Critical issues in group-III nitride MOVPE modeling

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One of the main features of III-nitride growth is quite high (compared to conventional III-V's) deposition temperatures. The decomposition of metalorganic precursors results in formation of atomic group-III metal species and/or complex molecules that may nucleate forming particles in the gas phase. Parasitic reactions between group-III and group-V precursors may serve as an additional material loss mechanism. Desorption of volatile group-III species from the growing surface is the principal mechanism controlling the ternary alloy composition. Modeling examples illustrating the role of theses mechanisms in AlN, AlGaN, and InGaN MOVPE are presented.

A detailed mechanism of gas-phase reactions of the initial precursor decomposition and formation of complex molecules that do not contribute to the growth [1] is combined to an original model of particle formation (Fig. 1) during AlN growth. The results of modeling of AlN deposition in a vertical high-speed rotating-disk reactor demonstrate a good agreement to the experimental data on the AlN growth rate as a function of the susceptor rotation rate (see Fig. 2). In addition, a qualitative reproduction of general trends reported in the literature (the reduction of the AlN growth rate with the operating temperature, pressure, and TMAl flow rate) is obtained. For InGaN MOVPE, it is shown that atomic indium produced by TMIn pyrolysis is capable of creating a high supersaturation in the gas phase, which results in nucleation and subsequent growth of liquid indium clusters. Detailed 3D modeling of InGaN MOVPE in a horizontal reactor has shown that the material losses due to condensation may reach 40 % at high indium gas-phase composition.

Elevated temperatures used to grow III-nitride compounds activate a chemical mechanism that is not pronounced during the growth of arsenides and phosphides: desorption of volatile group-III species from the growth surface. This mechanism manifests itself as a reduction of the Al incorporation into AlGaN with increasing group-III flow and increase in the Al content with the operating temperature [3] at temperatures above 1100 °C, when gallium desorption becomes intensive. Both tendencies have been reproduced quantitatively using a model of AlGaN MOVPE. In case of InGaN deposition, it has been found that interplay between gas-phase condensation of indium clusters and surface effects, such as indium desorption and elastic strain, determines to a great degree the indium incorporation.

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[2] J.R. Creighton, W.G. Breiland, and M.E. Coltrin, *Electrochem. Soc. Proc.*, **2002-3**, 28 (2002).
[3] S. Keller, G. Parish, P.T. Fini, S. Heikman, C.-H. Chen, N. Zhang, S.P. DenBaars, U.K. Mishra, Y.-F. Wu, *J. Appl. Phys.*, **86**, 5850 (1999).

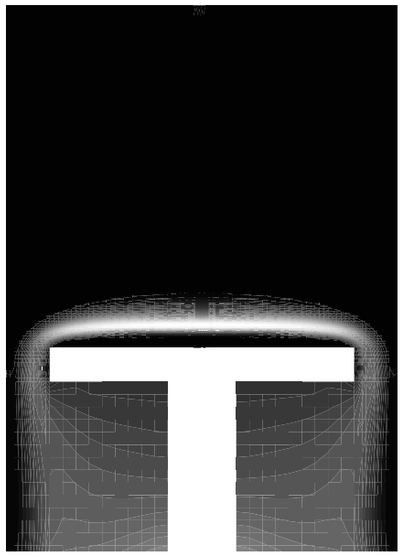

Figure 1. Layer of particles during AlN growth in a vertical reactor, predicted by the computations.

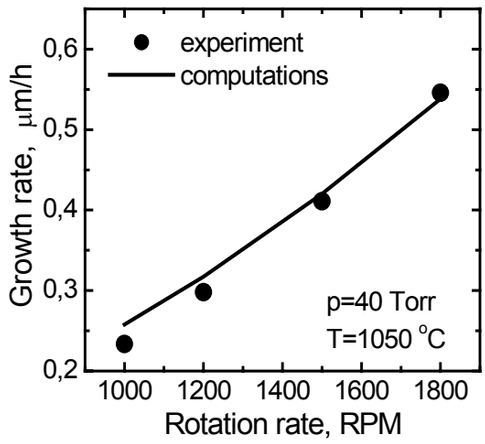

Figure 2. AlN growth rate as a function of the susceptor rotation rate. Experimental data from [2].