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

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Abstract: Gallium nitride (GaN) and its related nitride alloys with special physical properties are in technical areas of high interest. The growing of gallium nitride boules on non-native sapphire or silicon carbide requires complicated mechanisms of defect reduction in the lattice structure. Thus the production of gallium nitride substrates is a challenge. Hydride Vapor Phase Epitaxy (HVPE) is a promising technology for the production of large GaN bouls. In this study COMSOL Multiphisics is used for the simulation of non-isothermal flow and the mass transport. In this study a pseudo-3D simulation of non-isothermal flow and mass transport have been performed to analyze the influence of the reactor geometry and several process parameters.

Keywords: Multiphysics Simulation, Hydride Vapor Phase Epitaxy Reactor, Non-Isothermal Flow (nitf), Transport of Diluted Species (chds).

1. Introduction

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]. In the current state of technology this procedure is limited on the single-wafer manufacturing and not suitable for mass production. To get a better understanding of the processes inside such HVPE reactors, the flow and temperature fields and the concentration distribution of each species has to be considered in more detail. For this the selection of a suitable reactor was made and a model for multiphysics simulation was created.

2. Model creation

For the simulation only the main section of the reactor is considered. Simulation is limited to the area of the gas inlet nozzles to the substrate holder. Figure 1 shows the derived schematic cross section of the chosen HVPE reactor for GaN growth. GaCl is inlet in the middle of the gas nozzles. NH_3 and GaCl are separated by N_2 at the inlets to decrease parasitic reactions near the nozzles.

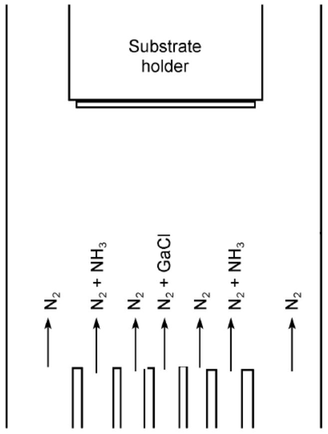

Figure 1. Schematic cross section of the gas inlet nozzles with incoming species and the substrate holder of the observed vertical HVPE reactor **[1]**

Starting from this part of the reactor, a rotationally symmetric 2D model geometry for the FEM simulation of Non-Isothermal Flow (nitf) was created. It is shown in Figure 2.

Figure 2 explains the structure of the FEM model. The reactor model has the border systems symmetry axis, inlets V_1 to V_4, wall, outlet, temperature, and the area of nitrogen. By setting up the model the following definitions have been used: at the inlets laminar gas flow conditions exist; at the wall no-slip boundary condition is satisfied; the equation of the state obeys the ideal gas law; Compressible fluid is adopted in the simulation and the flow is considered steady flow.

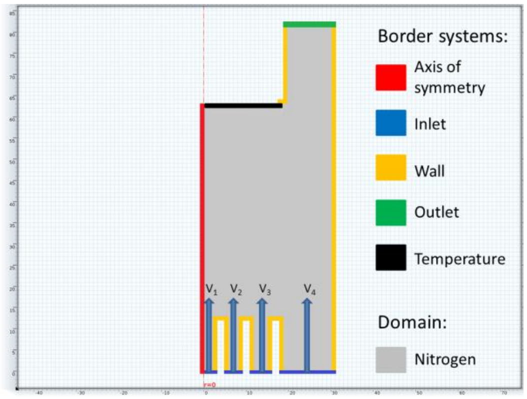

Figure 2. Axis symmetric reactor model with color-coded border systems and the flow area

The equations for conservation of mass, momentum, and energy are solved with the following boundary conditions. Gas inlets and gas outlets are defined as mass flow inlet and pressure-outlet, respectively. The temperature at the substrate-holder is 1320 K. In addition to the simulation of mass transfer the physical model Transport of Dilute Species (chds) was integrated. Therefore are separate boundary and domain conditions permit. For this the transport mechanisms are subject to convection with nitrogen as bulk fluid. For this purpose, three different sets of parameters from the literature were examined. The parameters used for the anisothermal flow and mass transport can be found in Table 1 to Table 3.

Table 1: Basic conditions I of literature **[1]**

Inlet	Species	Flow inlet temperature [K]	Flow inlet velocity [m/s]	GaCl or NH_3 ratio
V_1	GaCl-N_2	1120	0.06194	0.1650
V_2	N_2 1	1120	0.1032	/
V_3	NH_3-N_2	1120	0.06194	0.3781
V_4	N_2 2	1120	0.03943	/

The laminar flow rates are calculated by help of given mean inflow parameters from ZHAO et al [1], shown in Table 4.

In addition to the variation of the parameters a geometric variation was investigated. Here, the distance between the gas inlet nozzle and the substrate holder is changed. The resulting investigated distances are 40 mm, 50 mm and 60 mm.

Table 2: Basic conditions II of literature **[1]**

Inlet	Species	Flow inlet temperature [K]	Flow inlet velocity [m/s]	GaCl or NH_3 ratio
V_1	GaCl-N_2	1120	0.09291	0.1650
V_2	N_2 1	1120	0.1548	/
V_3	NH_3-N_2	1120	0.09291	0.3781
V_4	N_2 2	1120	0.05915	/

Table 3: Basic conditions III of literature **[1]**

Inlet	Species	Flow inlet temperature [K]	Flow inlet velocity [m/s]	GaCl or NH_3 ratio
V_1	GaCl-N_2	1120	0.21679	0.09945
V_2	N_2 1	1120	0.1548	/
V_3	NH_3-N_2	1120	0.12388	0.6450
V_4	N_2 2	1120	0.05915	/

Table 4: Volumetric flows in dependence on the respective speeds

Inlet	Area [mm^2]	$\dot{V}$[cm^3/S] to Table 1	$\dot{V}$ [cm^3/s] to Table 2	$\dot{V}$ [cm^3/s] to Table 3
V_1	28.27	1.7510	2.6266	6.1287
V_2	175.93	18.156	2.7234	2.7234
V_3	424.12	26.270	3.9405	52.540
V_4	2001.2	78.907	118.37	118.37

3. Meshing

In the present 2D model, triangular and rectangle mesh elements apply. Taking into account defined domain and boundary conditions of the model, the mesh was adjusted to the nitf-mode. The mesh has been improved and the surface layer mesh along the no-slip boundaries adjusted. The boundary layer mesh consists of rectangle mesh elements. Here also a boundary adjustment factor of 5, boundary layer stretch factor of 1,2 and the number of boundary layers with 2 have been defined. Inside, the model consists of a free triangular mesh. The mesh element sizes of the boundary layer mesh and the free triangular mesh can be adjusted independently. The mesh parameters are the same for all three geometric variations of the reactor model. Due to the axial length variation the mesh element number changes. As example, the mesh of the reactor model with an axial distance of 50 mm between gas inlet nozzles and substrate holder is shown in Figure 3. The mesh consists of 31.369 mesh elements and the results can be compared.

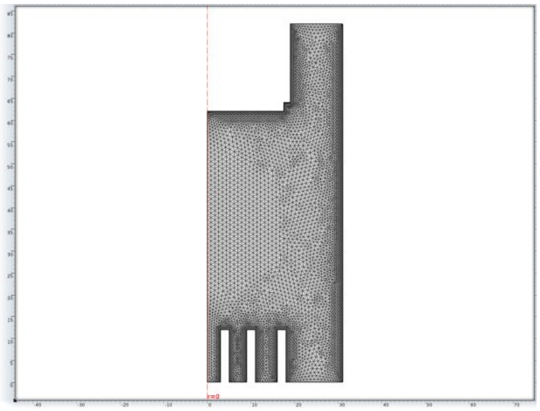

Figure 3. Mesh of the model with a distance of 50 mm from the inlet nozzle to the substrate holder

4. Results

In the further discussion the individual reactor models will be named as the designation reactor plus their nomenclature. Based on Table 5, the schema of the evaluated results will become more apparent.

Table 5: Schema of the evaluated results

Conditions from	Reactor 40	Reactor 50	Reaktor 60
Table 1	X	X	X
Table 2		X	
Table 3		X	

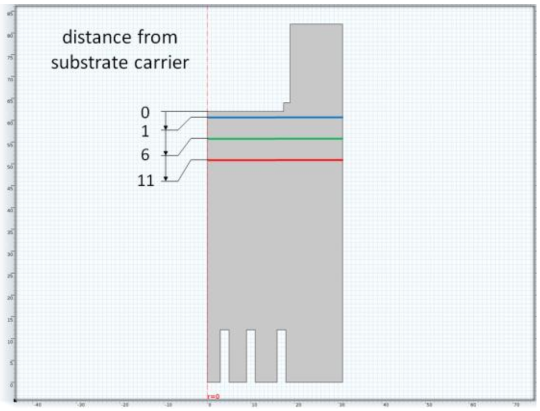

Figure 4. Representation of the measured line positions to reactor 50

For a detailed analyze all field sizes were evaluated along relevant measurement lines. Shown in Figure 4.

The color marked measuring lines are located in a distance of 1 mm, 6 mm and 11 mm in front of the substrate holder. This area is of great importance, because the chemical reactions of the individual species are be expected here.

4.1 Geometry variation

4.1.1 Geometry variation nitf

The velocity field of the reactor is shown in Figure 5.

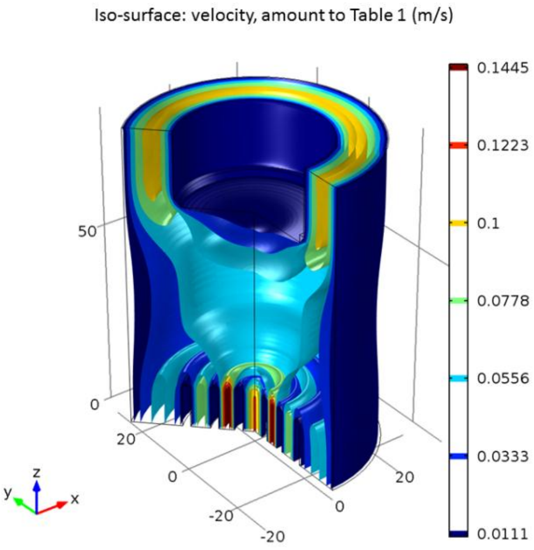

Figure 5. Sectional view of the velocity field of the reactor 50 based on iso-surfaces

The section view shows a representation of the whole reactor 50 by iso surfaces. The flow profile can be seen clearly. In the region of the gas inlet nozzle of intake V_2 the highest flow rates are found. This results from the nozzle cross section and inflow. Due to the increase in cross section in the behind lying area, there is a reduction in the flow velocity. The substrate carrier leads to further cross-sectional change in the reactor. From the reduction of the cross sectional area results a speed increase of the fluid in the area of the gas outlet. The results of the nitf simulation show, that a geometric distance variation of this magnitude has no effect on the speed in the range of 1 mm to 11 mm in front of the substrate holder. Thru reactor 50, the curve at the measurement lines is explained as example to all three reactors. This is shown in Figure 6.

When considering the measurement line 11 mm in front of substrate holder it can be seen that outgoing from the r-coordinate of 0 to the reactor wall, the temperature of 1148 K decreases about 20 K. With increasing rapprochement of the substrate holder, the temperature increases in the range of the r-coordinate 0. On the measuring line 1 mm in front of the substrate support it achieves approximately 1300 K and falls to the reactor wall to around 1150 K. The substrate holder extends on the r-coordinate of 0 to 19.

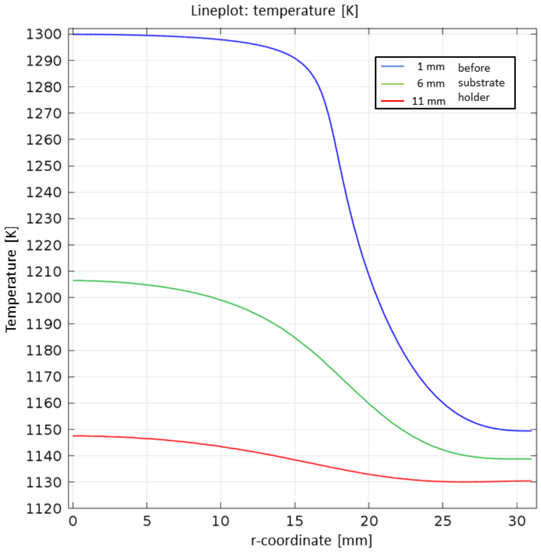

Figure 6. Representation of the temperature curves in the reactor 50, 1 mm, 6 mm and 11 mm in front of the substrate holder

It should be noted that in this region 1 mm in front of the substrate holder no constant temperature profile exists. The difference in temperature in this area is 75 K. The increased speeds in the region of the gas outlet transports the fluid from the colder areas of the reactor faster on the substrate holder, whereby there is no such strong warming. The temperature profile which is established by the flow profile and the boundary conditions of temperature is not influenced in the geometric variation.

4.1.2 Geometry variation chds

In the chds simulation the three species GaCl, N_2, and NH_3 are considered. In Figure 7, the concentration distributions of gallium chloride from the individual reactors are compared as main result. With increasing distance between the gas inlet nozzle and the substrate holder in comparison of same measuring lines, the concentration of gallium chloride decreases. When looking at individual reactors, the concentration of gallium chloride decreases in itself by reducing the distance to the substrate holder. Thus it can be shown, that the variation of the geometry has a considerable influence on the concentration distribution of gallium chloride in the range of the substrate carrier.

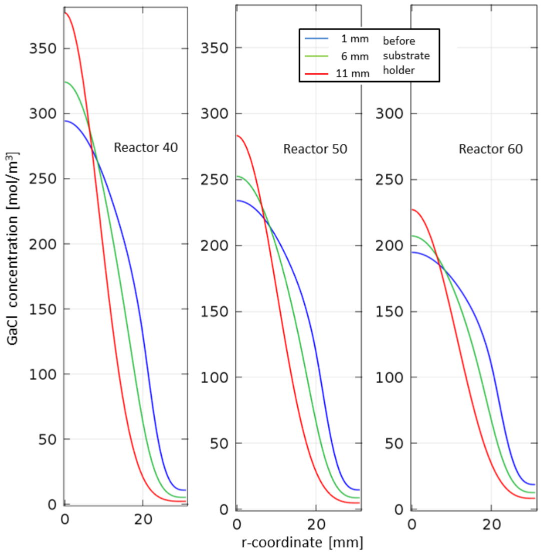

Figure 7. Representation of the concentration distributions of gallium chloride in reactor 40 to reactor 60 by means of defined measuring lines

4.2 Parameter variation

4.2.1 Parameter variation nitf

A comparison of the velocity fields on the defined measurement lines with variable parameters is given in Figure 8.

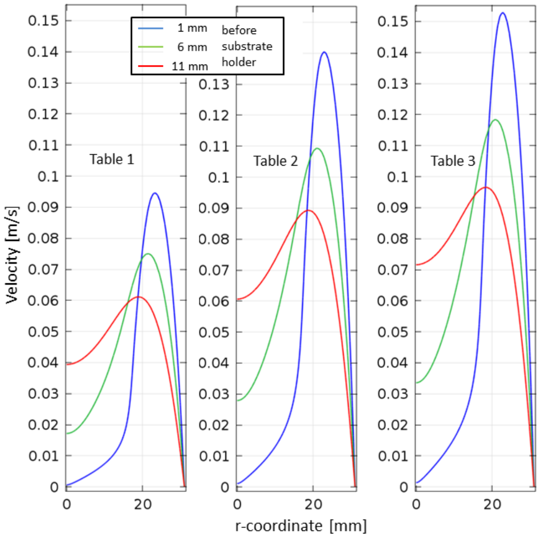

Figure 8. Representation of the velocity fields of the reactor 50 in response to the parameters from Table 1 to Table 3 on defined measuring lines

Due to the defined boundary conditions the inflow velocity at the gas inlet nozzles increases. It can clearly be seen that by variation of the parameters the velocity field can be affected at the measuring lines 11 mm to 1 mm in front of the reactor. Through the control of the velocity field also the temperature field can be influenced. With increasing velocity of the fluid, the temperature falls on the measurement lines in front of the substrate holder. This is due to the shorter time, which is available for heating the fluid.

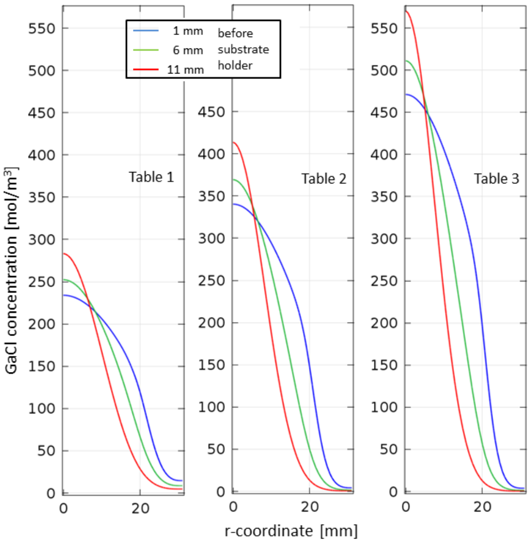

Figure 9. Representation of the concentration distributions of gallium chloride in reactor from the parameters of Table 1 to Table 3 by means of defined measuring lines

Reactor 50 with the parameters given in Table 1 has the lowest gallium chloride concentration. In direct comparison to the reactor 50 with the parameters of Table 1 to Table 2, the concentrations of the gas inlet nozzles is kept constant and the speed increased. This leads to an increase in concentration on the measuring lines on the substrate holder. In reactor 50 according to the parameters from Table 3, the gas inlet velocity is further increased, but the concentration of gallium chloride was reduced. However, further increases in the concentrations of the measured lines are listed. This justifies shorter diffusion processes. Generally it can be noted that, by an increase in speed of gallium chloride at the gas inlet, the concentration is increased in the region of the substrate holder. The velocity at the inlet in this case has a greater influence than the concentration.

5. Conclusions

By evaluating the results of the geometry variation could be shown, that the variation of the geometry has no marginal influence on the velocity and temperature field as consequence. By variation of the geometry, the concentration distribution of gallium chloride, nitrogen and ammonia, can be affected and thus controlled. When considering the parameters of variation of inflow velocities and concentrations of different species, their influence could be detected. By increased inflow velocities at the inlets, there is also a marked increase in fluid velocity throughout the reactor and measuring lines which are used for the evaluation. The increase of speed had also influence on the temperature field. With increasing speed, the temperatures decline in front of the substrate holder. This gives a distinct advantage. By control of the temperature field, thus it is possible to prevent premature separation reactions. The influence of parameter variation on the concentration distribution of each species was demonstrated. Thus it is theoretically possible, in the region of the substrate holder to set an almost constant concentration distribution profile of the individual reactants, and thus to control the deposition of gallium chloride reactions.

6. References

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