Reactor-scale Modeling of Silicon Epitaxy

Multiphysics Model of a Chemical Vapor Deposition (CVD) Process

This case study of epitaxial deposition of silicon film on a silicon substrate in a horizontal hot-wall reactor reproduces an earlier modeling study by Habuka *et al.* [1]. The steady-state finite element (FEM) model incorporates fluid flow, heat transfer, dilute species transport, and one-step Arrhenius kinetics at the wafer surface. Additionally, the transport properties of the gas species are all temperature dependent.

Epitaxy is the deposition of a crystalline layer on a crystalline substrate. It is a Chemical Vapor Deposition (CVD) process that is widely used in the semiconductor industry. Silicon epitaxy involves decomposition of chlorosilanes (commonly trichlorosilane or TCS) at high temperature (~ 900°C – 1150°C), with hydrogen as the reducing agent and carrier gas. Hydrogen gas is bubbled through liquid TCS to produce a dilute mixture of gaseous TCS in hydrogen carrier gas.

The deposition process steps involves the following physical phenomena:

- convective and diffusive transport of reactants from reactor entrance to the substrate (wafer),
- gas-phase reactions, and decomposition of reactants and products near heated wafer,
- species transport from gas stream through boundary layer to the wafer surface by diffusion,
- adsorption of reactants on the wafer surface,
- surface reactions,
- etching of deposited silicon by the HCL byproduct before it diffuses into the main flow, and
- transport of byproducts out of the chamber.

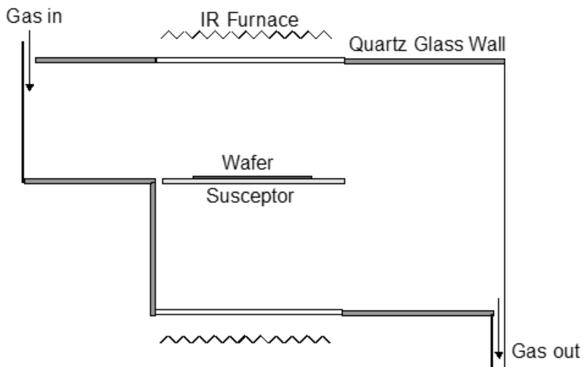

Figure 1: Schematic of the two-dimensional reactor [1]. Shaded walls are insulated. Figure not to scale.

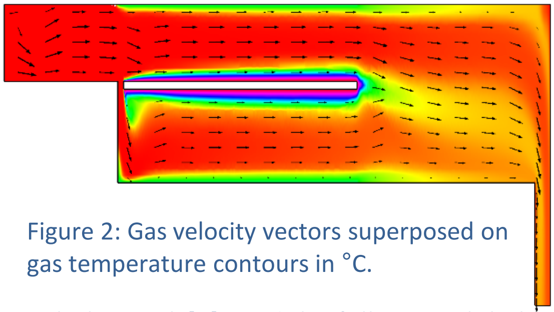

Figure 2: Gas velocity vectors superposed on gas temperature contours in °C.

Habuka *et al.* [1] used the following global, one-step approximation of the more complex chemistry [2]: $SiHCl_3 + H_2 \rightarrow Si + 3\ HCl$.

The effective rate coefficients for Arrhenius kinetics for this global reaction was taken from [1]. They had been computed by calibrating the model with experimental data.

The two-dimensional (2D) reactor schematic is shown in Figure 1. The end-to-end length is 0.705 m and the total height is 0.4 m. The wafer is radiantly-heated from above and below as shown. and operates at atmospheric pressure. The vertical walls on the left and right wall are kept at room temperature. The 8” wafer is located at the center of the 12” susceptor. The temperatures of both are assumed to be independently controlled to generate excellent uniformity at process temperatures ranging from 1120°C to 1180°C, with a nominal value of 1150°C.

The 2D FEM model was developed using COMSOL Multiphysics. The model uses the Non-Isothermal Fluid Flow, Heat Transfer and Transport of Concentrated Species physics components. The temperature dependence of all the transport properties of the three species (TCS, H_2 and HCl) were obtained from relationships given by Newman and Pollard [3]. The model takes less than five minutes to run the steady-state simulation.

Figure 2 shows the velocity vectors with superposed speed contours for the nominal operating conditions of TCS mass fraction of 0.71, wafer temperature of 1150°C, and top and bottom quartz wall temperatures of 477°C. The gas is heated up considerably by the susceptor and the wall, and speeds up along the wafer surface.

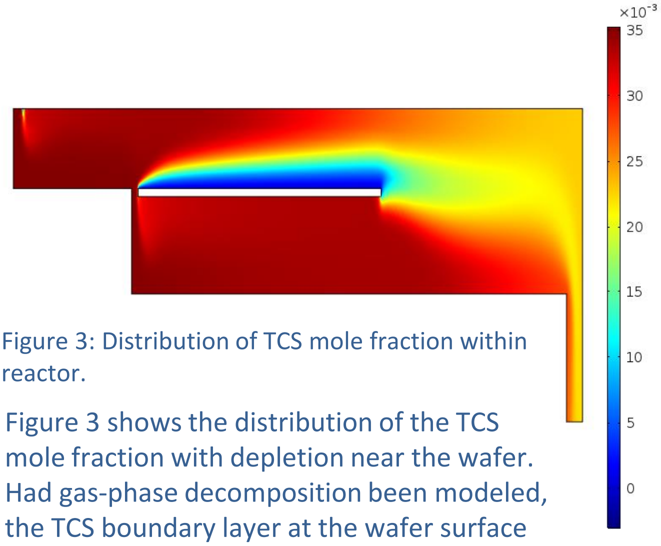

Figure 3: Distribution of TCS mole fraction within reactor.

Figure 3 shows the distribution of the TCS mole fraction with depletion near the wafer. Had gas-phase decomposition been modeled, the TCS boundary layer at the wafer surface would have been thicker.

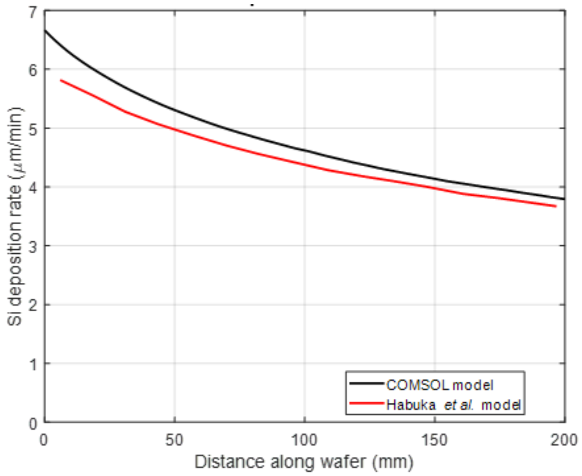

Figure 4: Deposition profile along flow direction. Comparison with Habuka, et al. [1].

Figure 4 shows that deposition rate uniformity is within 10% of those reported by Habuka *et al.* [1]. Figure 5 shows the effect of wafer rotation which significantly improves deposition uniformity, assuming that the typical rotation period is much smaller than the deposition period.

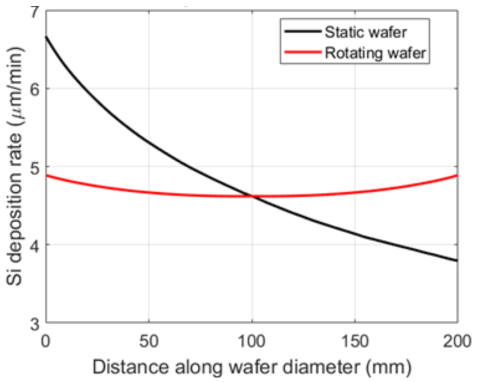

Figure 5: Deposition rates with and without wafer rotation.

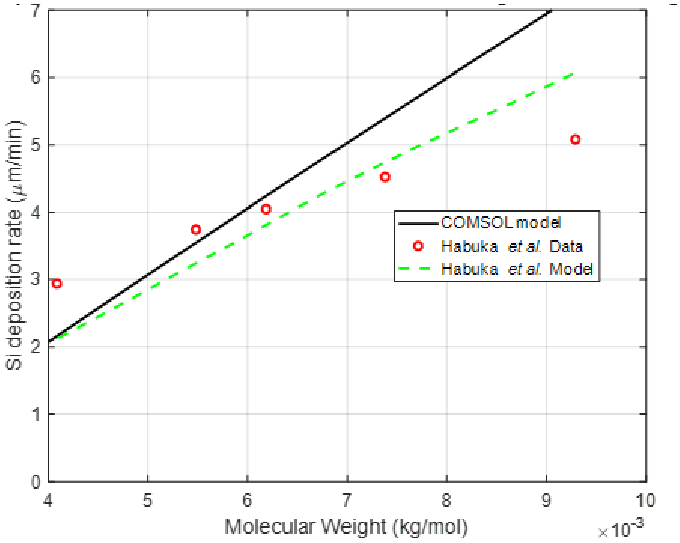

Figure 6: Average deposition rate as function of average molecular weight of gas at inlet. Nominal molecular weight is 6.67 kg/kg-mole (TCS mass fraction = 0.71).

The deposition rates computed for various TCS mass fractions are plotted in Figure 6. These results are in general agreement with Habuka's experimental data. The slight over-prediction of the deposition rate by the FEM model may be attributed to deposition on the insulated hot walls upstream of the wafer that is not modeled, and wafer temperature non-uniformities.

References:

[1] M. Habuka, Katayama, M. Shimda, K. Okuyama, "Numerical Evaluation of Silicon Thin Growth from $SiHCl_3$-H_2 Gas Mixture in a Horizontal Chemical Vapor Deposition Reactor," *Jpn. J. Appl. Phys.*, No. 33, p.1977-1985, 1994.

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[4] H. Habuka, T. Suzuki, S. Yamamoto, A. Nakamura, T. Takeuchi and M. Aihara, "Dominant Rate Process of Silicon Surface Etching by Hydrogen Chloride Gas," *Thin Solid Films*, No. 489, pp.104-110, 2005.

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