Modeling and process design of III-Nitride MOVPE at near-atmospheric pressure in Close Coupled Showerhead and Planetary Reactors

M. Dauelsberg[a], C. Martin[a], H. Protzmann[a], A. R. Boyd[b], E. J. Thrush[b], J. Käppeler[a], M. Heuken[a] R. A. Talalaev[c], E. V. Yakovlev[d], A. V. Kondratyev[d]

[a]AIXTRON AG, Kackertstr. 15-17, 52072 Aachen, Germany; [b]Thomas Swan Scientific Equipment Ltd. Buckingway Business Park, Cambridge CB4 5FQ, UK; [c]Semiconductor Technology Research GmbH, P. O. Box 1207, 91002 Erlangen, Germany; [d]Soft-Impact Ltd., P. O. Box 83, 194156 St. Petersburg, Russia,

This paper deals with the MOVPE growth of the group-III Nitride compounds GaN and AlGaN from TMGa, TMAl and NH_3 at higher process pressures up to near atmospheric pressure in commercial production scale multi-wafer reactors. Advanced model development and its validation by growth experiments are presented with particular emphasis on gas phase reaction kinetics and nucleation dynamics which are recognized to be crucial for Nitride MOVPE at elevated pressures. The impact of various process and reactor design parameters on the pressure dependence of GaN growth efficiency and AlGaN solid composition and their physical origin is discussed. The suitability for near atmospheric pressure growth of both the Close Coupled Showerhead reactor and the Planetary Reactor® is demonstrated. Process optimization strategies and reactor design criteria to approach higher pressures are derived from the analysis. Growth results underline the advantages of growing high temperature GaN at elevated pressures. In comparison with recently presented results [1] the model has been further refined, thus being capable of reproducing the effect of different reactor wall temperatures on the gas phase nucleation dynamics and pressure dependence during Nitride MOVPE.

The wide interest in near atmospheric pressure MOVPE of GaN-based heterostructures stems from the observation of lower threading dislocation density [2], better magnesium activation [3] and lower background impurity concentration [4] at elevated pressures. On the other hand, it is known that the growth efficiency of GaN and the Al-incorporation in AlGaN may be reduced at elevated pressures due to enhanced reaction kinetics, gas phase nucleation of reaction by-products and subsequent depletion of reactants. There is ample evidence of the occurrence of gas phase nucleation and cluster formation during MOVPE of group-III Nitrides and its dependence on various process parameters, e. g. from light scattering experiments [5].

The modeling approach is based on the simulation of mixed convective laminar flow coupled with heat transfer and chemical species mass transfer, using standard CFD (= Computational Fluid Dynamics) technology. The modeling of gas flow transport phenomena is supplemented by advanced reaction chemistry, thin film deposition and the gas phase nucleation dynamics of low volatility reaction by-products generated during the MOVPE of GaN and AlGaN at high temperatures.

The generation of adduct species, subsequent oligomerization, decomposition and the rate of formation of clusters (nano-particles) are found to control the group-III incorporation efficiency of GaN and AlGaN MOVPE in particular at elevated pressures. The effects of reactant dilution, residence time, flow pattern and thermal environment in the process chamber, as well as chamber size on the reaction kinetics, the rate of gas phase nucleation and the pressure dependence of Nitride MOVPE growth are analyzed and discussed. In figures 1 the effect of increasing the flow rate with increasing pressure in the Planetary Reactor® is exemplified. Figure 2 shows the pressure dependence of high temperature grown GaN for different chamber gap heights and reactor wall temperature in the Close Coupled Showerhead Reactor. Differences and communalities between the two reactor types Close Coupled Showerhead and Planetary Reactor® are debated.

[1] M. Dauelsberg, C. Martin, H. Protzmann[a], A. R. Boyd, E. J. Thrush, N. D. Gerrard, R. A. Talalaev, E. V. Yakovlev, A. V. Kondratyev, ICNS-6, Bremen, Germany, Aug. 28 – Sept. 2, 2005.
[2] P. Fini, X. Wu, E. J. Tarsa, Y. Golan, V. Srikant, S. Keller, S. P. DenBaars, J. S. Speck, Jpn. J. Appl. Phys. 37 (1998) 4460.
[3] P. Kozodoy, S. Keller, S. P. DenBaars, U. K. Mishra, J. Crystal Growth 195 (1998) 265.
[4] D. D. Koleske, A. E. Wickenden, R. L. Henry, M. E. Twigg, J. Crystal Growth 242 (2002) 55.
[5] J. R. Creighton, G. T. Wang, W. G. Breiland, M. E. Coltrin, J. of Crystal Growth 261 (2004) 204.

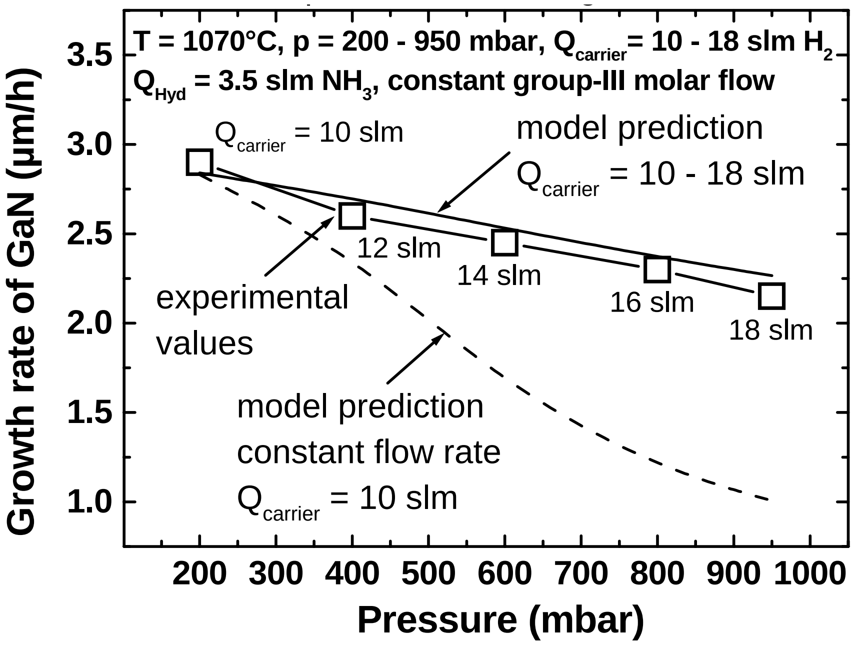

Figure 1. Dependence of GaN growth rate on pressure and carrier gas flow rate $Q_{carrier}$ in the Planetary Reactor® 6x2" configuration.

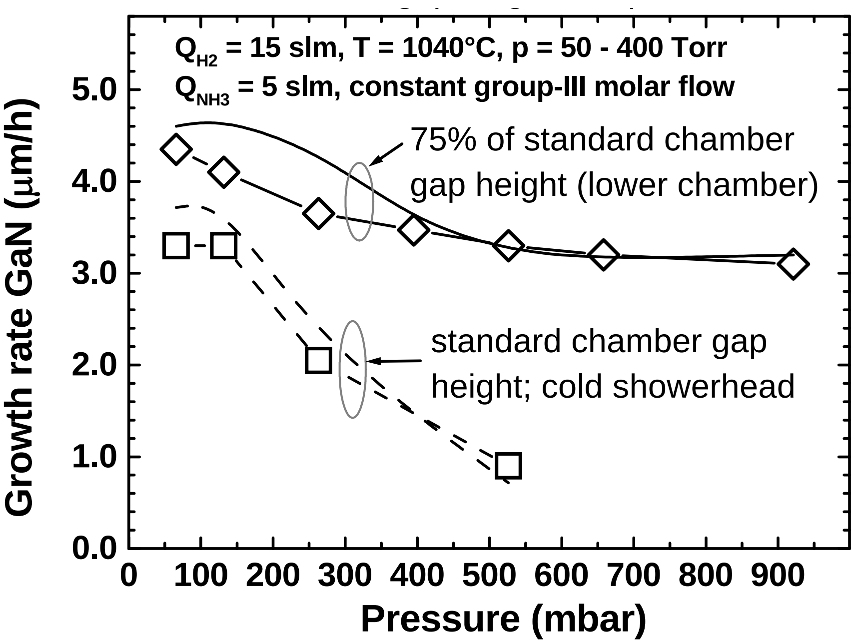

Figure 2. Pressure dependence of GaN growth rate in the 6x2" Close Coupled Showerhead Reactor, model prediction (lines without symbols) compared with experimental data (lines and symbols).