature gradient), the heavier molecules are driven away from the hot susceptor by the thermal diffusive force, and partly "saved" for downstream deposition. This is in agreement with the results obtained in [1]. There is an excellent agreement between the STORM results and the published results of Jensen et al [2].

[1] J. Ouazzani, K. Chiu, and F. Rosenberger, On the 2d Modelling of Horizontal CVD Reactors and its Limitations, J. Crystal Growth 91, 497-508 (1988).

[2] H.K. Moffat and K. F. Jensen, Three Dimensional Flow Effects in Silicon CVD in Horizontal Reactors, J. Electrochem. Soc., Vol 135, No. 2, 459-471 (1988).