Modeling and experimental analysis of GaN MOVPE in AIX 200 RF reactor

R.A. Talalaev [1)], **E.V. Yakovlev [1)]**, Yu.N. Makarov [2)], B.S. Yavich [3)], W.N. Wang [3)]
1) Soft−Impact Ltd., P.O.Box 83, 194156, St.Petersburg, Russia , 2) STR GmbH, P.O. Box 1207, D−91002 Erlangen, Germany , 3) Department of Physics, University of Bath, BA2 7AY, Bath, United Kingdom

Introduction

MOVPE of group III−nitride heterostructures for optoelectronic applications represents the complex process whose features differ significantly from conventional III−V growth procedure. High deposition temperatures and V/III ratios influence directly flow pattern, heat transfer and transport properties of the carrier gas/precursor mixture determining the overall deposition behavior. In this paper, we report on the combined modeling and experimental study of GaN MOVPE in AIX 200/4 RF−S horizontal reactor with separated supply of group−III and group−V precursors.

Detailed 3D simulations accounting for all relevant physical processes such as flow dynamics, heat transfer and precursor mixing and transport are performed in order to evaluate the influence of process parameter variation on the growth rate and uniformity. Gas−phase chemistry model includes the unimolecular gas−phase decomposition of trimethylgallium. Surface chemistry model [1] covers the whole range of deposition conditions that may be important for correct predictions: i.e., low temperature kinetically limited growth (parasitic deposition on reactor walls), mass transport limited growth at moderate temperatures, and growth limited by gallium desorption at elevated temperatures.

Effects of trimethylgallium and hydride flow rates and substitution of ammonia with nitrogen on the growth rate are studied and discussed by comparison of theoretical and experimental results.

Experimental

GaN epitaxial layers were grown on (0001) oriented 2” sapphire rotated substrates, using TMGa and NH_3 as precursors. A quartz plate separated the main reactant flows; as a result, TMGa with H_2 carrier gas were introduced into the upper stream, and NH_3 with H_2 or with a mixture of H_2 and N_2 carrier gases were supplied into the lower stream. Experimental results were obtained from growth runs that were performed at 200 mbar and 1140 or 1160 ^{o}C. The growth temperature was measured as a reference from the graphite susceptor bottom. To study growth rate variations in a single run by changing the input parameters, in− situ monitoring measurements of reflectivity were carried out.

Results and discussion

The design of the horizontal AIX 200/4 RF−S reactor includes some important features that should be properly incorporated into the global reactor model. Among these features, one can note the RF heated graphite susceptor consisting of two disks separated by a thin gap filled with hydrogen that provides the rotation of the upper susceptor disk and may lead to a temperature drop between the two disks up to 50 °C. Also, there is a cooling channel around the susceptor for the purpose of localization of heating area. Accurate prediction of the temperature distributions over the internal surfaces of the reactor liner (such as side walls and ceiling), heated mainly by radiation from the hot susceptor, is of great importance due to the following reasons. The overall efficiency of the growth process is determined by the degree of the utilization of TMGa and the products of its decomposition (primarily monomethylgallium (MMGa)), which, in turn, depends on the intensity of parasitic deposition on the side walls and ceiling. The parasitic deposition intensity is highest on the ceiling and is largely governed by two main factors: ceiling temperature and transport of trimethylgallium coming from the upper inlet and its mixing with ammonia and hydrogen supplied through the lower inlet. The presented computational model of the reactor includes the above geometrical details and physical−chemical mechanisms along with commonly considered flow dynamics, heat and mass transfer, and gas−phase chemical reactions.

Typical temperature distributions for the central cross−section of the reactor and over the ceiling are presented in Figs. 1−2. The distributions are given for the nominal deposition temperature 1160 °C, and one can see that under such operating conditions the maximal temperature on the ceiling may be as high as about 700 °C, which means that over some part of the ceiling parasitic deposition of GaN is limited by species transport to the ceiling rather than by low−temperature kinetics. The resulting distribution of the parasitic deposition rate over the ceiling is demonstrated in Fig. 3. The deposition intensity has a rather sharp maximum in the region located opposite the susceptor frontal edge due to relatively high temperatures and favorable transport conditions (TMGa supplied trough the upper inlet readily reaches these region) there. The “hole” on the parasitic rate distribution is related to the presence of the viewport opposite the wafer center, where hydrogen is supplied. Fig. 4 represents the growth rate mapping over the 2” wafer. The computed growth rate non−uniformity of about 25 % is close to the experimental observations.

Several parametric dependences of the growth rate have been computed. The enhancement of growth rate with the TMGa flow (see Fig. 5) is a well−known effect reproduced by the computations, but with some underestimation of the growth rate level. Fig. 6 shows that the growth rate decreases with increasing hydride flow supplied through the lower inlet (this increase is made by keeping the ammonia flow constant (3 SLM) and elevating the hydrogen flow), which is due to the effect of dilution of group−III species by the surrounding hydrogen/ammonia mixture.

It is interesting to consider how the composition of the mixture coming from the lower inlet influences the growth rate. Three series of experimental runs at fixed lower flow (8 SLM) have been performed, and the obtained results are given in Fig. 7. At first, the ammonia flow was increased with the corresponding decrease in the hydrogen flow rate. Then, nitrogen was added into the hydride mixture, and experiments were conducted at two constant ammonia flows (1.5 and 3 SLM) with gradual substitution of hydrogen with nitrogen. From the data collected, we can draw two main conclusions: (1) adding nitrogen into the hydrogen/ammonia mixture (at fixed total flow) affects the growth rate in a way very similar to the increase in the ammonia flow; (2) substitution of ammonia with nitrogen has a weak effect on the growth rate. Thus, substitution of hydrogen coming from the lower inlet with both ammonia and nitrogen has a practically the same effect on the growth rate. The computations performed for the ammonia flow of 3 SLM and varied H_2/N_2 ratio (see Fig. 7) fit well the experimental data. The growth rate drops by a factor of four as the nitrogen flow is raised from zero to 4.5 SLM, and this effect may be attributed to generally slower, compared to hydrogen, diffusion of TMGa and, consequently, MMGa in the denser nitrogen−containing mixture, as well as to delayed heating of the precursor mixing zone.

Conclusions

We have performed a combined experimental and modeling analysis of GaN MOVPE in the horizontal AIX 200/4 RF−S reactor. A computational model of the reactor, including the most important details of the reactor design and accounting for the physical−chemical mechanisms governing the growth process, in particular, low and moderate temperature parasitic deposition on the reactor walls, has been developed. It has been demonstrated that the parasitic deposition rate is highest on the ceiling due to the specificities of the heat transfer and mass transport in the reactor. The model verification has been performed using experimental data on the GaN growth rate under different operating conditions. A reasonable reproduction of the measured dependencies of the growth rate on the TMGa and hydride flow has been obtained without any fitting. In addition, it has been shown experimentally that the substitution of the hydrogen coming from the lower inlet with both nitrogen and ammonia has a similar effect on the growth rate that decreases as the hydride mixture composition is changed in favor of ammonia or nitrogen.

References

[1] R.A. Talalaev, E.V. Yakovlev, S.Yu. Karpov, Yu.N. Makarov, Journal of Crystal Growth, 230 (2001) 232.

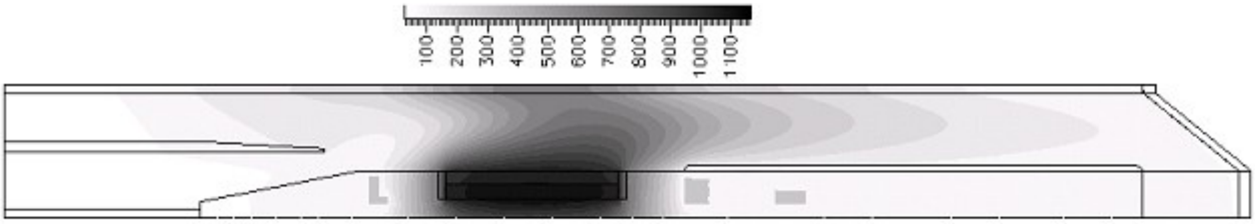

Fig. 1. Temperature distribution (°C) in the central cross-section of the liner.

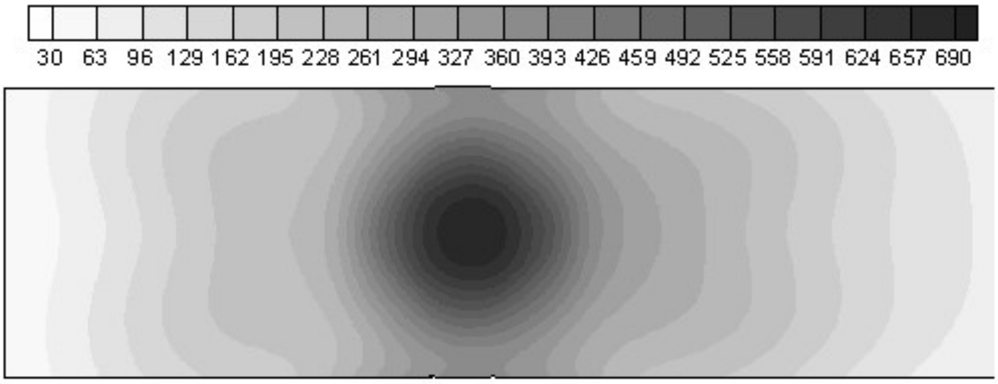

Fig. 2. Temperature distribution (°C) over the liner ceiling.

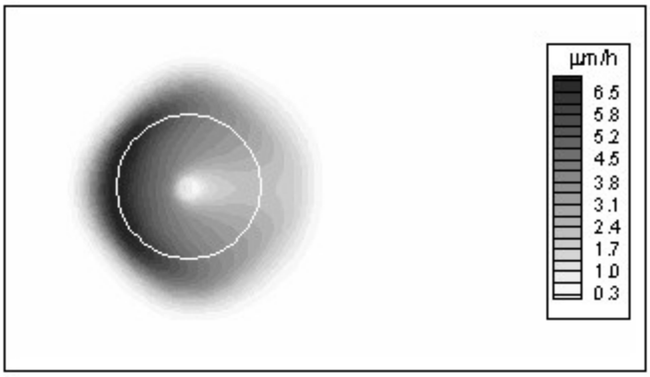

Fig. 3. Parasitic deposition rate over the ceiling. White circle indicates the wafer position.

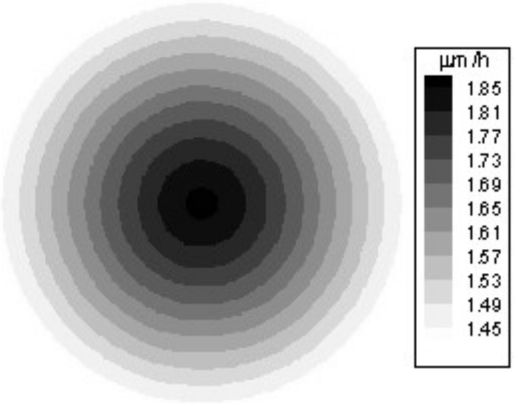

Fig. 4. Growth rate mapping over the 2" wafer.

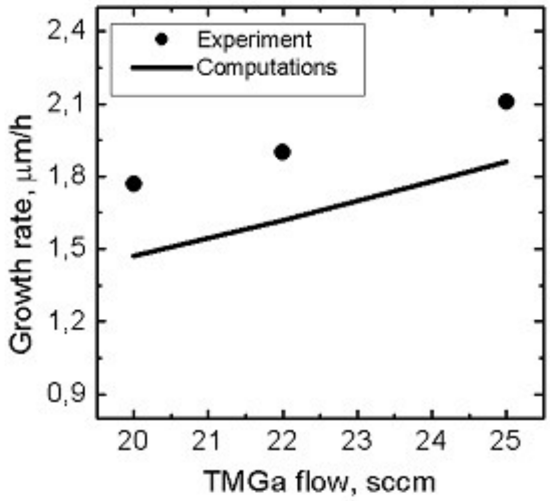

Fig. 5. Growth rate as a function of the TMGa flow

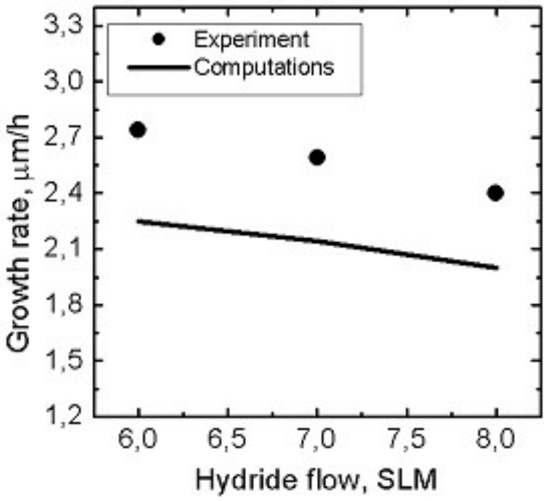

Fig. 6. Growth rate as a function of the flow via lower inlet at NH_3 flow = 3 SLM

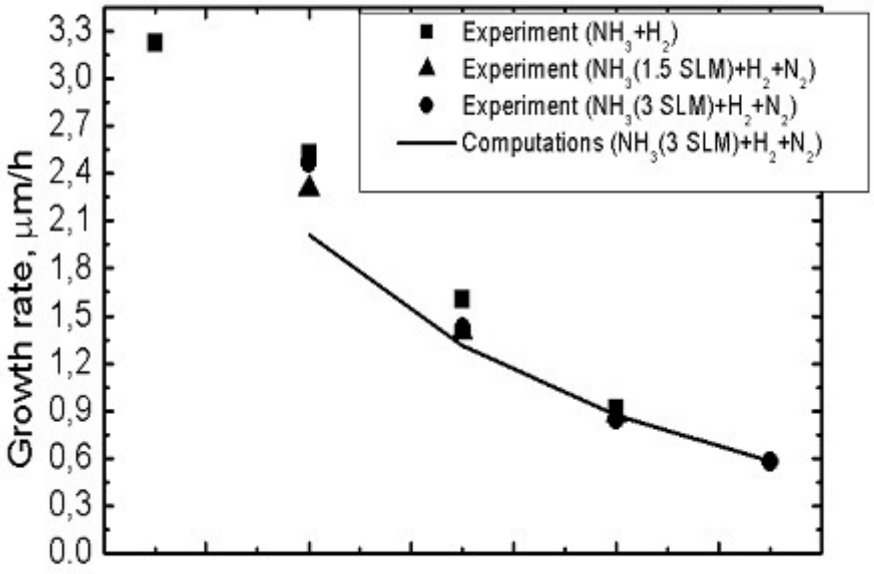

Fig. 7. Growth rate as function of the sum of ammonia and nitrogen flow via lower inlet