Using CHEMKIN for Materials and Microelectronics Applications

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Summary

This application note covers the various gas-to-surface chemistry simulations for materials and microelectronics applications that are possible using CHEMKIN.

Introduction

The development of microelectronic chips requires careful attention to materials processes involving gas-to-surface reactions. Commonly used processes such as chemical vapor deposition, atomic layer deposition, and plasma etching can be simulated using CHEMKIN. This application note describes how many of the reactor types in CHEMKIN can be used to simulate the gas-to-surface reactions for yield optimization, enhanced quality control and maximum performance.

Chemical Vapor Deposition

A number of CHEMKIN Reactor Models can be used for CVD simulations. Thermal CVD processes generally involve furnaces or heated surfaces. Simulations of CVD processes, therefore, often treat the temperature of the reactor or deposition surface as a fixed, experimentally determined input parameter, rather than a quantity that is obtained by solving an energy equation. The surface temperature is usually assumed to be equal to the temperature of the adjacent gas, except for processes performed at very low pressures. Because many CVD processes also have fairly long run times compared with startup and end-of-process transients, a steady-state simulation is often a good representation of a CVD process.

Generally, a low-dimensional simulation, such as an Equilibrium calculation or a PSR simulation, will be used to assess the chemistry, and possibly to simplify a reaction mechanism, before using it in higher-dimensional simulations. A multiple-phase equilibrium calculation can be used to determine the maximum possible deposition rate for a certain gas mixture, pressure and temperature. In a PSR simulation of a CVD process, the assumption is made that the chemical kinetics are rate limiting rather than mass transport effects or the inlet reagent supply rate. Higher dimensional simulations allow evaluation of the relative effects of chemical kinetics and mass transport. The reactor models in the CHEMKIN software can be used to simulate a number of reactor geometries used for CVD. The Plug Flow Reactor and Cylindrical Shear Flow Reactor Models can be used to model tube-furnace CVD systems, while the Planar Shear Flow Reactor can be used to model horizontal flow CVD systems. The Stagnation Flow Reactor Model can simulate a vertical showerhead system, while the Rotating Disk Reactor Model is for reactors in which high-speed rotation of the plate dominates the gas flow field.

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There are also specialized models (available from the Utilities menu in the CHEMKIN Interface) for the thermal analysis and modeling of the multi-wafer batch low-pressure CVD furnaces used in the fabrication of microelectronic devices.

Atomic Layer Deposition (ALD)

The CHEMKIN software includes several reactor models that can be used for simulating ALD processes. ALD is a technique used to deposit thin films of solid materials in a very controlled manner, and differs from CVD primarily in that it is a transient process with the deposition surface being exposed to pulses of alternating gases. Ideally, the deposition chemistry in ALD is self-limiting, with growth occurring in a layer-by-layer manner and the deposition thickness being controlled only by the number of cycles. ALD is also called: ALE, Atomic Layer Epitaxy, NLD, Nano Layer Deposition, ALCVD, Atomic Layer Chemical Vapor Deposition, and AVD, Atomic Vapor Deposition. There are also plasma enhanced variations such as PENLD, Plasma Enhanced Nano Layer Deposition. It is a relatively new technology, having made the transition from the research lab to production in the last decade.

The transient models within the CHEMKIN software are useful for optimizing pulse sequences and thus minimizing cycle times in ALD. The major advantage of ALD over CVD is the improved control over the deposition process and more conformal deposition. The inherently lower deposition rates, however, lead to longer process times and higher costs. During a pulse, it is important that enough molecules react with all parts of the substrate to be coated. But many of the precursor materials are expensive. Thus one of the process optimization goals is to reduce the amount of precursor that flows through the reactor but does not react at the surface. Considering the effects of finite-rate kinetics for surface reactions can be an important part of such an optimization, as reactions do not always behave in an ideal manner.

Plasma Etching

The CHEMKIN software includes a number of special features for modeling plasmas, most of which are demonstrated in these examples. For treating non-equilibrium plasmas, the plasma models allow you to specify different temperatures for the neutral gas, electrons, ions, and surfaces. A gas-phase reaction rate can be designated to depend on the electron temperature rather than the default neutral gas temperature. An electron-impact reaction can also be designated to involve a specified energy loss per collision. This option is used to describe excitation energy losses for electrons in solving the electron energy equation, without explicitly defining each vibrationally or electronically excited-state as a separate species within the corresponding thermodynamic data. For surface reactions, ion-assisted reactions can have yields that depend on the ion energy. Such reactions can also be designated as Bohm reactions, which mean that the ion flux is limited by the Bohm velocity of the ions, rather than by the ion's thermal speed. This factor has been introduced to account for the fact that the ion interaction with the surface will be subject to transport limitations, such that a gradient near the walls in the ion density will occur. A zero-dimensional model cannot capture this effect, such that a Bohm-flux correction model is used.

About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN, the *de facto* standard for modeling gas-phase and surface chemistry that provides engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design also offers the KINetics software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the plant. Reaction Design serves more than 350 customers in the commercial, government and academic markets.

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