Modelling of MOCVD Reactor: New 3D Approach

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Abstract. The paper presents comparison of two different 3D models of vertical, rotating disc MOCVD reactor used for 3D GaN structure growth. The first one is based on the reactor symmetry, while the second, novel one incorporates only single line of showerhead nozzles. It is shown that both of them can be applied interchangeably regarding the phenomena taking place within the processing area. Moreover, the importance of boundary conditions regarding proper modelling of showerhead cooling and the significance of thermal radiation on temperature field within the modelled structure are presented and analysed. The last phenomenon is erroneously neglected in most of the hitherto studies.

1. Introduction
Metal-Organic Chemical Vapour Deposition (MOCVD) is one of the most widely used epitaxial technologies to manufacture electronic devices, especially for optoelectronic applications. Even though, this thin-film deposition technique is used for mass production, it is highly complex process involving reacting flow of organometallic and hydrides precursors accompanied by carrier gasses [1–4]. Its complexity is especially intricate in the case of three-dimensional structure growth, like the 3D GaN column structures destined to solid state lighting. This application is in the scope of authors interest. The pillar design of LEDs allows getting even more than 10 times bigger active area in comparison to the planar solutions [5–7]. Moreover, the vertical alignment of junctions assures lower influence of thermal expansion mismatch between the columns and the substrate, as well as it results in low defect concentration regardless of the material type. These benefits cause that 3D LEDs and their production techniques, with special emphasis on MOCVD, gain more and more attention of various research groups, nowadays [5–13]. The studies are oriented on understanding the selective growth of semiconductor materials [5–8], as well as on experimental and numerical analyses of MOCVD parameters and their influence on the growth processes [9–13].

There are several constructions of MOCVD reactors with both lateral and vertical gas flow [14] but from the point of view of optoelectronic applications more popular are close coupled showerhead reactors [5-7,10]. The outline of such a reactor is presented in figure 1. The reactants are introduced through a showerhead located over a susceptor and flow down towards its surface, where the film deposition process occurs. The susceptor is in a form of the rotating, heated disc, while the showerhead is water cooled, so huge temperature differences can be observed inside the chamber. The forced flow of the carrier gasses and the precursors may be influenced by the buoyancy force and the rotational motion of the susceptor. As the result, the three-dimensional velocity field inside the reactor
is observed, what is crucial from the point of view of modelling. Moreover, the chemical reactions are mostly temperature activated, so the knowledge of the temperature field inside the chamber with special emphasis on the processing area is a must to properly analyse the growth mechanism.

![Outline of MOCVD vertical, rotating disc reactor.](image)

Although, MOCVD reactors have been under numerical investigations for several decades already [1–13], the constructions of particular reactors differ significantly and the differences of elaborated models are significant and dependent on type, shape and dimensions of analysed chambers. Fotiadis et al. [9] studied vertical reactors under wide range of operating parameters such as susceptor and chamber walls temperatures, pressure, inlet flow rate and susceptor rotational speed. The test reactor had 140 mm in diameter susceptor and was characterised by the high distance between the gas inlet and the processing area changing in the range from 40 to 240 mm. The conducted analyses showed that the reactor geometry is of crucial importance to reduce buoyancy induced vortexes and to achieve high uniformity of thin-film layer deposition. Furthermore, Zhong et al. [10] conducted 2D simulations of the similar reactor but with much smaller distance between the susceptor and the showerhead equalled to 10 mm. They concentrated on transient flows and the possibility of temporary oscillations that might increase the growth rates of semiconductor compounds and might result in structure inhomogeneity. On the contrary, Mitrovic et al. [11, 12] focused on high-speed rotating MOCVD reactors characterised by susceptors with diameters of 300 and 450 mm and the distance between the susceptor and the showerhead of 75 and 125 mm, respectively. Their “pressure-rotational rate” diagrams allows predicting the influence of the carrier gases and reactants flow on the growth rate under wide range of varying conditions in big chambers, when the rotational speed remarkably exceeds 100 rpm.

In general, one can conclude the 3D models are necessary to accurately describe the temperature and the velocity fields inside the disc rotating MOCVD reactors. On the other hand, the questions regarding importance of different phenomena are still raising. For example, in the most of papers [8, 10–13], the radiation heat transfer mechanism is neglected, even though some authors in their early studies [9] state clearly that such an attitude is not allowed in MOCVD reactors. Furthermore, the showerheads are usually represented as a uniform velocity boundary condition [1,2,9–13] and the cooling of either showerhead or chamber walls is implemented in the form of constant temperature boundary condition [10–13]. These assumptions can, however, influence the temperature field in the reactor chamber and may affect the precursors decomposition and the modelled growth process [1–4].

The paper presents the new, reduced 3D model of empty MOCVD reactor used further by the authors to investigate the processes of 3D GaN structure growth. The worked out model allows reducing the usage of computational resources, simultaneously assuring high accuracy of the conducted simulations. Its advantages have been proven in the numerical investigations dealing with the influence of different boundary conditions and assumptions on the temperature and velocity distribution within the considered MOCVD chamber. The carried out investigations are comprehensive taking into account previous studies [8–13].
2. Reduced model of MOCVD reactor

The MOCVD reactor under consideration is a close coupled showerhead reactor of Thomas Swan Scientific Equipment Ltd. that cross-section is schematically presented in figure 1. A graphite susceptor with the diameter of 140 mm is located in 175 mm in diameter, cylindrical chamber, that is closed from the upper side by a water-cooled showerhead. The shower itself contains almost 2000 tubes covering in total the area of almost 135 cm². The diameter of each nozzle is 0.6 mm. The distance between the susceptor and the showerhead equals to 11 mm. The outlet is located around the susceptor as it is marked in figure 1.

2.1. Models: assumptions and boundary conditions

Due to the distribution of the tubes at the area of the showerhead, the symmetry has been found and a model covering a quarter of the reactor chamber has been elaborated. The outline of the model, named Q-type, is shown in figure 2a. The complexity of the geometry incorporating matrix of tubes as well as planned introduction of processed samples with 3D GaN structures into the simulations, have forced us to work on much simpler model. The requirement to have a 3D analysis and the design of intricate matrix of showerhead tubes lead us to the second model, named SR-type solution. It is presented in figure 2b, and it covers only a single row of nozzles sliced from Q-type model. In both the cases, the susceptor is marked in red and represents a uniform graphite layer coated with 100 µm silicon carbide.

![Figure 2. The geometry outline for the model covering a) the quarter of the reactor chamber (Q-type) b) the single row of showerhead tubes (SR-type).](image)

In order to examine the models, the numerical analyses have been conducted with the aid of ANSYS CFX software with the dense mesh covering 5 to 8 inflation layers at every solid surface. Moreover, within the processing area, the first layer thickness has been limited to several micrometers to assure fine grid and an accurate modelling of the main area of interest. It was verified that further refining of the discretisation mesh does not influence the velocity and the temperature fields within the modelled structures.

The simulations with both the models have been conducted for the following assumptions and boundary conditions:

- carrier gas is 100% H₂ (the properties of the fluids are described with the aid of ideal gas law);
- reference pressure in the chamber is 25 kPa and the outlet relative pressure equals to 0 Pa;
- uniform temperature of 1000°C at the bottom area of the susceptor is assumed;
- uniform temperature of 50°C at the tube inlets and at the surface of showerhead (water cooling) is applied;
- radiation thermal model with 0.2 emissivity of various walls bounding the gas flow is incorporated (no heat absorption or scattering within fluid domain has been analysed);
- uniform velocities at the inlets of showerhead tubes ranging from 3000 ÷ 12000 sccm are assumed;
• both stationary solution and the rotation of the susceptor are investigated (rotational speed \( \omega \) equals to 100 rpm).

The values of linear velocities at the nozzle inlets are calculate from the volumetric flow rates according to the formulas:

\[
V_Q = \frac{Q_X}{60 \cdot N \cdot A_{TUBE}}
\]

\[
V_{SR} = V_Q \frac{N}{2\pi N^2_{SR}} = \frac{Q_X}{60 \cdot (2\pi N^2_{SR}) A_{TUBE}}
\]

where: \( V_Q \) and \( V_{SR} \) are linear inlet velocities for Q and SR-solution respectively [m/s]; 
\( N \) – number of tubes in the showerhead [-]; 
\( N_{SR} \) – number of tubes in SR-model showerhead [-]; 
\( A_{TUBE} \) – cross-sectional area of the single tube in the showerhead [mm\(^2\)]; 
\( Q_X \) is a nonstandard volumetric flow at temperature \( T_X \) and pressure \( p_X \) calculated according to the formula:

\[
Q_X = Q_{STD} \frac{p_{STD} T_X}{p_X T_{STD}}
\]

where: \( Q_{STD} \) is a standard volumetric flow [secm] at the standard conditions \( p_{STD} \) and \( T_{STD} \) of 103 kPa and 273 K;

2.2. Results and discussion

The most important information that must be obtained from the numerical results is temperature distribution within the processing area and velocity profiles in the modelled chamber. Hence, the results have been analysed along several lines located along the susceptor radius at the susceptor surface and over it. The lines and their descriptions are gathered in table 1, and the exemplary ones are presented graphically in figure 3.

| NAME | LOCATION |
|------|----------|
| ALONG | along the radius of the susceptor on its surface |
| 500 \( \mu \)m | 500 \( \mu \)m over the line ALONG |
| 1 mm | 1 mm over the line ALONG |
| 3 mm | 3 mm over the line ALONG |
| 5 mm | 5 mm over the line ALONG |

Figure 3. Streamlines in Q-model with two marked lines along which the results are gathered in SR-type and Q-type MOCVD models.
Verification of the reduced 3D model (SR-solution) has covered the comparison of temperature and velocity fields obtained with the aid of both models. Exemplary velocity and temperature distributions versus the distance from the susceptor origin along the four lines defined in table 1 are shown in figure 4 and figure 5, respectively. The results have been obtained for the highest analysed volumetric flow rate of 12000 sccm, and the stationary susceptor.

![Velocity distribution along four lines in SR-type and Q-type MOCVD models.](image1)

**Figure 4.** Velocity distribution along four lines in SR-type and Q-type MOCVD models.

![Temperature distribution along two lines in SR-type and Q-type MOCVD models.](image2)

**Figure 5.** Temperature distribution along two lines in SR-type and Q-type MOCVD models.

Conducted simulations shown a good conformity among Q-type and the reduced models. The observed differences in the temperature and velocity fields are located outside the processing area and they should have no influence on the growth conditions. Both models allow analysing heat and mass transfer phenomena inside MOCVD reactor with respect to the different operating conditions (type of carrier gases, flow rates pressure etc.).

Furthermore, the impact of the susceptor rotation has been analysed. The simulations have been repeated for both types of the models with implemented domain rotation for the whole analysed range.
of inlet velocities. The exemplary results along four lines obtained for the highest volumetric flow rate are presented in figure 6, figure 7 and figure 8, respectively. Figure 6 shows lateral ($V_X$ – along the susceptor radius, $V_Y$ – along the susceptor surface perpendicular to its radius) and vertical ($V_Z$ – perpendicular to the susceptor surface) velocity components, while the resultant vector magnitude is illustrated in figure 7. The velocities are given for the coordinate system that refers to the susceptor as a stationary domain. Figure 8 presents temperature distributions. For clarity, the figures do not show the results obtained for the Q-type model.

The susceptor rotation introduces the lateral velocity component perpendicular to the susceptor radius, hence it influences the velocity field in the chamber. It should be emphasised that the $V_X$ and $V_Z$ components distributions obtained for the two analysed cases with and without rotation are comparable. The characteristics almost cover with each other. Furthermore, the 3D flow almost does not affect the temperature field within the tested range. The obtained temperature uniformity in the processing zone is high and the observed differences are located in the area outside the samples’ location (beyond 0.06 m) and they are negligible (below 4°C). Nevertheless, the implementation of rotation is a must to predict properly the growth kinetics inside the reactor. The results gained with the aid of Q-type model with implemented rotation are in good conformity with the characteristics shown in figure 6, figure 7 and figure 8; hence, the two presented models can be applied interchangeably.

![Figure 6. Lateral and vertical velocity components distribution along four lines in SR-type model with and without susceptor rotation.](image)
3. Different boundary conditions

Next, with the aid of the reduced SR-type model, the verification of various boundary conditions representing the showerhead cooling has been conducted. In comparison to the previously used assumptions, the constant temperature at the surface of the showerhead has been replaced among simulations by three versions corresponding to different heat exchange between the chamber and the surrounding:

- adiabatic boundary condition named “Adiabatic” – heat is transported only by the cold gases flowing through the reactor chamber,
- constant temperature boundary condition of 50°C named “With T=const” – it represents ideal cooling of the showerhead,
- convective boundary condition of 1000 W/m²K with reference temperature of 50°C named “With Conv.” – it characterises the real water cooling systems.
Exemplary temperature distributions for adiabatic, convective and constant temperature boundary conditions obtained for the highest examined velocity are shown in figure 9. To improve readability, the number of characteristics is reduced to the results gathered along the susceptor and along the line located 500 µm over the previous one.

Firstly, adiabatic boundary condition results in lower temperature gradients within the modelled chamber. Incorporation of reactor cooling with the aid of only impinging cold gases gives poorer heat transfer rate and it does not describe properly the water-cooled showerhead of the investigated MOCVD reactor. Secondly, both, the constant temperature and the convective boundary conditions allow to receive comparable temperature distribution within the processing area. The difference between the temperature gradients at 1 mm distance from the susceptor surface, obtained for the two cases, does not exceed 1.5°C. Moreover, the average temperature at the showerhead surface for the convective boundary condition is only about 45°C higher in comparison to the constant temperature value of 50°C assigned at this boundary. This difference should not affect the growth process. In consequence, the constant temperature assumptions is proper and allows for adequate modelling of MOCVD reactors with cooled showerheads.

4. Thermal radiation
The last investigated and hereby presented problem is an influence of the radiation transport mechanism on the heat exchange process within the MOCVD reactor. The series of numerical simulations has been conducted mainly for the SR-type model for the all the assumptions and the boundary conditions defined in section 2 except thermal radiation model. Hence, regarding the thermal radiation the three cases have been analysed and they are presented below:

- thermal radiation model is switched off,
- thermal radiation with 0.2 emissivity of various walls bounding the gas flow is incorporated,
- thermal radiation with 0.2 emissivity of walls of MOCVD chamber and 0.8 emissivity of graphite susceptor coated with SiC layer is implemented.

Exemplary results obtained for the highest and the lowest analysed velocity for the model without and with thermal radiation are shown in figure 10. Furthermore, figure 11 presents the solution incorporating thermal model with different emissivity of the susceptor surface. Lower value of 0.2 corresponds to the surface emissivity of all the remaining walls bounding the chamber that can be made of either quartz or stainless steel. Higher emissivity of 0.8 characterises the properties of the
graphite susceptor with SiC coating. Similarly, as previously, temperature distributions are presented along the radius line of the susceptor and along the line located 500 µm over the previous one.

Figure 10. Temperature distribution along two lines in SR-type model: constant temperature boundary conditions with thermal radiation model switched on (0.2 emissivity) and off for two inlet velocities.

Figure 11. Temperature distribution along two lines in SR-type model: constant temperature boundary conditions with thermal radiation model and different emissivity values of the susceptor.

The curves presented in figure 10 show that both, inlet velocity and thermal radiation influence the obtained temperature distribution within the processing area, even though the impact on the temperature field of the first parameter is insignificant within the tested flow rates. Incorporation of radiation heat transfer mechanism induces higher heat exchange rates, that are further increased by higher emissivity values of the susceptor surface. For the constant temperature boundary condition at the bottom surface of the susceptor equalled to 1000°C, the temperature at the susceptor, where the growth process takes place, is more than 8°C lower for 0.2 emissivity and about 21°C lower for
0.8 emissivity in comparison to the model without radiation heat transport. Even for the lower emissivity of the gas flow limiting areas and lack of absorption and scattering mechanisms within the fluid domain the radiation cannot be neglected.

5. Conclusions
The paper presents the new, 3D reduced model of the close coupled showerhead MOCVD reactor. The comparison of the results obtained with the aid of the new solution and the 3D model based on the symmetry of the chamber are in good conformity with each other. It has been proven that the novel approach incorporating only single line of nozzles allowed analysing phenomena taking place within the modelled chamber. Moreover, the importance of boundary conditions regarding proper modelling of the showerhead cooling are emphasised. Either constant temperature boundary condition or convective boundary condition must be used. Thermal radiation is a very important heat transport mechanism within MOCVD chamber where the huge temperature gradients between the showerhead and the susceptor are present.

6. References
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