Equipment Simulation - State of the Art and Future Challenges

Chr. Werner
SIEMENS, Corporate Research and Development,
Application Center Microelectronics, Munich, Germany

1 Introduction

Process and device simulation have been used for more than a decade now and a number of programs have proven their ability to predict doping profiles and electrical behaviour prior to manufacturing the devices. The aim of equipment simulation is to extend the simulation technology also to support the design of the reactors used in the manufacturing process of semiconductor devices and to provide a better physical and chemical understanding of the parameters that control the technological processes.

In this paper we will review the current models for heat and mass transport used in the simulations and indicate the areas of necessary further developments. Actual applications to problems in a submicron manufacturing environment will illustrate the presentation.

2 Theory

2.1 Differential equations

The gas flow in the reactor is simulated by a numerical solution of the hydrodynamic transport equations in the gas, i.e. the mass-, chemical-species-, momentum-, and energy-continuity equations.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial}{\partial t}(\rho u_i) + \nabla \cdot (\rho \mathbf{u} u_i) = \nabla \cdot (\mu_m \nabla u_i) - \frac{\partial p}{\partial x_i} + C_i$$

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \mathbf{u} H) = \nabla \cdot (\kappa_m \nabla T) + S_h$$

$$\frac{\partial}{\partial t}(\rho m_i) + \nabla \cdot (\rho \mathbf{u} m_i) = \nabla \cdot \mathbf{j}_i + G_i$$

where ρ is the density of the mixture, t is time, and $\mathbf{u}$ is the velocity vector, μ_m is viscosity of the mixture, p is pressure, and C_i represents viscous terms in addition to those expressed by μ_m. H is specific enthalpy that is related to the temperature through heat capacity C_p by $dH = C_p dT$, κ_m is thermal conductivity of the mixture, T is temperature, and S_h is the rate of heat generation per volume. With m_i we express the mass fraction and with $\mathbf{j}_i$ the mass current density of species 'i', and G_i is the generation term in the bulk. The ideal gas law $P = \rho RT$ is included to express the correct relation between density, pressure, and temperature.

In the general case the diffusion current $\mathbf{j}_i$ is not only driven by the concentration gradient of the species i but also of all the other species and of the temperature

$$\mathbf{j}_i = -D_i^T \nabla(lnT) - \sum \rho D_{ij} \nabla m_j$$

where D_{ij} and D_i^T are the multicomponent diffusion and thermodiffusion coefficients, respectively.

2.2 Physical models

2.2.1 Transport parameters

The transport parameters viscosity μ, thermal conductivity κ, and diffusion coefficients D_{ij} and D_i^T are derived from statistical thermodynamics using the Lennard-Jones molecular interaction potential. A comprehensive description of all the equations and transport models used in CVD simulation can be found in the new book of Kleijn and Werner [1].

New extensions try to extend the applicability of flow simulation into the transition regime to free molecular flow. This is important for pressures below 5 Pa as they are used in sputter deposition or plasma etching reactors.

The Direct Simulation Monte Carlo method (DSMC) [2] can model that regime with sufficient accuracy, but because of the high computational effort of this method it is still hoped that by the inclusion of special slip boundary conditions and modified transport properties the validity of the hydrodynamic approach can be extended at least down to moderately low pressures.

2.2.2 Radiation

In state of the art processing reactors the temperature is fixed on most of the external walls either by regulated heating or by water cooling, This can be modelled by appropriate Dirichlet boundary conditions.

For internal surfaces with absorptivity $a(x)$, emissivity $e(x)$, and reflectivity $r(x)$ we have to consider

a radiative heat flux of

$$q(x) = \int a(x)R(x,x')e(x')[T(x')]^4 dx' - e(x)[T(x)]^4$$

where the radiative heat exchange matrix $R(x,x')$ is calculated from the view factors $A(x,x')$ by the integral equation

$$R(x,x') = A(x,x') + \int A(x,x'')r(x'')R(x'',x')dx''$$

Usually the grey diffusive approximation has been used in radiation modeling [3]. which assumes the coefficients e, a and r to be independent of radiation wavelength, but so far no systematic investigation of its validity has been published. Indeed we would suspect that especially for reactors with lamp heating more realistic reflection models might be essential to yield accurate simulation results.

2.2.3 Chemistry

The chemistry of a CVD process is considered by a boundary condition in the mass diffusion equations on the reacting wafer surface as

$$\rho m_i u + j_i = \frac{M_i}{M_d} \rho_d \, R_d(T, p, m_1, m_2, ..)$$

where ρ_d, M_d and R_d are the mass density, the molecular weight and the deposition rate of the layer to be deposited.

For most of the CVD processes we have only rudimentary models concerning the chemical reactions [4]. In the simulations usually rough overall reactions are used, which utilize empirical parameters fitted to measured deposition rate data. Though the simulation programs would allow to handle at least half a dozen reactions with a number of intermediate species, a bottleneck seems to exist in the experimental determination of all the necessary kinetic data.

2.2.4 Plasma modeling

In plasma enhanced deposition or etch processes the activation energy for the chemical reactions is provided via a highly non-equilibrium process, in which a low density of free electrons is excited by an RF field to energies much higher than the ambient temperature. Modeling the plasma with sufficient accuracy requires enormous computer resources and has been performed so far only for 1-D geometry [5]. Inclusions of plasma properties into realistic reactor modeling so far have used highly simplifying assumptions concerning the electronic energy distribution function and the chemical reactions involved in the deposition [6, 7]. More work is definitely necessary to provide a reliable plasma simulation capability with affordable computer resources.

3 Applications

A commercial fluid flow simulator [8] was utilised to solve the transport equations in 3 dimensions after appropriate subroutines had been added to describe the physical and chemical properties of the respective processes. Typical calulation times of about 1 h on an Apollo 10000 workstation have been needed for a geometry with 3000 gridpoints.

In this paper we will show a variety of examples from the industrial application, which we had to solve in a manufacturing environment for submicron silicon devices for our memory and logic products of the 16 M and 64 M generations.

3.1 Temperature distribution in a RTP reactor

A very important question in RTP reactor optimization is the temperature profile at the substrate, which can sensitively influence the deposition homogeneity. We have performed a simulation study of a RTP-CVD reactor for Si/Ge epitaxy, where the substrate is held on small quartz pins and is heated from below by radiation through a quartz window [9]. The measured temperature profile across the substrate exhibits a strong decrease at the edges due to enhanced energy losses in that regions, which could be very well reproduced by simulation.

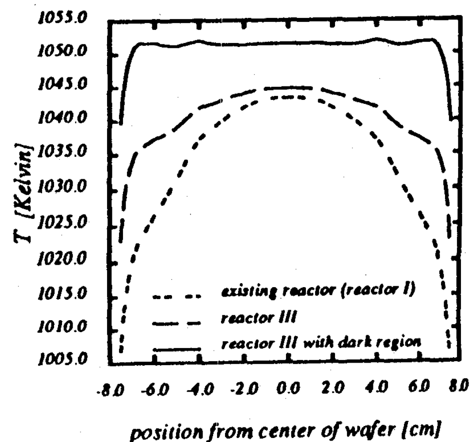

Fig. 1: Optimization of the temperature profile in an RTP reactor

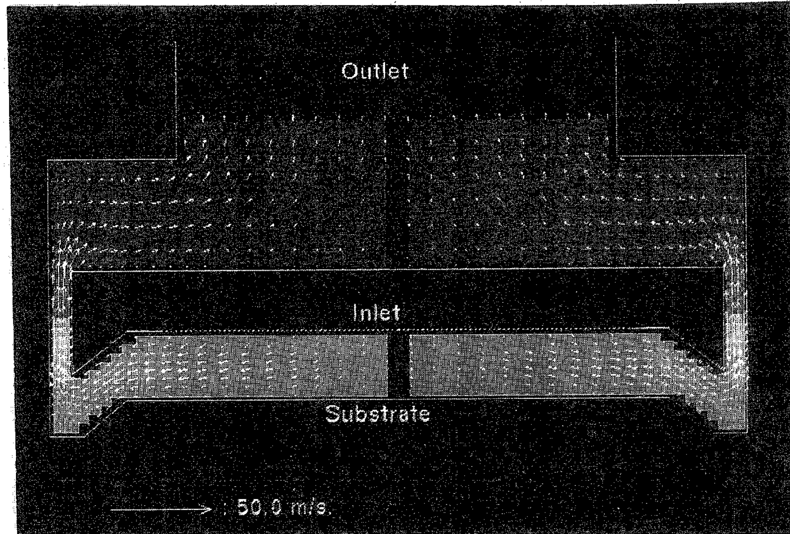

Fig. 2: Velocity of gas flow and pressure contours inside the CVD reactor. A significant pressure drop can be seen where the gas streams upwards to the outlet port.

We have performed a careful optimization using the simulation, where both the geometry of the reactor chamber and the reflectivity of the inner walls have been changed to compensate for the heat loss at the edge of the substrate. The results of this optimization is depicted in Fig.1 which shows a factor 4 homogeneity improvement over the original reactor design.

3.2 Chemical Vapor deposition of tungsten films

In Figure 2 we show the gas flow and the pressure distribution in a cold wall, single wafer, tungsten CVD reactor based on the reduction of tungsten hexafluoride by silane.

In the reactor simulated, the wafer is placed on a hot susceptor at the bottom of the reaction chamber. The gases are introduced through a broad showerhead inlet above the wafer and are extracted at the top of the reactor. A typical application for reactor optimization is shown in Figure 3, where we plot the tungsten deposition rate along the wafer radius for different spacings between the showerhead and the susceptor. At smaller spacings we have a larger pressure drop across the wafer radius, which leads to a higher deposition nonuniformity.

3.3 Sputtering reactor for titanium deposition

Sputter reactors operate at a pressure below 1 Pascal, where the mean free path of the molecules is comparable to the dimensions of the reactor. The gas flow in these reactors can be described by the Direct Simulation Monte Carlo (DSMC) method, in which the motion of a representative set of molecules is simulated directly. The method was applied to simulate a titanium deposition process in a state-of-the-art sputter reactor for 8" wafers [9].

Fig.4 shows the molar concentration of titanium in a sputter reactor without collimator at 0.13 Pascal. The top wall is the target, the bottom wall the substrate. In Fig.5 the deposition rate profiles at the substrate are depicted for different reactor configurations.

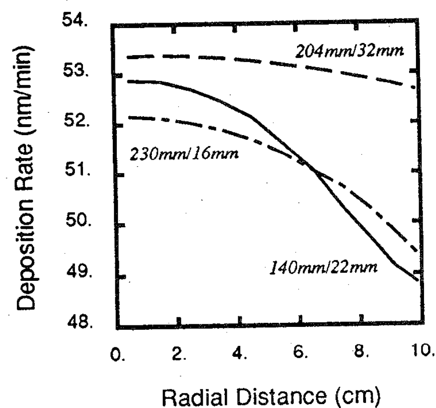

Fig. 3: Deposition rate uniformity for a tungsten cold-wall CVD reactor for different reactor geometries. Numbers denote the showerhead diameter and chamber height.

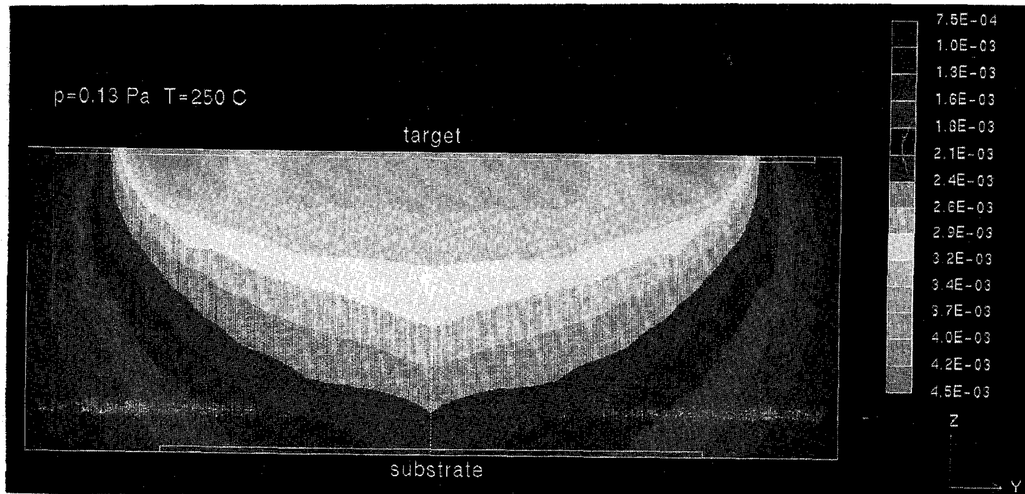

Fig. 4: Distribution of titanium concentration in the sputtering reactor calculated with the Direct Simulation Monte Carlo method.

4 Conclusions

In comparison with the better established topics of process and device simulation, equipment simulation can be regarded to be still in its beginning. Nevertheless, a number of groups at universities and in industry are actively working to improve the physical and chemical models used in the simulation and to develop user friendly simulation tools.

From the results obtained so far we can expect, that equipment simulation can be utilized as efficiently for the development of future manufacturing equipment as process and device simulation has been used for transistor optimization already for more than a decade.

Acknowledgement: The author would like to thank his colleagues R.P.Brinkmann, A.Kersch, Ch.Hopfmann, and M.Hierlemann for critical discussions on various aspects of this article. Moreover, fruitful coperation with Klavs Jensen from MIT and Chris Kleijn from Delft university is greatfully acknowledged.

References

[1] C.R. Kleijn and Chr. Werner, *"Modeling of chemical Vapor Deposition of Tungsten Films"*, Birkhäuser Verlag, Basel 1993

[2] K.Nanbu et al. *Rarefied Gas Dynamics*, Aachen 1990, p.913

[3] A. Kersch, et al., H. Schäfer, Chr. Werner, Digest of Techn. Papers, Intern. El. Dev. Meeting, Washington 1991 p.883

[4] Klavs Jensen, Chemical Engineering Science, **42**, p.923-958, 1987

[5] M.J. Kushner, J. Appl. Phys. **63**, 2532 (1988)

[6] S.K. Park and D.J. Economou, Journ. El.chem. Soc. **137**, 2103, (1990)

[7] D.B. Graves and K.F. Jensen, IEEE Trans. Plasma Physics **PS-14** [2] 78 (1986).

[8] H.I. Rosten and D.B. Spalding, *The PHOENICS Beginner's Guide*, Wimbledon, (1987). Other programs appropriate for equipment simulation include FLUENT (Creare.x Inc., New Hampshire 1990) and FIDAP (Fluid Dynamics International, Evanston, Illinois 1990).

[9] A. Kersch, et al.,W. Morokoff, Chr. Werner, B. Vollmer, D. Restaino, Digest of Techn. Papers, Intern. El. Dev. Meeting, San Francisco 1992, p.181

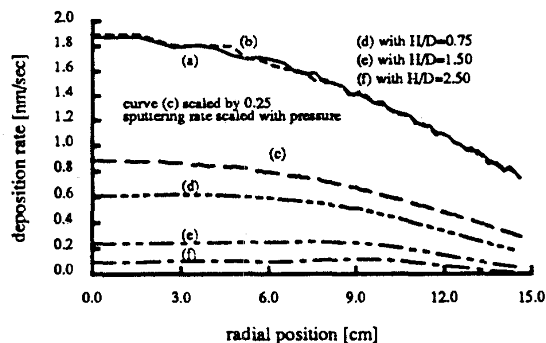

Fig.5: Deposition rate profiles along a radius across the substrate for different working conditions: a)-c) without collimator: a) 0.13 Pa, $T_{sub} = 250^oC$, b) 0.13 Pa, $T_{sub} = 50^oC$, c) 0.7 Pa, $T_{sub} = 50^oC$ d)-f) collimators with different aspect ratios, 0.13 Pa, $T_{sub} = 250^oC$.