Critical Evaluation of Multi-Component Diffusion Models for Simulation of MOVPE reactors

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Metal-Organic Vapor Epitaxy (MOVPE) is a process widely used in the LED industry to deposit epitaxial films. For example, films based on Nitride materials are processed mainly to blue to green LED chips which are the basis for illumination devices in industrial, automotive and solid state lighting today.

MOVPE is a highly complex vapor deposition process. Gasses are deployed unmixed to a flow flange which distributes carrier gasses (H2, N2), precursors for metal atoms (TMGa, TEGa, TMAl, TMIn) and precursors for nitrogen atoms (NH3) to a reactor chamber. In this chamber the gasses are mixed while transported towards the species boundary layer on top of the hot wafer. In this boundary layer diffusion is the rate limiting process and gasses diffuse through it, react at the hot wafer surface and form the epitaxial film. The reactors are usually at low pressures (< 500 mbar) and the gas mixtures in the reactor chamber can be assumed to be ideal, as the metal-organic precursors are only present in very low concentrations.

Modeling a MOVPE reactor with the goal to predict growth rate distributions on the wafer in a given reactor, involves the simultaneous solution of the Navier-Stokes, energy and mass conservation equations for the different species in the multi-component gas mixture, as well as gas phase and surface reactions models.

Accordingly, the growth rate of the epitaxial film is proportional to the mass fraction outside the boundary layer at the wafer surface and inversely proportional to the velocity boundary layer thickness:

$$GR \sim \frac{Y_{MO}}{\delta}$$

Thus, not only the boundary layer thickness but also the distribution of the metal-organic precursor outside the boundary layer is of importance for the accurate calculation of the growth rate. In MOVPE reactors diffusion processes are fast and of the order of or not much smaller in magnitude than convective transport, therefore, the distribution of gas phase species changes considerably during transport from the flow flange to the boundary layer (unmixed at the flow flange – mixed outside species boundary layer).

While we believe that the boundary layer thickness is calculated quite accurately in CFD models for the MOVPE process, recently, we suspect that some of the deviations in simulated growth rates and experimental ones are due to models for multi-component diffusion available in commercial CFD codes like CFD-ACE or ANSYS Fluent, typically used in the semiconductor industry today. Both codes do not solve the exact Stefan-Maxwell equations, which should provide the most accurate solutions compared to simple diffusion models, such as Fickian diffusion or to approximations of the Stefan-Maxwell equations.

To evaluate the errors made using such approximations, simulations of several test problems are carried out with the commercial CFD code CFD-ACE, ANSYS Fluent and an academic code developed in OpenFOAM which solves the Stefan-Maxwell equations without approximation. One- and two-dimensional test problems reported in literature (Kumar & Mazumder, 2007) (Mazumder, 2006) are solved as well as a simple axis-symmetric quasi-3D model for a commercial MOVPE reactor.

First, it is established that the OpenFOAM implementation of the exact Stefan Maxwell equations produces results consistent with literature data. Then simulations with the quasi-3D model are carried out using real operation conditions.

While in the academic cases the studied gas mixtures are different from relevant epitaxial growth gas compositions, in the axis-symmetric cases such conditions can be studied. The deviation in GaN growth rates between the exact solution in the academic code and approximations of the Stefan-Maxwell equations in the commercial code is established. This allows us to estimate the uncertainty in commercial code simulation results, and suggests if improvements to the commercial code models are necessary.

Literature

Kumar, A., & Mazumder, S. (2007). Assessment of the dilute approximation for the prediction of combined heat and mass transfer rates in multi-component systems.

Mazumder, S. (2006). Critical assessment of the stability and convergence of the equations of multicomponent diffusion.