Pseudo-3D Multiphysics Simulation of a Hydride Vapor Phase Epitaxy Reactor

Matthias Hackert-Oschätzchen[1], Michael Penzel[1], Philipp Plänitz[2], Andreas Schubert[3]

[1]Chemnitz University of Technology, Chemnitz, Germany

[2]GWT-TUD, Dresden, Germany

[3]Chemnitz University of Technology, Chemnitz, Germany; Fraunhofer Institute for Machine Tools and Forming Technology IWU, Chemnitz, Germany

Abstract

GaN and its ternary alloys (InAlN, InGaN, AlGaN) opened the road to efficient solid state lighting by white light emitting diodes (LED) and led to important changes in the field of high capacity data storage by the blue laser diode (LD). GaN is a direct band gap semiconductor with a band gap of 3,42 eV at room temperature. It has god chemical and physical properties such as high saturated electron drift velocity, high thermal conductivity, high hardness, high breakdown field strength, good chemical stability and low dielectric constant. Hydride vapor phase epitaxy (HVPE) is considered as the most perspective growth technique to provide large size GaN-boules. Main advantage compared to other growth factor techniques is the achievable high growth rate. The cost effective growth of free standing GaN substrates requires the boule growth approach [1,2]. Within this study a complex multiphysics model of a HVPE reactor shown by ZHAO et al. was developed [1]. The specific parameters of the gas inlets have been derived from this literature. Figure 1 shows a scheme of the cross section of the vertical HVPE reactor. The growing boule is placed upside-down above the gas injector head. Precursors are GaCl and ammonia. The inlet of GaCl is in middle of the reactor. Two nitrogen streams are applied as barrier next to the inlet of ammonia, to avoid parasitic reactions near the inlets.

The usage of COMSOL Multiphysics with a pseudo-3D geometry approach was based on literature data. Afterwards compressible non-isothermal fluid flow and transport of diluted species were added. Therefore results from the complete coupling of fluid dynamics and thermodynamics were applied for the calculation of the concentration distributions of all species. As example of the results Figure 2 shows the concentration for ammonia. It can be derived, that the nitrogen flow barrier works well under the given conditions. Furthermore the model was used to characterize the reactor design by help of parametric studies. Therefore three different geometry variations, each with three different gas inlet parameters have been evaluated.

Reference

[1] ZHAO, C. et al.: Simulation of growing GaN in vertical HVPE reactor. Z. SCIENCE CHINA Physics, Mechanics & Astronomy, (2010), Bd. 53, Nr. 1, DOI: 10.1007/s11433-010-0108-z, S. 72-75.
[2] Schineller, B., Kaeppeler, J., Heuken, M.: Vertical-HVPE as a Production Method for Free-Standing GaN-Substrates. Konferenzprotokoll, AIXTRON AG, Austin, Texas, USA, 2007.

Figures used in the abstract

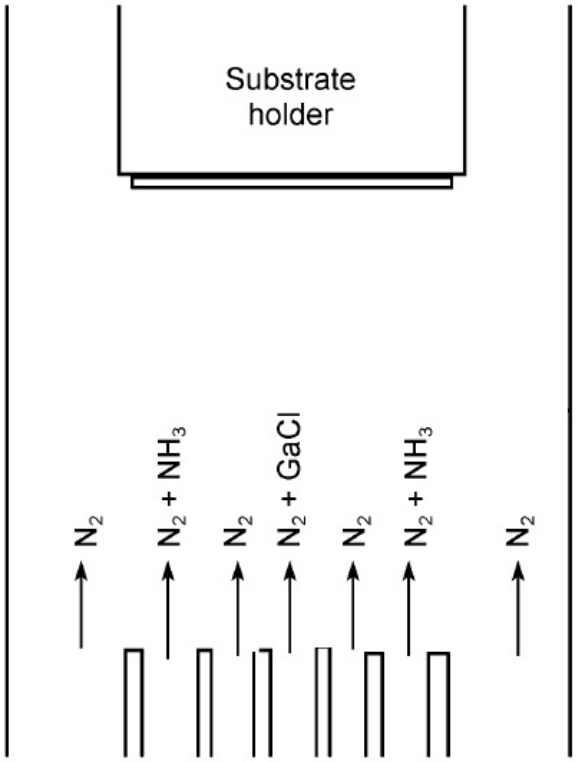

Figure 1: Scheme of the HVPE reactor for GaN growth [1].

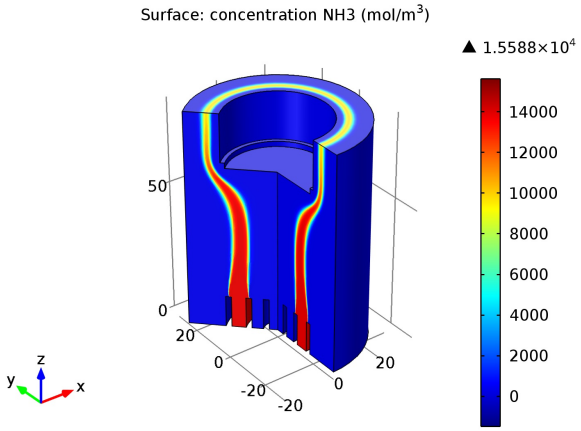

Figure 2: Concentration distribution of ammonia.