Journal of Crystal Growth 406 (2014) 53–58

Contents lists available at ScienceDirect

Journal of Crystal Growth

journal homepage: www.elsevier.com/locate/jcrysgro

Numerical simulation of the gallium nitride thin film layer grown on 6-inch wafer by commercial multi-wafer hydride vapor phase epitaxy

Xue-Feng Han [a], Min-Jae Hur [a], Jae-Hak Lee [b], Yoo-jin Lee [b], Chung-seok Oh [b], Kyung-Woo Yi [a,*]

[a] *Department of Materials Science and Engineering, Seoul National University, Seoul 151-744, Republic of Korea*
[b] *TGO tech, Hwasung-City, Gyeonggi-Do, 445-812, Republic of Korea*

ARTICLE INFO

Article history:
Received 17 April 2014
Received in revised form
3 June 2014
Accepted 19 August 2014
Communicated by R. M. Biefeld
Available online 27 August 2014

Keywords:
A1. Computer simulation
A1. Fluid flow
A3. Multi-wafer HVPE
B1. GaN

ABSTRACT

In this study, experimental analysis and numerical simulation analysis have been exploited to investigate the effect of the flow rate of the carrier gas and the effect of the temperature in a new multi-wafer hydride vapor phase epitaxy (HVPE) device. The numerical calculation results have shown the same trend with the experimental results demonstrating that increasing the carrier gas flow rate could shift the maximum value position of the deposition rate to increase the uniformity of the deposition rate distribution within the wafer. The species fraction and the fluid flow also have been investigated to further explain the effect of the carrier gas. Furthermore, temperature effect is also studied to show that in a relatively high temperature, the uniformity of the deposition rate in this equipment is better. The uniformity of the deposition thickness is evaluated through the analysis of standard deviation.

1. Introduction

Gallium nitride has a direct band gap which is widely used in the LED (light emitting diodes) and LD (laser diodes) fabrications. After the excellent work and numerous contributions from the Nichia Corporation's research team [1], the GaN growth method has received a lot of attentions from many research groups and companies. At present, high nitrogen pressure solution growth (HNPSG), metal-organic chemical vapor deposition (MOCVD) and hydride vapor phase epitaxy (HVPE) are feasible to produce the GaN film. Among them, only HNPSG has the ability to produce the dislocation-free GaN single crystal and the directional growth experiment has been conducted by Bockowski et al. [2]. But this method seems not to be a hot topic across the commercial LED companies due to its harsh conditions such as high temperature of 2000 K and high pressure of 2 GPa. Meanwhile, the GaN film grown by MOCVD based on the trimethylgallium (TMGa) has a good quality with a much lower cost in comparison with HNPSG. Thus this method is favored in LED product application. Also, because of the widespread use of MOCVD such as TiN deposition, grapheme deposition, GaAs deposition, it has been studied very thoroughly during the past years [3–7]. However, the constantly increasing illuminating LED market demands a more cost-effective way to produce the GaN film. As a consequence, improving the quality of the GaN film produced by HVPE which exploits a cheaper reactant GaCl and has a larger growth rate becomes a critical research work.

Many researches have been published before, from the atomic scale simulation [8–10], molecular-dynamics study [11,12] to computer fluid dynamics (CFD) [3,13–17]. Especially for the CFD calculation, previous studies have provided considerable insights into the effect of the equipment geometry [17,18], the effect of the temperature [19], the effect of the carrier gas [15] and the effect of the GaCl synthesis reaction [13]. Most of them are focusing on the experimental stage other than mass production stage. Thus we hope that our work will make a distribution to help people think about the method to improve the quality of the mass production by HVPE. In traditional HVPE equipment, there are usually two pipes to transport the reacting gases, and sometimes the carrier gas is input through another pipe. Alternatively, reacting gases can be mixed with the carrier gas to deposit. In order to improve the uniformity of the deposition thickness at the wafer, the wafer is rotated with the susceptor. And through the remarkable studies on the traditional HVPE equipment, a nice uniformity of GaN thin film can be controlled. To increase the productivity, a device capable of depositing several 6-inch wafers has been developed. The computational and experimental study of this equipment will be the subject of this paper.

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* Corresponding author.

http://dx.doi.org/10.1016/j.jcrysgro.2014.08.018

2. Experiment procedure

2.1. Experiment

A new design of multi-wafer HVPE equipment is used to deposit the GaN epi-layer in our experiment. As shown in Fig. 1(a), six 6-inch wafers are placed on the susceptor, the reacting gases and carrier gas are transported from the center pipe and flow out through the peripheral wall. To increase the throughput, the susceptor is designed large enough to hold many wafers. Compared to the single-wafer equipment, the control of the uniformity of the deposition thickness in all of the wafers becomes more difficult. Since the susceptor is very large, the wafers near the nozzle deposit more quickly than the wafers far away from the nozzle due to the transport phenomena. The similar phenomena are also presented in the conventional equipment [15–17]. With the increase of the susceptors size, the transport effect becomes more obvious and the uniformity becomes much lower. To overcome the transport effect, carrier gas is utilized to dilute and transport the reacting gases. Actually, the method to introduce the carrier gas is diverse: carrier gas can be injected separated with reacting gases [19]; carrier gas can be also mixed into reacting gases [16]. Besides, the geometry of the gas pipes has an effect on the distribution of the gas species [17]. In our experiment, with other conditions constant, two different flow rates of carrier gas are used to investigate how the carrier gas influence the GaN deposition rate distribution. The thickness of the GaN deposition is measured by the epi-layer thickness mapping device named PL+A310, which exploits the interference phenomena of the crystal surface and the interface between the crystal and substrate. To reduce the cost of the experiment, 6-inch wafer is replaced by the three 2-inch wafers in a row as shown in Fig. 1(b).

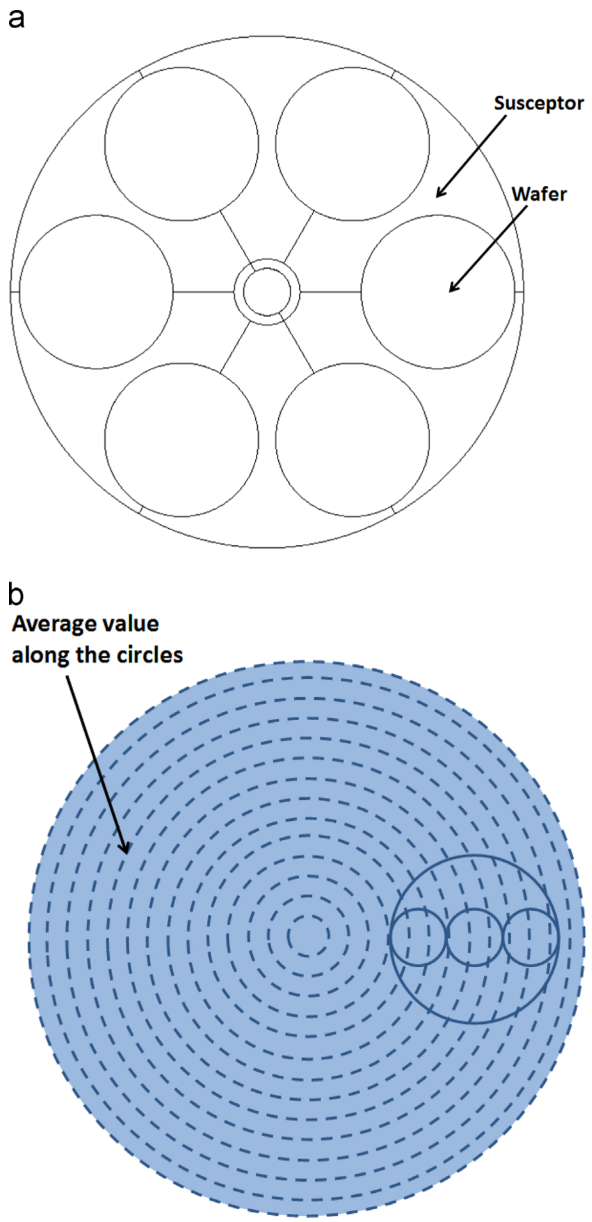

Fig. 1. (a) Schematic configuration of the equipment from the top view and (b) method of measuring the thickness distribution.

2.2. Calculation

Moreover, to ensure all of the wafers have the same deposition thickness, the behavior and the distribution of each gas species should be analyzed in detail. Since the deposition and reaction occurred at high temperature in a hermetic chamber, the phenomena are hard to investigate by the experiments. The analysis work is implemented by the CFD software CFD-ACE. The simulation domain is including the susceptor, wafers, gas inlets and gas outlets. The model is made of 316,545 unstructured grids. Since the actual experiment is conducted under a long time at a constant temperature and pressure, steady state was assumed in the simulation.

The main phenomena such as flow, mass transfer and chemical reaction have been considered in this simulation. The gravity is 9.8 m/s^2, temperature is 1223 K, and pressure is 101,325 Pa. For the volume conditions, the gases obey the ideal gas law; the viscosity is calculated by mix kinetic theory; the heat capacity is by the JANNAF method; heat conduction is by mix kinetic theory. For the boundary conditions, all of the external walls are adiabatic; the gases flow into the model at a constant volume per minute; the outlets are designated as a constant pressure. The chemical reaction occurs at the surface of the wafers and susceptors.

To make the calculation more efficient, some assumptions have been made: 1. Considering the temperature difference within the susceptor is very small, the temperature of the whole equipment is set as constant. 2. The depositions occur not only at the wafers but also at the susceptor according to the observation of the experiment, and both of the GaN deposition rates are regarded as same value. 3. Gas phase reaction including the decomposition of NH_3 and the formation of NH_4Cl has not been considered due to their effects are not obvious in the previous study [16]. 4. Turbulence would not be included due to the maximum Reynolds number is 1514.74.

The primary equations applied in this simulation are as following:

1. Flow equation

$$\rho\frac{Dv}{Dt}=\eta\nabla^2 v-\nabla P+\rho g$$

$$\frac{\partial\rho}{\partial t}=\nabla(\rho\vec{v})=0$$

2. Deposition equation

$$J_i=\alpha_i\beta_i(P_i^w-P_i^e)$$
$$i=\mathrm{GaCl},\ \mathrm{NH_3H_2},\ \mathrm{N_2}\quad \beta_i=(2\pi\mu_i RT)^{-1/2}$$

Here, p, η, t, ρ, T and u are the pressure, viscosity, time, density, temperature and velocity vector, respectively. μ_i is the molar mass, R is the gas constant, p^w is the partial pressure at the surface, p^e is the saturated vapor pressure, and α is the sticking probability.