Equipment and Process Simulation of Compound Semiconductor MOCVD in the Production Scale Multiwafer Planetary Reactor

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Abstract

The article addresses the use of computational modelling during the equipment design and process development of the Planetary Reactor®, an industrial production scale multiwafer reactor for the MOCVD (Metalorganic Chemical Vapour Deposition) of epitaxial compound semiconductor thin films. MOCVD equipment and process simulation is based on the coupled computation of gas flow field, heat transfer, including rf induction and thermal radiation, and chemical species mass transport and reaction kinetics on 2D axisymmetric and 3D computational domains.

1 Introduction

Compound semiconductor heterostructures are the basis for optoelectronic and electronic devices that can be found in numerous consumer products as well as in telecom and data transmission equipment, like lasers, modulators and detectors for fiber optics, or HBTs (Hetero Bipolar Transistors) and HEMTs (High Electron Mobility Transistor) as high frequency power amplifiers for wireless communication. In the near future Ultra High Brightness Light Emitting Diodes (UHB-LEDs) are likely to replace the conventional light bulb in practically any application from domestic and office lighting to traffic signals and outdoor advertising. Metal Organic Chemical Vapor Deposition (MOCVD) is the technique of choice to meet the requirements for high volume production in the compound semiconductor industry. During MOCVD processing a dilute mixture of reactive gases decompose and thin epitaxial layers of III-V materials, like AlGaAs, InGaAsP, InGaN and related compounds, are deposited in a low pressure reactor with substrate temperatures of 600°-800°C for conventional III-V materials and up to 1200°C for GaN based layers. [1] reviews the MOCVD growth of compound semiconductors.
The present paper introduces the use of equipment level computational modelling in the field of compound semiconductor MOCVD. Simulation has been applied to

further develop, improve and optimise equipment performance and process design of the Planetary Reactor® [2], an industrial production scale MOCVD reactor for multiwafer processing of up to 7x6" (or 49x2" equivalently) substrates. Model features and software requirements to describe the MOCVD process are discussed, model validity is demonstrated by comparison between predicted and measured growth rate distributions in the Planetary Reactor®, determined by X-ray diffractrometry. The impact of modelling and simulation on key design issues for the performance of MOCVD reactors is addressed, i.e. gas inlet design, control of reactor scale species depletion, and thermal management, in order to meet stringent production requirements, such as growth rate uniformity, compositional control of multinary III-V layers, and precursor species utilisation efficiency, while ensuring reproducibility and process stability in an industrial volume production environment.

2 Modelling approach

The computational model of the MOCVD growth process is based on first principle prediction of coupled flow, heat and mass transfer by solving the corresponding transport equations on 2D or 3D domains supplemented with appropriate boundary conditions. The MOCVD process model features multi-disciplinary physics and chemistry, as thermal radiation transfer, the electromagnetics for rf induction heating, gas phase and surface chemistry. See [3] for a comprehensive overview of CVD model approaches, and [4] for previous work on Planetary Reactor® modelling. Radiation propagation is computed by Monte-Carlo ray tracing; spectrally dependent optical properties of semitransparent walls and coated surfaces are taken into account. The transport equations are solved by a pressure based Finite-Volume method on unstructured grids [5].

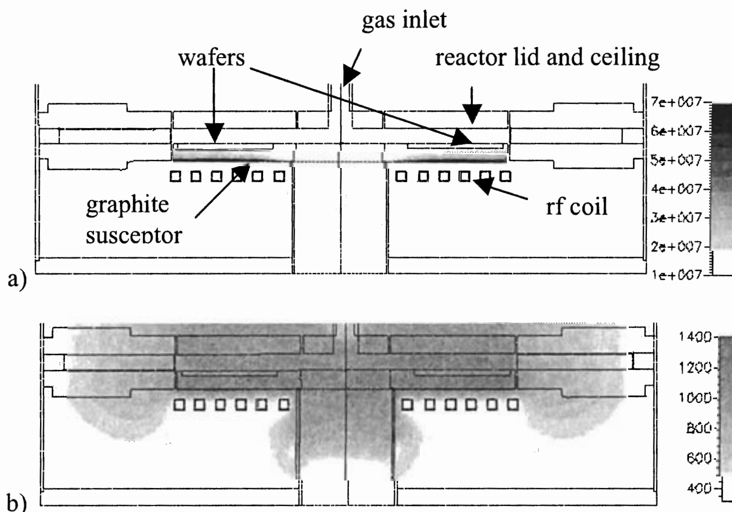

Fig. 1. Calculated inductive power density (W/m^3) distribution (a) and temperature (Kelvin) distribution (b) in the Planetary Reactor® at T = 1150°C (generic design of the reactor).

3 Results

The accurate prediction of detailed heat transfer in the process environment, including thermal radiation as the predominant mode of heat transfer and electromagnetic induction in a rf induction heated system, is a crucial prerequisite for the determination of species distribution, as well as layer thickness and composition. Thermal control and uniformity in the growth area up to a level of $\pm 1°C$ are needed to meet uniformity requirements during MOCVD growth of multinary layers, as e.g. InGaN or InGaAsP due the high temperature sensitivity of species incorporation, composition and resulting material properties. Fig. 1 shows the heat source distribution in the graphite susceptor of the Planetary Reactor® at typical process conditions for high temperature growth of GaN based layers, as resulting from the coupled computation of electromagnetic induction, heat transfer and flow.

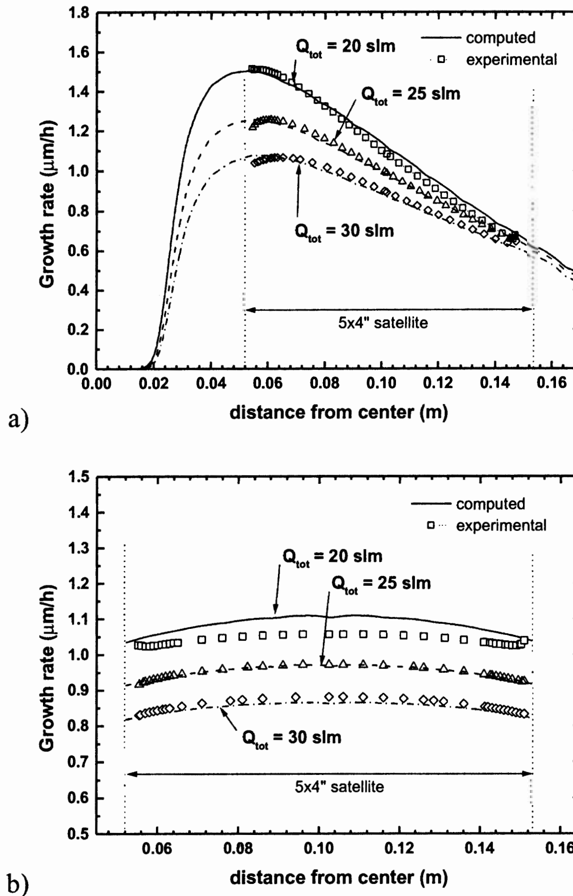

Fig. 2. Computed (lines) and measured (symbols) growth rate profiles of $Al_xGa_{1-x}As$ (x=0.28) in the Planetary Reactor® AIX 2400G3 on static (a) and rotated (b) substrates for various carrier gas flow rates. Growth temperature T = 600°C, process pressure p = 100 mbar.

Equipment and process modelling has been extensively used to reveal parametric dependencies of growth rate uniformity and precursor efficiency on a wide variety of process conditions and combinations thereof, as e.g. flow rates, flow rate split ratio between multiple gas inlets, and precursor partial pressures, as shown in Fig. 2 for carrier flow rates. The design of a multiple flow gas injector was also supported by the detailed 3D-simulation of coupled flow, heat transfer, and species mass transfer around the injection zone. A series of design criteria had to be satisfied, like the absence of local separation and return flow, separating different precursors, matching of flow rates, and thermal management to avoid pre-reaction and condensation of decomposition by-products. This allowed for the optimisation of a rather large number of geometry and process related parameters, which is prohibitive for a time consuming, purely empirical approach based on expensive cycles of re-designing, building of hardware components, and testing under process conditions.

4 Conclusion

Computational modelling of the MOCVD process is used for equipment and process optimisation in an industrial multiwafer Planetary Reactor®. The modelling approach is based on the solution of coupled incompressible gas flow, heat transfer, including rf induction and thermal radiation transfer, and chemical species mass transport and reaction kinetics. Key issues of modelling efforts include global heat transfer and thermal management in the rf induction heated system up to growth temperatures of 1150°C (e.g. during MOCVD of Nitride thin films), the analysis of parametric dependence of layer thickness uniformity, and the design of crucial components, like gas injectors. Equipment optimisation and process tuning resulted in a growth rate uniformity of GaAs of < 1% on 6" substrates and photoluminescence uniformity of < 1 nm standard deviation on the usable substrate area.

5 Acknowledgements

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