Modeling of heat and mass transfer in an SiC CVD reactor as a tool to design modern materials for high power electronics applications

T. Wejrzanowski[1], J. Skibinski[1], A. K. Lewandowska[2] & K. J. Kurzydlowski[1]
[1]*Faculty of Materials Science Engineering, Warsaw University of Technology, Poland*
[2]*Faculty of Power and Aeronautical Engineering, Warsaw University of Technology, Poland*

Abstract

Silicon carbide (SiC) is a wide bandgap material with the potential for high-power and high-temperature electronics. Nowadays, the most efficient manufacturing process is Chemical Vapor Deposition (CVD) at a temperature of about 1900K. The performance of SiC devices is limited by the material quality of SiC substrates and their epitaxial structures, which depend highly on the processing conditions.

In the present study, the quantitative relationship between heat and mass transfer in the hot wall CVD reactor and the epitaxial growth of SiC is addressed. Epitaxial growth means crystal growth that progresses while inheriting the laminar structure and the orientation of substrate crystals. From a technological point of view, it is important to cover the wafer with a thin film of homogeneous thickness. Since there are many parameters that influence a reaction on the crystal area, such as temperature, pressure, gas flow, reactor geometry, it is difficult to design the optimal process.

According to the fact that it is impossible to experimentally determine the exact distribution of heat and mass transfer inside the reactor during the crystal growth, modeling is the only solution to understanding the process precisely. Numerical simulations allow us to understand the process by calculation of heat and mass transfer distribution during the epitaxial growth of SiC. The reactor walls are induction heated during the growth process. Gases are introduced to the reactor at

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room temperature and are heated during the flow inside the reactor chamber. The main heating mechanism inside the reactor is convection. Additionally, the plate on which SiC is grown is rotating during the process, which affects the mass distribution.
Keywords: Finite Volume Method, epitaxial growth, chemical vapor deposition, silicon carbide.

1 Introduction

The fundamental parameters of silicon carbide (SiC) material are very attractive for applications such as high power transistors HEMTs (High Electron Mobility Transistors), bipolar transistors IGBTs (Insulated Gate Bipolar Transistor), field effect transistors MOSFETs (Metal-Oxide Semiconductor Field-Effect Transistor), MESFETs (Metal Semiconductor Field Effect Transistor), JFETs (Junction gate Field Effect Transitor), high power blue diodes, LEDs and laser diodes [1].

Epitaxial growth is a widely used method for manufacturing such semiconductors, because epitaxial layers can be created as a single crystal, without grain boundaries and other defects, so it produces crystals of highest quality [2]. Chemical vapor deposition (CVD) is an accepted epitaxial method to grow 6H- and 4H-SiC layers and p-n structures [3]. Since there are many parameters influencing reactions on crystal growth area such as temperature, pressure, mass flow rate of inlet gases, it is difficult to design optimal process.

High quality of the crystal can be obtained with the appropriate operating conditions of the reactor during the process [4]. It is impossible to determine heat and mass transfer distribution in the reactor experimentally due to high temperature of the process and flow disturbance that measuring probe would introduce. Numerical simulations allow to understand the process by determining distribution of temperature and flow velocity during the epitaxial growth of silicon carbide.

This study concerns influence of heating temperature and mass flow rate of inlet gases on the process of crystal growth in CVD reactor. In order to investigate this subject a series of computer simulations and experimental processes have been performed. Numerical simulations were performed using ANSYS Fluent software.

2 Case study

The numerical model of hot wall SiC CVD reactor was created. The model allows to simulate the conditions inside the reactor during the process of silicon carbide crystal growth. The purpose of this work was to study the influence of process input parameters on crystal growth of silicon carbide.

2.1 CVD reactor

The CVD reactor Gemini 1 (Figure 1) studied in this work is used for manufacturing of monocrystalline silicon carbide. Numerical model of CVD reactor was developed. Geometry of the reactor is presented on Figure 2. The reactor walls and

the disc on which silicon carbide base is placed are made of graphite, material chosen due to its inductive properties. The graphite chamber is wrapped with an induction coil and is induction heated during epitaxial growth. Experimental measurements show that the graphite disc has constant temperature during the process. Additionally, the disc is rotating during the process, which allows to obtain more homogeneous growth rate on the silicon carbide plate. The rotation also influences mass fraction distribution of the reagents over the chemical reactions area. Inlet gases are introduced to the reactor as a homogeneous mixture in room temperature. Gases are heated by reactor walls, so the main heat transfer mechanism is convection.

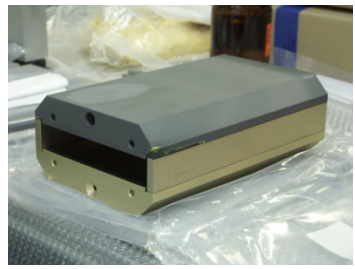

Figure 1: SiC CVD epitaxial growth reactor.

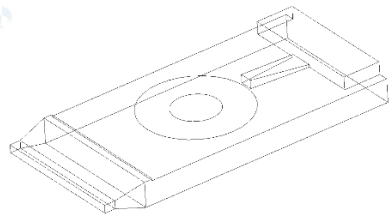

Figure 2: Geometry of the reactor.

The finite element mesh of 4.500.000 triangular elements has been created for the geometry of the reactor. The mesh is refined over the chemical reaction area, since it's the area of biggest importance, and mesh should be the most accurate above it.

2.3 Assumptions

The graphite walls of reactor chamber are constantly heated during the whole process. Experimental measurements exhibited that graphite disc has constant temperature during epitaxial growth. According to the above facts, the induction heating was not included in the model, instead temperature on reactor walls was assumed constant.

The influence of material walls roughness on the fluid flow was considered. Roughness of graphite was investigated using Atomic Force Microscope

(Figure 3). However, literature indicates that in case of laminar flow wall roughness has no influence on the fluid, so it can be neglected [6].

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 properly define the physical properties of the gases for studied case, all gases were assumed act as an ideal gas, so their density could be determined according to Clapeyron equation:

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

2.5 Boundary conditions

Boundary conditions of performed simulations are listed in Table 1.

Table 1: Input parameters.

Parameter	Value
Inlet temperature [K]	300
Heating temperature [K]	1893
Operating pressure [mbar]	200
SiH_4 [l/min]	0.02
C_3H_8 [l/min]	0.012
H_2 [l/min]	10,65,80,90

Temperature on walls, working pressure and both silane and propane mass flow rates stay constant for each case, whereas hydrogen mass flow rate takes four different values: 10, 65, 80 and 90 l/min. Each simulation was performed for plate rotating 18 rad/s and stationary plate.

2.4 Numerical simulations

ANSYS Fluent software used for calculations solves a set of differential equations describing mass and heat transfer. Solver uses the Finite Volume Method which allows to choose 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 density profile of inlet gases species model of ANSYS Fluent was used. For given problem the diffusion energy source option was used, which allowed to include the effect of enthalpy transport due to species diffusion in energy transport equation.

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

Energy equation solved by Fluent software has following form:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\underset{v}{\rightarrow}(\rho E + p)) = \nabla \cdot (k_{eff}\nabla T - \sum_j h_j \underset{J_j}{\rightarrow} + \left(\bar{\bar{\tau}}_{eff} \cdot \underset{v}{\rightarrow}\right) \tag{2}$$

In the above formula three terms represent energy transfer: conduction, species diffusion and viscous dissipation.

The diffusion energy source in pressure-based solver solves the species diffusion term:

$$\nabla \cdot (\sum_j h_j \underset{J_j}{\rightarrow}) \tag{3}$$

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

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot \left(\underset{v}{\rightarrow} \rho h\right) = \nabla(k \nabla T) + S_h \tag{4}$$

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

3 Results

It was observed experimentally, that the crystal growth area is moving with variation of hydrogen mass flow rate. For H2 flow rate of 10 l/min, crystal growth area is beyond the wafer, and no layer was obtained in the experiment.

It was found that whatever the mass flow rate is, temperature is not homogeneous over the plate. The values of temperature increase with the decrease of hydrogen mass flow rate (Fig. 3). The temperature of gases on the inlet of the reactor the reactor is 300 K whereas walls are heated to 1893 K.

Flow parameters change according to hydrogen mass flow rate. The higher the hydrogen mass flow rate is, the faster the gas flows inside the reactor (Fig. 4). Velocity profile in reactor depends on temperature of the walls, mass flow rate on the inlet and rotation of the plate. Reactor geometry has a symmetric plane but because of the rotation of the plate, velocity profile inside the reactor does not have such plane. This asymmetric flow changes the proportion of hydrogen and gases that participate in chemical reactions over plate.

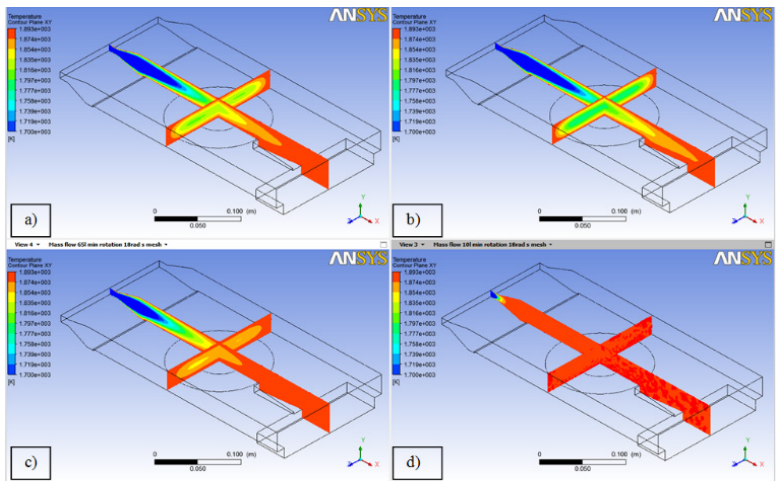

Figure 3: Temperature distribution inside the SiC CVD reactor for different mass flow rates: a) 80 l/min; b) 90 l/min; c) 65 l/min; d) 10 l/min.

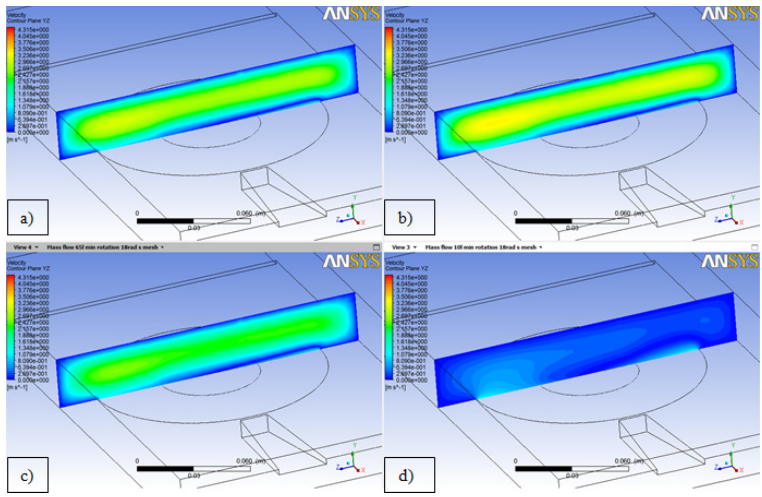

Figure 4: Velocity profile with change of hydrogen mass flow rate: a) 80 l/min; b) 90 l/min; c) 65 l/min; d) 10 l/min.

However the rotation of the plate does not influence temperature distribution over the silicon carbide plate.

Summary results of temperature gradient over the chemical reaction area are shown on the chart in Figure 5. For the same heating temperatures, but different hydrogen mass flow rates, temperature distribution shifts inside the reactor. Surface deposition rate depends on temperature, hence changes in temperature

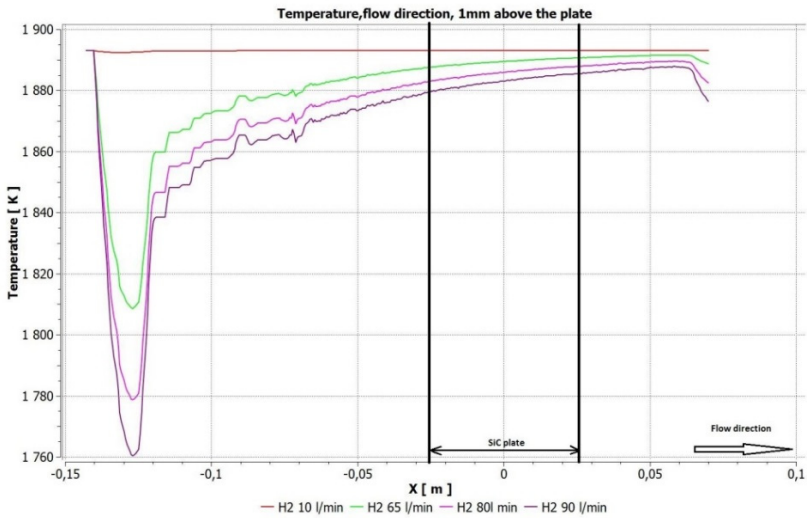

Figure 5: Temperature gradient over the SiC plate for different mass flow rates of hydrogen.

gradient result in chemical reactions area movement. For example, temperature gradient movement indicates, that for hydrogen mass flow rates of 80 and 90 l/min chemical reactions area should move about 4cm.

4 Conclusions

The model of Chemical Vapor Deposition reactor for simulations of heat and mass transfer has been developed. Results showed, that regardless the temperature of the heating element, temperature and density of reagents over the crystal growth area are not homogeneous. The value of temperature over the silicon carbide crystal depends on hydrogen mass flow rate. Experimental data together with numerical simulations will allow to determine the dependence of temperature gradient over the SiC plate and the chemical reaction area movement. Determination of valid temperature range of gases over the crystal growth area for the process of epitaxial growth allows to optimize the process parameters and to obtain the crystal of best quality.

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References

[1] Park, Yoon Soo. “SiC materials and devices”, Semiconductors and Semimetals, Vol. 52, San Diego: Academic press.
[2] S.K. Lilov, Yu.M. Tairov, V.F. Tsvetkov, “Study of silicon carbide epitaxial growth kinetics in the SiC-C system”, Journal of Crystal Growth, Volume 46, Issue 2, February (1979), pp. 269-273.
[3] Wang, Y.A. Davis R.F. “Growth rate and surface microstructure in 6H-SiC thin films grown by chemical vapour deposition”, J. Electron. Mater. 20:869.
[4] Xianfeng, Zhiming Chen, Jianping Ma, Xiang Zan, Hongbin Pu, Gang Lu, “Epitaxial growth of cubic silicon carbide on silicon by sublimation method”, Optical Materials, Volume 23, (2003), pp. 39-42.
[5] Li Zhe Yang, Li Yun, Chen, Han Pin, “Influence of silicon cluster on epitaxial growth of silicon carbide”, Science China Physics, Mechanics and Astronomy, Online.
[6] Guobing Zhou, Shi-Chune Yao, “Effect of surface roughness on laminar liquid flow in micro-channels”, Applied Thermal Engineering, Volume 31, Issues 2-3 (2011) 228-234.
[7] Baliga, B.J. “High voltage silicon carbide devices”, Mat. Res. Soc. Symp. Proc. 512: 77-88, 1998.