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Influence of hydrogen volumetric flow rate on temperature distribution in CVD reactor based on epi-growth of SiC

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Abstract

In the present paper the quantitative relationship between the heat and mass transfer in the Aixtron VP508 hot wall CVD reactor and the epitaxial growth of silicon carbide is determined. The aim of this study was to estimate optimal process conditions for obtaining monocrystalline silicon carbide epi-layers with the most homogenous thickness. Since there are many parameters influencing reactions on the crystal area, such as temperature, pressure, gas flow and reactor geometry, it is difficult to design an optimal process. Detailed 3D modeling was used to gain insight into the process conditions, as it is problematic to experimentally determine the exact distribution of heat and mass transfer inside the reactor during epitaxial growth. Numerical simulations allow one to understand the process by calculating the heat and mass transfer distribution during the epitaxial growth of silicon carbide. The present approach was applied to enhance the performance of the Aixtron VP508 reactor.

Keywords: Finite Volume Method, epitaxial growth, chemical vapor deposition, silicon carbide

1. Introduction

Silicon carbide is a wide bandgap material with potential for high-power and high-temperature electronics. The fundamental parameters of SiC are very attractive for applications such as high power transistors HEMTs (High Electron Mobility Transistors), bipolar transistors IGBTs (Insulated Gate Bipolar Transistors), field effect transistors MOSFETs (Metal-Oxide Semiconductor Field-Effect Transistors), MESFETs (Metal Semiconductor Field Effect Transistors), JFETs (Junction Gate Field Effect Transistors), high power blue diodes, LEDs and laser diodes [1].

Epitaxial growth is a method widely used for manufacturing such semiconductor structures, because epitaxial layers can be created as single crystal layers, which means that crystals of the highest quality can be produced [2]. Low epi-defect concentration is required for the fabrication of silicon carbide transistors [3]. Chemical vapor deposition (CVD) is an accepted epitaxial growth method of 6H- and 4H-SiC layers, which can be used as p-n structures [4]. Since there are many parameters influencing reactions on the substrate, such as temperature, pressure and volumetric flow rate of inlet gases, it is difficult to design an optimal process.

High quality crystals can be produced if there are appropriate operating conditions in the reactor during the process [5]. It is difficult to experimentally determine the heat and mass transfer distribution in the reactor due to the high temperature of the process and flow disturbance introduced by the measuring probe. Numerical simulations allow one to better understand the process by determining the distribution of temperature and flow velocity during the epitaxial growth of silicon carbide.

Commercial reactors are widely used in production lines and R&D laboratories throughout the world and have become a common tool for designing new materials and

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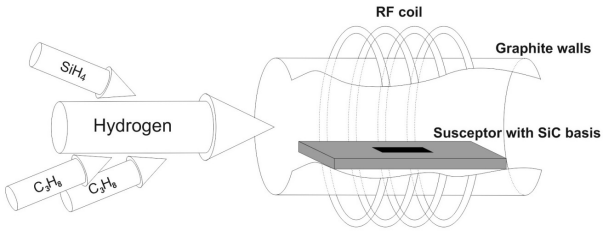

Figure 1: Schematic diagram of silicon carbide epitaxial growth in CVD process

Figure 2: Chamber of Aixtron VP508GFR CVD reactor

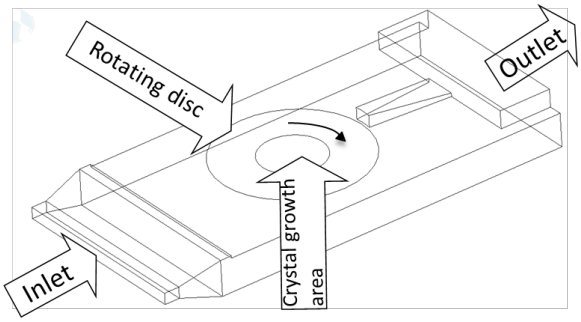

Figure 3: Schematic model of the CVD reactor

devices. As a result, the development of the predictive models of commercial systems has recently become an interesting subject of research. Lofgren et al. modeled heat and mass transfer in the Linkoping CVD reactor [6, 7]. Pawlowski et al. [8] performed modeling analysis of MOVPE GaN in the Thomas Swan close-coupled shower head 3×2 inch reactor. Optimization of the growth rate uniformity for nitrogen and hydrogen carrier gases was performed in [9] for the growth of AlGaAs in the AIX 200 horizontal single wafer reactor. Two different gas inlet configurations were considered in [10] to analyze the homogeneity of AlAs/GaAs structures in the AIX 200 reactor. The SR6000 numerical model was developed and studied in the Horizontal MOVPE reactor in [11] together with planetary and vertical reactors. The modeling results of MOVPE GaN in the AIX 200/4 HT reactor with a separate supply of group-III and group-V precursors were reported in [12] for two configurations of the separation plate, and the computations matched well the character of the growth rate distribution along the flow direction.

In this work modeling and an experimental study of silicon carbide epitaxial layers grown in the Aixtron VP508 Chemical Vapor Deposition reactor were carried out. The effect of the volumetric flow rate of inlet gases (precursors and carrier gas) on the distribution of temperature and gas flow, which strongly influence the crystal thickness, was studied and a comparison of numerical and experimental results was made.

2. Experimental procedure

This study is focused on the influence of hydrogen volumetric flow rate on the process of SiC epitaxial growth. Silicon carbide epitaxial layers were grown on silicon carbide substrates in the Aixtron VP508 chemical vapor deposition reactor (CVD). A schematic diagram of the epitaxial growth process is shown on Fig. 1.

In the experiment, 4H-SiC substrates were used for epitaxial processes. For the homoepitaxial growth of 4H-SiC layers C_3H_8, SiH_4 precursors for carbon and silicon sources, diluted in H_2, were used. At the first growth stage we performed in situ etching of the surface of the silicon substrate by hydrogen to obtain the appropriate surface roughness of the substrates without any scratches [13]. Inlet gases used for the deposition of the silicon carbide layer were silane (SiH_4, = 20 ml/min), propane (C_3H_8, = 12 ml/min) used as precursors and hydrogen (H_2 = (10, 65, 80, 90) l/min) as a carrier gas. The reactor pressure was constant at 75 mbar, whereas the temperature was 1620°C. Experimental data regarding the influence of the hydrogen volumetric flow rate on the thickness distribution was used to verify the modeling results.

3. Numerical model

A numerical model of the hot wall SiC CVD reactor was created in order to simulate the conditions inside the reactor during the growth process of silicon carbide layers. The purpose of this work was to study the influence of input gas parameters on the homogeneity of the silicon carbide epilayers.

The Aixtron VP508 Chemical Vapor Deposition reactor (Fig. 2) studied in this work was used for the deposition of

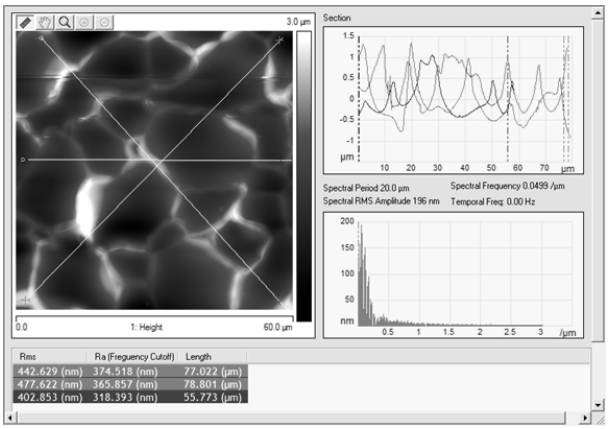

Figure 4: Profile of the graphite plate surface obtained from AFM characterization

Table 1: Input parameters

Parameter	Value
Inlet temperature, K	300
Heating temperature, K	1893
Operating pressure, mbar	200
Rotational speed of the disc, rad/s	18
SiH_4, l/min	0.02
C_3H_8, l/min	0.012
H_2, l/min	10, 65, 80, 90

monocrystalline silicon carbide epitaxial layers. A numerical model of the CVD reactor was developed. The geometry of the reactor is presented in Fig. 3. The reactor walls and the disc on which silicon carbide base is placed are made of graphite covered by TaC, a material chosen for its inductive properties. The graphite chamber is wrapped in induction graphite isolation and is inductively heated during epitaxial growth. Experimental measurements show that the graphite disc remains at a constant temperature during the process. Additionally, the disc is rotating during the process, resulting in a more homogeneous growth rate on the silicon carbide substrate. The rotation also affects the mass fraction distribution of the precursors over the crystal growth area. Inlet gases are introduced to the reactor as a homogeneous mixture. Gases are heated by reactor walls, so the main heat transfer mechanism is convection.

A mesh of 4,500,000 elements was created for the geometry of the reactor chamber. The mesh is refined over the crystal growth area, since it is the area of the greatest importance and the mesh should be at its most accurate above it.

The graphite walls of the reactor chamber are constantly heated during the whole epitaxial process. Experimental measurements showed that the surface of the graphite disc remains at a constant temperature during epitaxial growth. Inductive heating was not included in the model and the temperature on the reactor walls was assumed constant instead.

The influence of the roughness of the material walls on the fluid flow was considered. The roughness of graphite was investigated using Atomic Force Microscopy (Fig. 4). However, the literature indicates that, in the case of laminar flow, wall roughness has no influence on the fluid, so it can be neglected [14].

The gas mixture introduced to the reactor in silicon carbide epitaxial growth process is composed of hydrogen (H_2), silane (SiH_4) and propane (C_3H_8). To define the physical properties of the gases for the studied case, all gases were assumed to act as an ideal gas, so their density could be determined according to the Clapeyron equation:

$$\rho = \frac{pM}{RT} \tag{1}$$

The flow in the reactor is considered as compressible, so the pressure in the Clapeyron equation is calculated as a sum of the local relative pressure predicted by Fluent and the operating pressure.

The boundary conditions of the performed simulations are listed in Table 1.

The temperature on the walls, working pressure and both silane and propane volumetric flow rates stay constant in all instances, whereas the hydrogen volumetric flow rate takes four different values: 10, 65, 80 and 90 l/min. Each simulation was performed for a plate rotating 18 rad/s and a stationary plate.

ANSYS Fluent software used for calculations solves a set of differential equations describing the mass and heat transfer. The software is based on the Finite Volume Method, which allows you to determine the physical properties of the model, numerical algorithms and discretization schemes. As a result temperature, velocity, density and pressure distributions inside the reactor chamber are calculated.

To properly designate the density profile of inlet gases species model of ANSYS Fluent was used. For a given problem the diffusion energy source option was used, which takes into account the effect of enthalpy transport due to species diffusion in the energy transport equation.

ANSYS Fluent solver solves a set of governing equations. This includes both the mass and momentum equation and

the energy equation.
The energy equation solved by Fluent software takes the following form:

$$\partial/\partial t\,(\rho E) + \nabla \cdot \left(\vec{v}\,(\rho E + p)\right) = \nabla \cdot \left(k_{eff}\nabla T - \sum_j h_{j\vec{J_j}} + \left(\bar{\bar{\tau}}_{eff}\cdot\vec{v}\right)\right) \quad (2)$$

In the abovementioned formula three terms represent energy transfer, namely conduction, species diffusion and viscous dissipation.
The diffusion energy source in pressure-based solver solves the species diffusion term:

$$\nabla \cdot \left(\sum_j h_{j\vec{J_j}}\right) \quad (3)$$

The energy equation in the solid region (in this case the rotating plate region) is described by the formula:

$$\frac{\delta}{\delta t}(\rho h) + \nabla \cdot (\vec{v}\rho h) = \nabla(k\nabla T) + S_h \quad (4)$$

The term $\nabla\cdot(\vec{v}\rho h)$ describes the convective heat transfer due to the rotational motion of the solid.

4. Results and discussion

Heat and mass transfer distribution inside the CVD reactor during the epitaxial growth process were studied. Accurate prediction of the temperature distribution influences the overall efficiency of the crystal growth process, because the growth rate is determined by the decomposition of the precursors and then appropriate chemical reaction on the substrate surface. This depends on the intensity of parasitic deposition on the reactor walls [15]. Parasitic deposition is governed by the temperature distribution on the reactor walls heated by induction graphite.
To study the influence of the hydrogen volumetric flow rate on the silicon carbide layer thickness homogeneity a series of simulations with working volumetric flow rates of 10, 65, 80 and 90 l/min was performed. The calculated temperature distribution over the SiC growth area in CVD processes is shown in Fig. 5.
It was found that temperature is homogeneous over the epitaxial growth area only in the case of the H_2 volumetric flow rate of 10 l/min. The temperature values increase when the hydrogen volumetric flow rate decreases (Fig. 6).
Flow parameters change according to the hydrogen volumetric flow rate. The higher the hydrogen volumetric flow rate, the faster the gas flows inside the reactor (Fig. 7). The velocity profile in the reactor depends on the temperature of the walls, volumetric flow rate on the inlet and

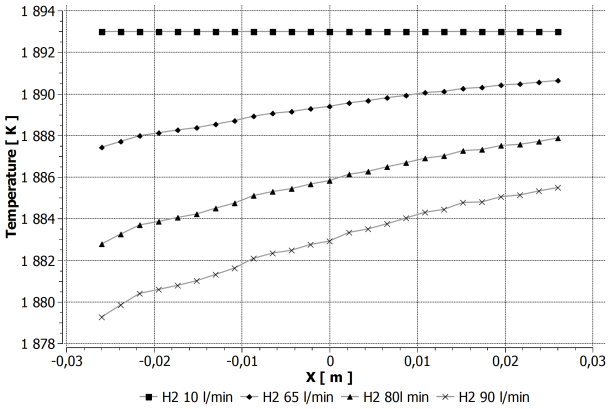

Figure 6: Temperature gradient over the SiC plate for different volumetric flow rates of hydrogen

Table 2: Homogeneity of silicon carbide layer thickness

Hydrogen volumetric flow rate, l/min	Mean crystal thickness, μm	Standard deviation	Coefficient of variation
90	2.26	0.269	0.119
80	1.91	0.196	0.103
65	1.90	0.103	0.08

rotation of the plate. Reactor geometry has a symmetric plane but because of the rotation of the plate, the velocity profile inside the reactor does not have such a plane. This asymmetric flow changes the proportion of hydrogen and gases that participate in chemical reactions over the plate.
The present experiment shows that the chemical reactions area moves depending on the hydrogen volumetric flow rate. The silicon carbide layer was not obtained in the experiment performed for the H_2 volumetric flow rate of 10 l/min because the chemical reaction area moved out of the epitaxial growth zone of the reactor, which in fact is the substrate. Homogeneity of the obtained SiC layer was investigated. Mean layer thickness, standard deviation and the coefficient of variation were calculated (Table 2).
Similar values of mean layer thickness were obtained for processes with the volumetric flow rates of 65 and 80 l/min. To distinguish the difference between the obtained crystals, both the standard deviation and coefficient of variation were calculated. Standard deviation is a measure of the amount of variation from the average; lower values indicate that the data points are closer to the mean value. Coefficient of variation is the ratio of standard deviation to the mean value, and shows the extent of variability in relation to the mean value. Results show that the most

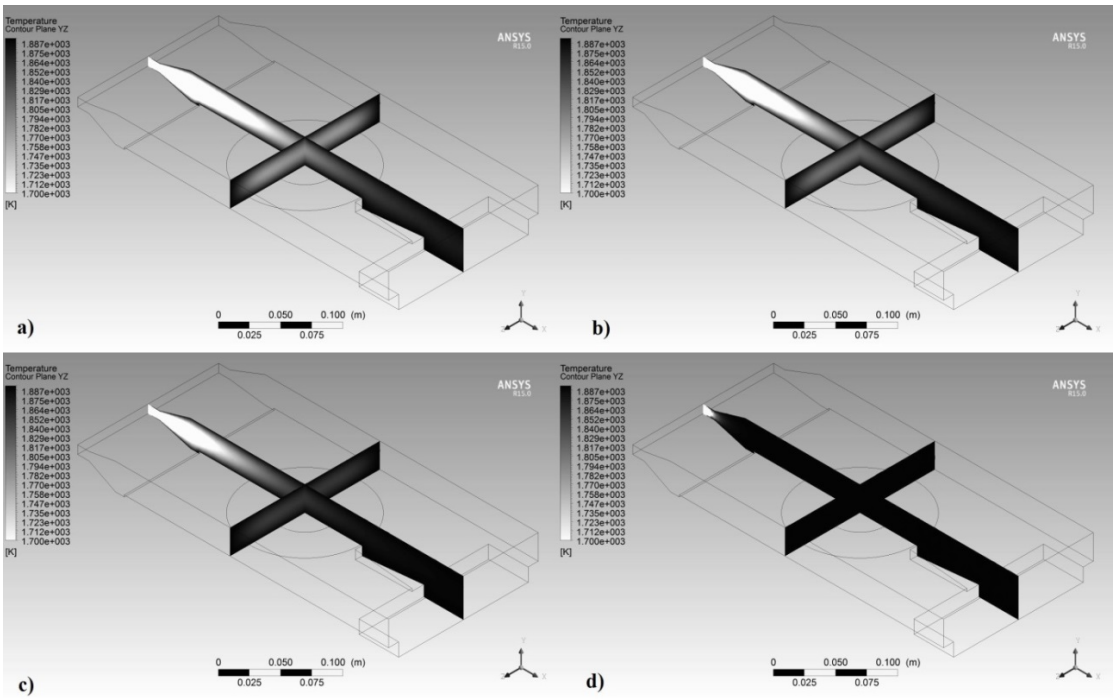

Figure 5: Temperature distribution inside the SiC CVD reactor for different volumetric flow rates: a) 90 l/min; b) 80 l/min; c) 65 l/min; d) 10 l/min

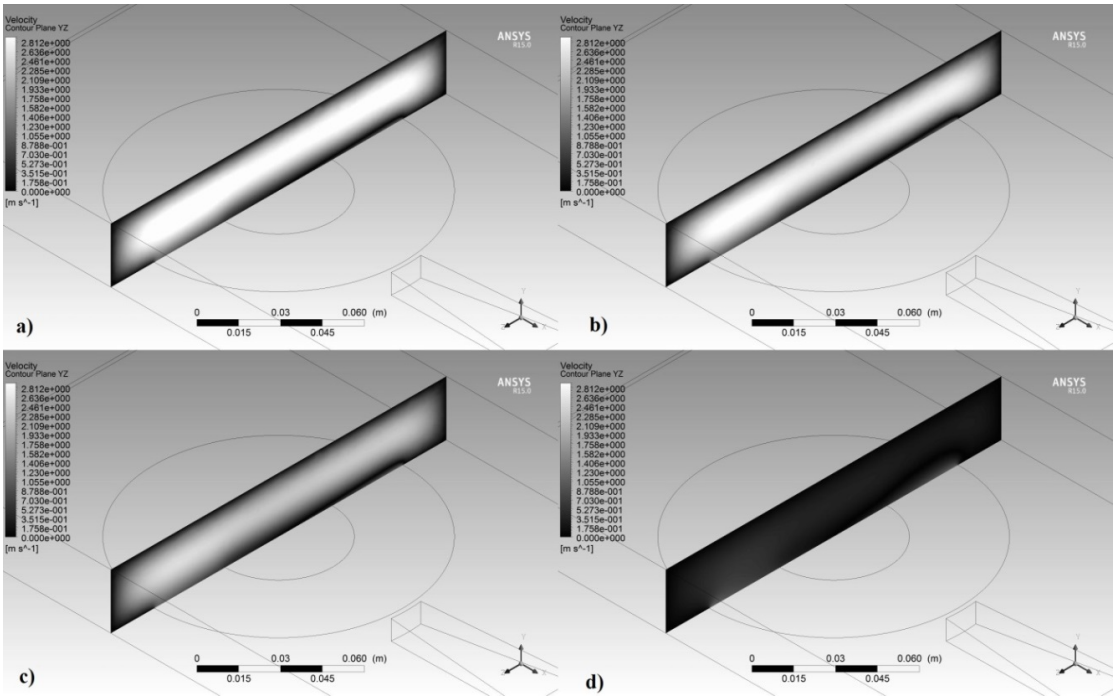

Figure 7: Velocity profile with change of hydrogen volumetric flow rate: a) 80 l/min; b) 90 l/min; c) 65 l/min; d) 10 l/min

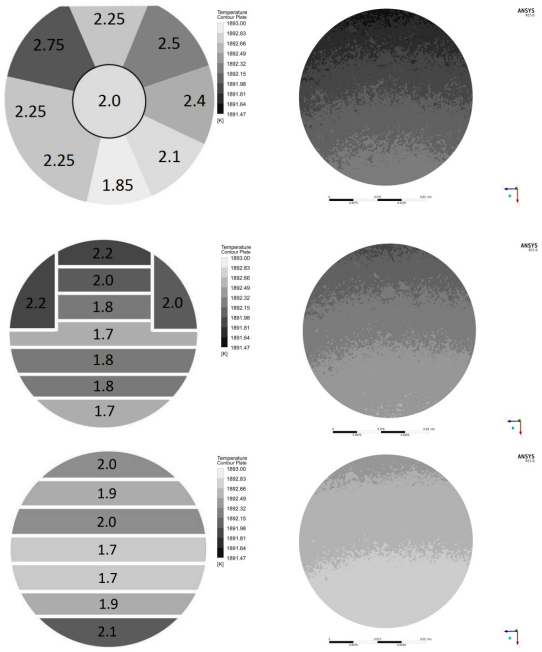

Figure 8: Comparison of SiC layer thickness homogeneity obtained experimentally with calculated temperature distributions for hydrogen volumetric flow rates of: a) 90 l/min ; b) 80 l/min ; c) 65 l/min.

homogeneous layers are obtained for the highest temperature values over the epitaxial growth area obtained for the H_2 volumetric flow rate of 65 l/min.

Modeling outcomes showed that changing the hydrogen volumetric flow rate results in a temperature distribution shift inside the reactor. Since one of the factors influencing the surface deposition rate is temperature, changes in temperature gradient result in movement of the chemical reaction area. The simulation results indicate that for the hydrogen volumetric flow rates of 80 and 90 l/min the temperature values are shifted about 2.5 cm, and the shift for the hydrogen volumetric flow rates of 65 and 80 l/min is about 4.5 cm.

5. Conclusions

A model of the Aixtron VP508 Chemical Vapor Deposition reactor was developed for simulations of heat and mass transfer. Results show that the value of temperature over the silicon carbide growth area depends on the hydrogen volumetric flow rate. The temperature over the epitaxial growth area is homogeneous only for the hydrogen volumetric flow rate of 10 l/min, but for such a low volumetric flow rate the chemical reaction area moves out of the epitaxial growth zone of the reactor. The dependence of the temperature gradient over the SiC plate and the silicon carbide layer thickness homogenity were investigated using experimental data together with numerical simulations. By determining a valid range of temperature over the epitaxial growth area during the epitaxial process, the authors were able to optimize the process parameters to obtain the most homegenous thickness, which is crucial for growing devices based on silcon carbide.

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