Title:

SIMULATION OF THIN FILM FORMATION

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Simulation of Thin Film Formation

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Abstract

This project aims to develop modeling and simulation tools to describe the chemical and physical processes important to the manufacture of thin films on semiconductor substrates. We have developed software simulation tools that model chemical and physical vapor deposition processes on silicon surfaces. In addition, the chemistry of several important etching processes has been investigated with large-scale atomistic simulations.

Background and Research Objectives

This research effort is aimed toward the development and application of modeling and simulation tools to problems in the formation of thin films on semiconductor substrates. Patterned thin films of conductive and insulating materials form the basis for the manufacture of electrical circuit elements important to the function of semiconductor devices. The development of predictive modeling tools that are capable of describing the topography of deposited and etched material layers will greatly assist the manufacturing process, by eliminating or reducing the expense associated with making trial wafers. Developing the computational tools requires the ability to describe the reaction chemistry that occurs both in the vapor phase of a reactor, as well as the chemistry that occurs at the surface of the substrate. In addition, it is necessary that we be able to describe the evolution of the full three-dimensional geometry of the material films on wafers with features on the sub-micron size. Once the film is formed, we then seek to characterize the film in terms of its structure and behavior.

Importance to LANL's Science and Technology Base and National R&D Needs

This research supports the Laboratory's core competencies in Modeling and Simulation and in High Performance Computing.

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The full predictive simulation capabilities being developed require not only large computing resources, but also the development of innovative new strategies to solve the mathematical equations that govern the chemical and physical processes being modeled.

These effects include the transport of material from the reactor volume to the substrate surface, the nonlinear kinetics of the gas and surface phase chemistry, and the development of robust mesh generation software needed to faithfully represent the geometry and composition of the materials being simulated.

Scientific Approach and Accomplishments

This project has been organized into two related thrust areas. In the first, we have performed theoretical calculations designed to predict the chemical behavior of the materials used to deposit or etch thin films on surfaces. In the second thrust, we have developed the simulation software that uses this chemical reactivity information to simulate the growth or etching of films on surfaces.

In the first thrust, we have investigated the chemistry that is important to the etching of silicon surfaces using highly reactive chlorine ions that may be generated in plasma etching reactors. These calculations use molecular dynamics, in which we follow the motion of chlorine ions impacting silicon surfaces using classical mechanics [1]. This approach requires the development of reliable interatomic potentials to describe the forces that occur between the reacting silicon and chlorine atoms [2]. Further applications of this work have also been published [3,4].

Plasma reactors can also be used to deposit films on surfaces, and using similar computational tools, we have collaborated with colleagues at Motorola, Inc., to study the deposition of metals onto semiconductor surfaces [5]. However, when metals are deposited at high energies (such as are obtained with plasma reactors) onto surfaces, they can sputter (knock off) atoms from the surface. We have studied the effects of this sputtering process, especially for processes where we seek to deposit copper onto metal surfaces [6,7].

In the second thrust, we have developed simulation software, TopoSim-3D, to describe both the chemical and physical processes that are involved in the formation of thin films. This software models the time dependence of the evolution of a thin film. There are three major processes that need to be considered, as well as a major computational effort

required to maintain a faithful representation of the deposition geometry. The physical and chemical processes modeled include (a) the transport of materials from the vapor phase of a reactor to the surface where the film is growing, (b) the reactive chemistry that occurs at the vapor-surface interface, and (c) the motion of the vapor/surface interface as material is either deposited or removed by the chemistry. The complete description of the process then requires that we build and maintain a three dimensional computational mesh that describes the shape of the vapor/material interface.

The transport of material through the vapor phase is based on a low-pressure assumption that material travels in straight-line trajectories from the reactor volume to the material surface. In general, the material surface may be characterized by small-scale (submicron-sized) features such as holes or trenches. In such cases, the entire purpose of performing a simulation may be to ensure that the reactor conditions are set so that deposited material fills these features without leaving voids in them. A void in a trench that is being filled with a metal (to make a conducting wire, for example) will greatly affect the properties of the final conductor, in terms of its electrical resistivity and reliability. The principal computational issue to consider is the visibility of one part of the material surface from another. If material hitting the surface does not stick there, it may bounce off in another direction, ultimately to land at another place on the surface, but only if that new place is visible from the first. Sophisticated methods were incorporated into TopoSim-3D to address these visibility concerns, which if treated in the most direct fashion can become very computationally intensive.

The chemistry that occurs at the surface is handled using the chemical kinetics software libraries (CHEMKIN and SURFACE CHEMKIN, [8]) developed at Sandia National Laboratory. This software makes it possible to define detailed reaction mechanisms for processes that occur both in the gas phase and at the material surface. The net effect of the mechanism is to describe how material is deposited or removed at the surface on the atomic and molecular level. The parameters that govern the rates of these processes are what is computed from the studies of the first thrust area.

A major concern of TopoSim-3D is the interaction between the physics of material transport and the chemistry that occurs at the surface. Any material that arrives at the surface and does not react there may then leave ("bounce off") only to appear as arriving material at some remote surface location (visible from the first). Since the overall rate of reaction at any point on the surface depends on the total amount of material arriving there,

TopoSim-3D must solve the mathematical equations governing the combined transport and chemistry in an iterative way. We first guess how much material arrives at any point on the surface, compute reaction rates from that, and from the amount of material that does not react locally, transport non-reacted material to other surface locations, updating our estimate of how much material arrives at the remote location. This process is iterated until the amount of material that leaves one from one surface location is globally consistent with the amount of material that arrives at all other locations.

Once we have an estimate of the rate at which the surface will grow at any one point on the surface, we move the entire interface and prepare to go back to the beginning and start up a new time step. But when we move the points on the computational mesh that describe the position of the material surface, the mesh gets distorted. Once too much distortion accumulates, we need to refine the mesh so that we maintain a numerically meaningful description of the shape of the surface. The mesh description of the surface is handled by the **LaGriT** software library, developed at Los Alamos [9].

Applications of TopoSim-3D to typical deposition geometries are described in Los Alamos publications [10] and conference proceedings [11]. Additional applications have been made to a model where we simultaneously simulate both the deposition of material onto a polycrystalline structure, and follow the simultaneous grain growth of the deposited material [12].

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