Algorithms and Models for Simulation of MOCVD of III-V Layers in the Planetary Reactor

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Abstract

Advances in development of mathematical models and numerial techniques for modelling of MOCVD in the Planetary Reactor^{TM} are presented. Importance of coupled flow and mass transport calculations, accurate modelling of radiative heat transfer and complex chemical interactions is discussed. Advantages and disadvantages of block–structured and unstructured grid algorithms are considered.

1. Introduction

In recent years mathematical modelling and numerical simulation of metalorganic chemical vapour deposition (MOCVD) has become useful to find the optimal set of process parameters and to investigate growth mechanisms. This work is concerned with modelling of growth of III-V semiconductors in the multiwafer Planetary Reactor^{TM}, which is especially suitable for large scale production of heterostructures for various kinds of semiconductor devices due to the high degree of growth rate and compositional uniformity across the wafer and good utilization of precursor materials [1, 2]. In the reactor to be modelled, several wafers are placed on rotating satellites which in turn rotate around the central axis of the susceptor plate. Group III metalorganics and group V hydrides, both mixed with the H_2 carrier, are introduced through separate inlet channels at the center of the reactor flowing radially outwards along the growing layers. The ceiling plate is thermally coupled to the water cooled reactor top by a cooling gas mixture of Ar and H_2 that allows for controlling of the ceiling temperature through its composition.

Simplified modelling aproaches have been applied to predict growth rate profiles and to optimize technical design in this type of CVD reactor [3, 2]. However, mass transport calculations have been done in a separate step after flow and temperature prediction and radiation heat transfer has been considered in a simplified manner.

An advanced approach was proposed in [4, 5] taking into account coupled flow, heat transfer and mass transport, including chemical reactions and formation of deposits on the reactor ceiling. The aim of this work is to develop further the mathematical models and algorithms used for modelling of growth in the Planetary Reactor^{TM}.

2. Mathematical models

The mathematical model for MOCVD growth consists in the solution of coupled partial differential equations which describe conservation of total mass and momentum, heat transfer and the chemical species' mass transport in the reactor, including multicomponent diffusion and chemical reactions. Flow is coupled with mass transport of the predominant gas phase species H_2, AsH_3, TMGa and MMGa. Coupling of flow and mass transport is crucial in modelling of growth in the Planetary Reactor^{TM}, since the molar weight of the gas mixture is not uniform, especially near the entrance region where strong intermixing occurs between the flows coming from two inlet channels.

Thermal radiative heat transfer is modelled by assuming a non-participating gas mixture and semi-transparent grey-diffusive quartz walls. Radiative heat transfer is coupled with heat conduction in the quartz wall and solid parts of the reactor, including thermal solid/fluid interaction, and conductive heat transfer in the cooling gas above the ceiling plate. Detailed modelling of radiative heat transfer is crucial for the accurate determination of the temperature distribution at the ceiling plate. The ceiling temperature influences sensitively the kind and thickness of deposits. If the ceiling temperature is too high - deposition of polycristalline GaAs can take place, whereas if it is too cold - condensation of As can occur. Therefore, accurate calculation of the temperature distribution on the ceiling is important to reduce the deposits. Wave length dependencies of radiative properties of the quartz wall and the effect of deposits on radiative properties and, therefore, on the ceiling temperature are shown to be important to predict temperature distribution on the ceiling [6, 7]. In Fig 1 isotherms (a) and streamlines (b) of the flow in the reactor are shown. Heating of the nozzle and ceiling due to radiative heat transport can be seen.

By modelling of the species' mass transport homogeneous decomposition of TMGa to MMGa and deposition of polycrystalline GaAs on the ceiling are taken into account. Growth of III-V heterostructure layers on the wafer is performed at mass transport limited growth conditions. The growth rate is determined by mass transport of the group III species only, because arsine (AsH_3) is introduced into the reactor at high

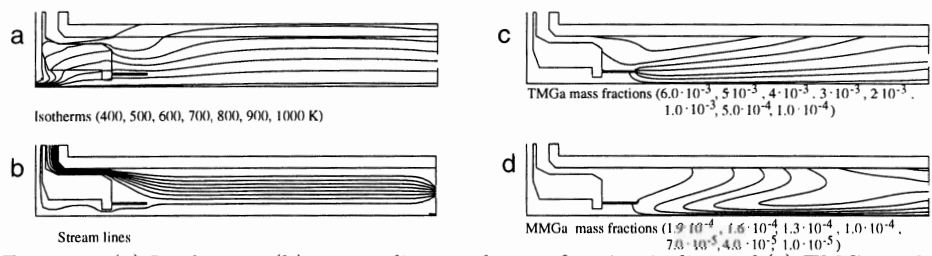

Figure 1: (a) Isotherms, (b) stream lines and mass fraction isolines of (c) TMGa and (d) MMGa in the reaction chamber. Growth conditions: inlet flow ratio between upper and lower inlet R= 85, total flow rate F= $21.5\frac{l}{min}$, $F_{AsH_3} = 100\frac{l}{min}$, growth temperature $T_g = 750°$ und system pressure $P_0 = 200$ mbar.

excess. TMGa (c) and MMGa (d) mass fraction distributions are shown in Fig. 1. Homogeneous decomposition of TMGa occurs actively in the heated gas near the susceptor. Verification of the models is performed by comparison of calculated and measured growth rate distributions (Fig. 2). Polycrystalline deposit grows on the quartz ceiling at kinetically limited conditions due to the lower temperature on the cooled ceiling compared to the substrate. Therefore, a heterogeneous rate law is assumed as mass transport boundary condition on the ceiling. Thickness of the deposited GaAs film on the ceiling can be affected by the cooling gas composition (Ar/H_2 ratio), this can be seen in Fig. 3. The model predicts reasonably the thickness of the deposits and effect of the cooling gas composition, as shown in Fig. 3, and modelling can help to adjust the optimal Ar/H_2 ratio to reduce the formation of the polycrystalline deposit on the ceiling.

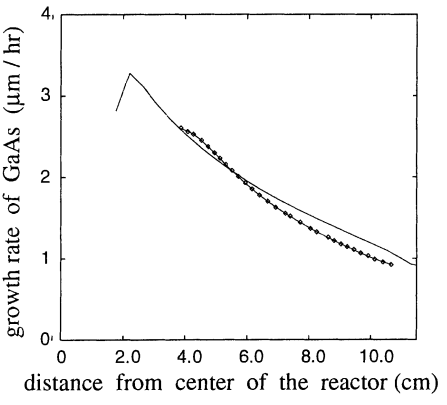

Figure 2: Calculated (—) and measured (-◇-) growth rates on the non-rotating wafer at a flow ratio of R=85; total flow rate F=17.2 $\frac{l}{min}$, T_g = 750° und P_0=200 mbar.

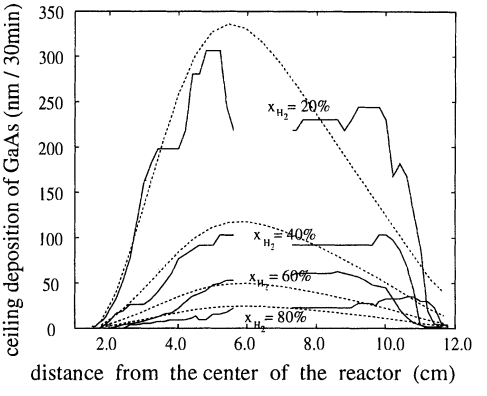

Figure 3: Measured (-) and calculated (- - -) layer thickness of ceiling deposits for cooling gas compositions x_{H_2}=20%, x_{H_2}=40%, x_{H_2}=60%, and x_{H_2}=80%; F=21.5 $\frac{l}{min}$, R=53 $\frac{l}{min}$, F_{AsH_3}=50 $\frac{l}{min}$ T_g= 750°, P_0=200 mbar.

3. Numerical algorithms

The models described above are implemented into two different solution procedures:

- a finite volume method using block-structured non-orthogonal collocated grids for two-dimensional flows as described in detail in [7].
- a procedure using an unstructured grid finite volume algorithm with adaptive local grid refinement [8].

The first approach seems to be very effective in terms of accuracy and convergence rate, especially because fast solution procedures and a multigrid method based on a Full Approximation Scheme for the non-linear coupled systems of equations can be employed for a speed up of the convergence rate. The disadvantage of the block-structured approach appears with resolving the complex reactor geometry and with

grid generation. In the case of unstructured grids, it is easier to introduce the complex reactor configuration, for example, provided from CAD, and automatic grid generation is possible, which makes this approach advantageous for the optimization of the reactor geometry and design. Another advantage of the unstructured grid approach is the possibility for an easy incorporation of an adaptive local grid refinement. Additional grid volumes are introduced automatically at the parts of the computational domain, where accuracy of the calculations does not satisfy a preselected criteria. However, the unstructured grid approach requires significantly more computing time and memory on a comparably fine grid than the blockstructured one . In Figure 4 the grids generated for the reactor are shown using both numerical approaches.

An optimal way to combine the advantages of both approaches is to use hybride unstructured/structured grids. In this case it would be possible to preserve the high accuracy and convergence rate of structured algorithms and the geometrical flexibility of the unstructured approach. This will be a topic for forthcoming research.

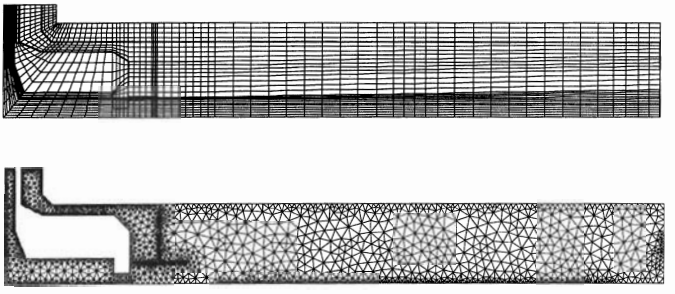

Figure 4: Comparison of structured (on top) and unstructured grids (on bottom)

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