Verification of Thermo-Fluidic CVD Reactor Model

Z Lisik, M Turczynski, L Ruta[1] and E Raj
Lodz University of Technology, Department of Semiconductor and Optoelectronic Devices, Wolczanska 211/215, 90-924 Lodz, Poland

[1]E-mail: lukasz.ruta@p.lodz.pl

Abstract. Presented paper describes the numerical model of CVD (Chemical Vapour Deposition) reactor created in ANSYS CFX, whose main purpose is the evaluation of numerical approaches used to modelling of heat and mass transfer inside the reactor chamber. Verification of the worked out CVD model has been conducted with measurements under various thermal, pressure and gas flow rate conditions. Good agreement between experimental and numerical results confirms correctness of the elaborated model.

1. Introduction

Nowadays, the rapid development is observed in the area of semiconductor device manufacturing. Among the main technological steps, the processes oriented on thin-films deposition or growth of epitaxial layers are of crucial and still growing importance for microelectronics. Chemical vapour deposition (CVD) is one of them. Traditional CVD methods require high temperatures of 900-1000°C (or even higher) demanded for the activation of chemical reactions leading to the decomposition of gaseous reactants called precursors. As the result, the particles (atoms) necessary for deposited layer are released and the new layer grows on the surface of the heated substrate. The CVD technology is applied in many areas of industry when the epitaxial grow or thin layer coating surface are required, e.g. in production of protective coating on glass and metal, active and dielectric layers for semiconductor devices or multilayer structures for LEDs and lasers applications [1].

High temperatures required to thermal decomposition of precursors is, however, a serious limitation of traditional CVD in some processes e.g. limiting the number of materials that can be used as substrates. To reduce the process temperature to 400-500°C and omit this disadvantage, additional methods that allow enhancing the chemical reaction rates in lower temperatures are necessary. It can be achieved using the electrical activation of gaseous environment with the aid of plasma, like in the Plasma Enhanced Chemical Vapour Deposition (PECVD) technology. This is, presently, the most popular technology of low temperature CVD deposition [2].

The proper run of CVD processes is very sensitive to such factors as the state of gaseous environment or temperature field inside the reactor chamber. These parameters should be controlled and monitored during the reactor operation. Unfortunately, usually the reactor design does not allow or reduces possibility of full monitoring of the conditions inside the chambers during the deposition processes. For example, in the case of silicon carbide annealing processes that demand high and uniform temperature distribution inside the processing area, opaque crucibles are used that make impossible even the pyrometric temperature measurements [3]. One of the way to manage the problem is to employ numerical simulations that allow designing of multi-dimensional models of the heat and mass flow in the chamber under different operating conditions. Such numerical investigations of the phenomena taking place in CVD reactors have been already carried out and published [4-7]. Unfortunately, it was difficult to verify the correctness of the numerical approaches used in the models by direct measurements in the working reactors. Therefore, it has been found that it would be desired to perform some investigation aimed at the evaluation of the usually used numerical approaches, in which the simulations would be compared with the experiments carried out in a specially adopted CVD reactor. Such an investigation dealing with the experimental evaluation of the heat and mass transfer modelling inside a CVD reactor has been carried out and are reported in the paper.

2. CVD reactor used for experiments

As the object of investigations, the CVD reactor (Texas Instrument with build-in feasibility of enhancing chemical reaction rates with the aid of plasma) was chosen, as a typical reactor used to process thin film growth, which we could adopted to the planned experiments. Its photo is shown in figure 1. The diameter of its chamber was 59,5 cm, the diameter of the heating plate with susceptor playing the role of bottom electrode was 56 cm. The installed heater allowed to get the maximum temperature in the reactor reaching 400°C The working gas is supplied from the bottom and it flows along the susceptor to the outlet placed in the centre of the chamber.

Figure 1. The photo of the CVD reactor.

The preparation of CVD reactor to the experiments dealing with the examination of numerical approaches covered the arrangement of the reactor to create appropriate conditions for the considered measurements. As the result, the setup allows to carry out the experiments with atmospheric or lower gas pressure in the chamber, for gas flows changing from 0 up to 1000 sccm and the heater temperature of up to 300°C controlled by additional thermocouple. The adaptation of the reactor chamber to monitoring the temperature of processing samples was the other necessary modification. Its main part consisted of a set of thermocouples with measurement setup that have been introduced into the reactor chamber. Beside the thermocouple measurement system, the IR measurement procedure was also considered and appropriate tests have been performed. The CVD chamber covers two default quartz glass windows installed in the chamber walls, on the top and in the side wall, as it is shown in figure 2. In the first case, the window is placed directly above a small hole in the upper electrode, which allows monitoring the limited area of heating plate e.g. with the tested sample, whereas in the second case, the side window assures much wider field of view. In order to allow IR monitoring via the windows, their quartz-glass panes, having low transparency in the IR range, has been replaced the germanium ones.

(a) (b)

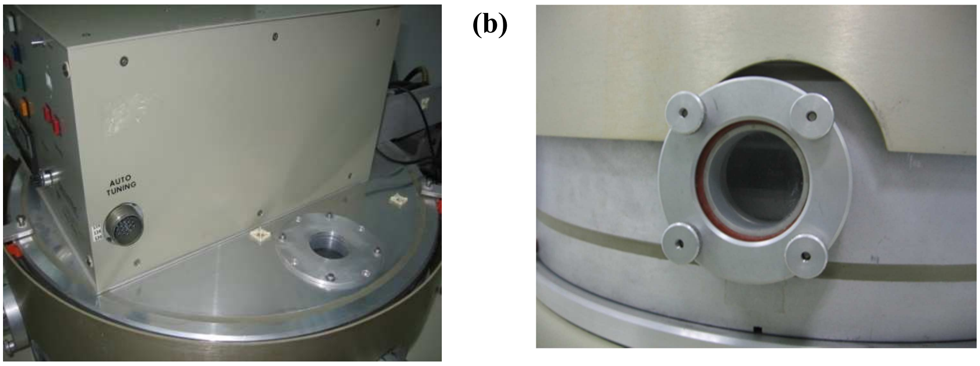

Figure 2. Windows in CVD reactor: (a) top quartz window, (b) side wall window.

In the IR measurements, the thermovision camera JENOPTIK VARIOCAM HR640 was used. The examples of IR pictures of the heated susceptor with and without a silicon pellet on it, taken directly by IR camera, are presented in figure 3. As it can be noticed, the colours of the susceptor "flows" whereas the difference between silicon pellet and the rest of susceptor is drastically large although their real temperatures are rather similar. To large extent, it is connected with the changes in the local measurement conditions such as the differences in emissivity, as it takes place in the case of the susceptor and silicon pellet. To be more useful, the pictures were converted in numerical scaling process by a special software, which reduced these adverse effects giving more realistic presentation of the temperature distribution.

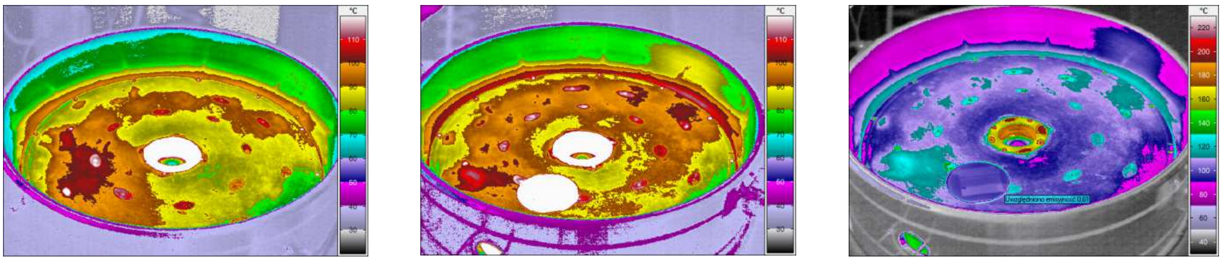

Figure 3. IR pictures of heated suceptor at atmospheric pressure taken directly by IR camera (a) without silicon pellet, (b) with silicon pellet, (c) with silicon pellet after the scaling process.

3. Model of heat and mass transfer in CVD reactor

The 3D numerical model of heat and mass transfer in CVD reactor shown in figure 2 has been developed using commercial software ANSYS CFX [8] and it is limited to the domain shown in figure 4. As in typical models of such reactors [9-11], it covers the area of reactor chamber limited by its walls, the electrodes marked in red and the inlet and outlet tubes for working gases. The dimensions of the modelled structure are depicted in figure 4b. Since the model was designed to verify the used numerical approaches by the comparison of computed and measured results obtained for the same conditions, it imposed the basic assumptions for the carried out simulations that were as follows:

- Nitrogen is used as a working gas and its properties changes in agreement with the ideal gas law.
- Gas flow rate is constant and varies among simulations in the range 0 ÷ 1000 sccm.
- Reference pressure inside the chamber is in the range 7,6 mbar - 1 bar.
- Relative pressure at the outlet equals to 0 bar.
- Thermal boundary conditions on the wall surfaces are changing, being the subject of investigations.

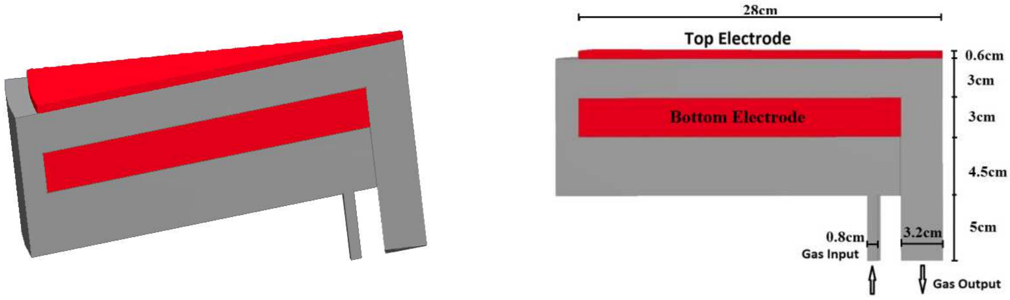

Figure 4. The geometry outline for the PECVD reactor chamber 3D model (a) spatial view of the model domain covering 15º-wedge chamber part, (b) radial cross section.

In the modeled CVD reactor, the heater in a form of a heating coil coated by the isolating ceramics is built into the bottom electrode that plays the role of susceptor. It means that the heat dissipation inside the bottom electrode, generally, is not homogeneous, which can lead to some inhomogeneity in the temperature distribution on the electrode surface influencing the gas-susceptor heat exchange. To verify such a possibility, the test measurements of the temperature distribution have been done using IR and thermocouple methods.

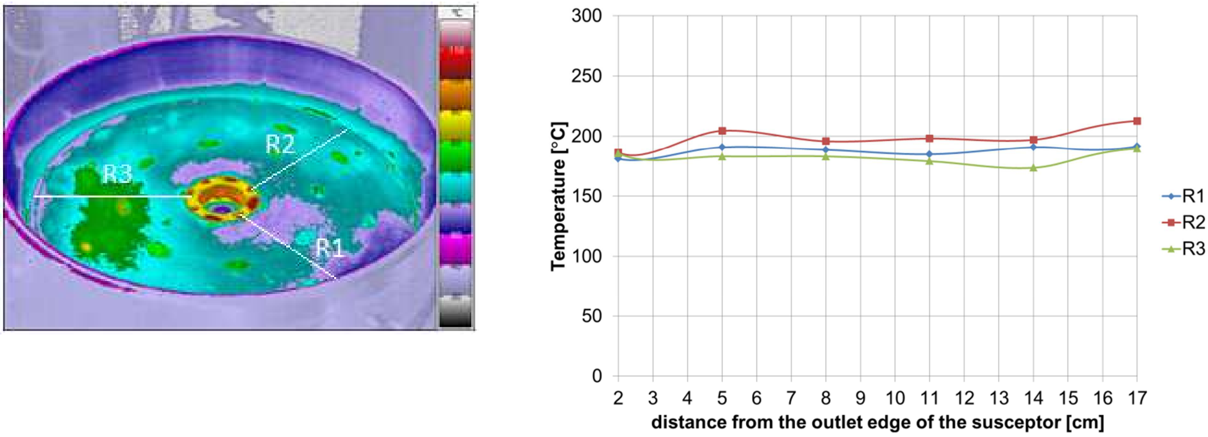

Figure 5. Temperature fluctuation on the susceptor surface represented by: IR measurements (left) and thermocouple measurements along three chosen radiuses (right).

The representative results are shown in figure 5. The IR measurements gave after the scaling process the color distribution like this one shown in figure 5a with an area of larger temperature observed always at the same place. The difference is larger than 16°C, which cannot be treated as reliable taking into account the uncertainty of the used IR temperature measurement method. Therefore, they have been followed by thermocouple measurements along the radiuses marked in figure 5a. The temperature deviations along the chosen radiuses are shown in figure 5b. They confirmed that no significant differences between the temperature distributions along the radiuses occurred and the "warmer" area indicated in figure 5a represents rather the fluctuation of measurement conditions only.

Nevertheless in figure 5b, some variations in the temperature measured along the radiuses are noticeable with a magnitude about 5 ÷ 8°C in relation to its average value. They look like stochastic ones without any relation to the heating coil location on the one hand and their magnitude is very small of the order of a few percents, on the other hand. It allows us representing the heater as a homogeneous layer located in the middle of the bottom electrode, as it is shown in figure 6. Its temperature T_S has been assumed as a constant one varying among simulations in the range 0 ÷ 300°C.

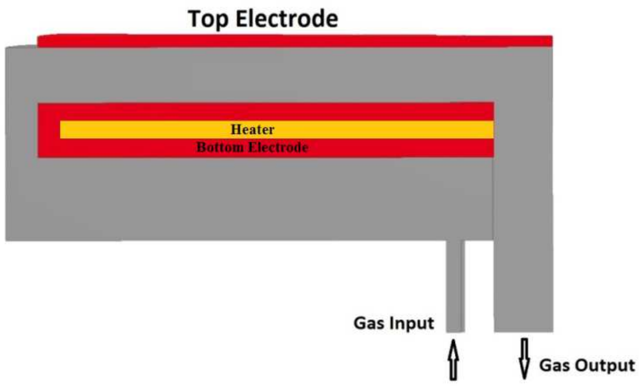

Figure 6. Sketch of the model domain presenting localization of the heater inside bottom electrode.

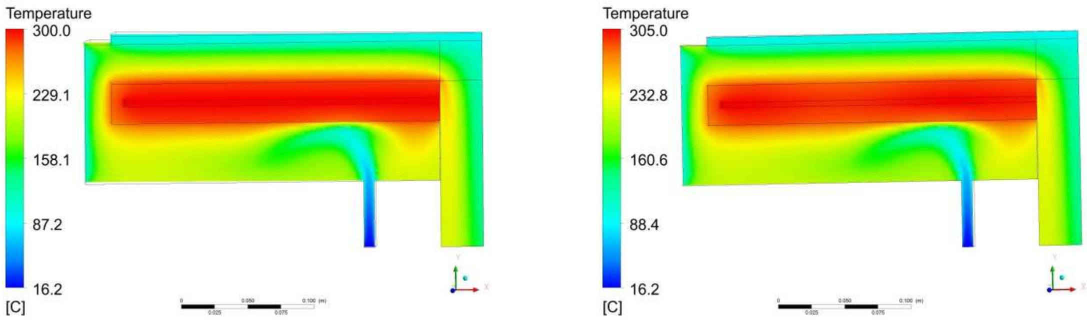

Figure 7. Temperature distributions obtained for: (a) homogeneous heater temperature distribution (b) sinewave heater temperature distribution ($T_{Saverage}$ = 300°C, sinewave magnitude ± 5°C).

In order to check if the presence of some disturbances in the heater temperature can affect the temperature distribution inside the reactor chamber working area, the comparative simulations for the same operating conditions and the average heater temperature but with homogeneous and sinewave distribution along the heater have been conducted. The obtained temperature distributions shown in figure 7 are almost identical, which confirms the correctness of proposed assumption.

4. Results of investigation

Using the model described above, series of simulations have been carried out changing the temperature enforced at the bottom electrode, the pressure and the gas flow inside the chamber. Moreover the heat exchange with the surrounding has been modelled with the aid of different boundary conditions at the walls of the chamber. In the case of adiabatic boundary condition, no heat transfer occurs, what means that the dissipated heat is removed by the working gas only. The isothermal and convective boundary conditions correspond to different intensity of heat exchange with the surrounding determined by the temperature of cooling system implemented at the chamber walls.
Moreover, the influence of thermal radiation on the total heat transfer within the reactor chamber has been investigated. All the simulations were followed by the comparative measurements using the built-in thermocouple measurement system. As the basic reference, the temperatures T_1 and T_2 located at the surface of the heating plate as it is shown in figure 8, were used in majority of experiments.

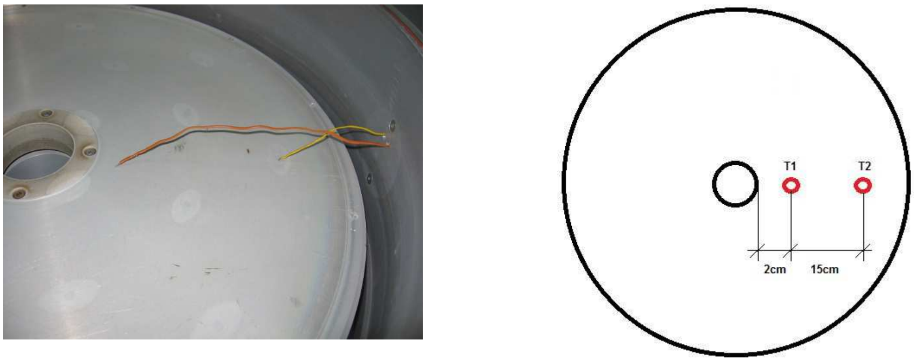

Figure 8. Localization of thermocouples in the chamber: general view (left) and the definition of two check points (right).

Series of simulations and experiments have been performed for different sets of parameters determining the operating conditions giving the full insight into the heat and mass transport processes in the reactor chamber. Below, some representative results are presented and discussed.

Figure 9 shows the simulation results covering the distributions of temperature and gas streamlines in the reactor chamber obtained for the adiabatic boundary condition on the surfaces limiting the modeled structure and the presence of radiative heat exchange inside the chamber with emissivity set to 0.2. The analysis has been carried out for the gas flow rate 1000 sccm, the pressure inside the chamber 1 bar and the heater temperature of 300°C. The temperatures measured in experiment were essentially lower than the one, obtained in the simulations. For example, the measured temperature T_1 on the susceptor was 275°C, whereas the value T_1 obtained in the simulation was 296°C. This difference may indicate that the heat removal by the gas flow is not the dominant process in the investigated reactor chamber.

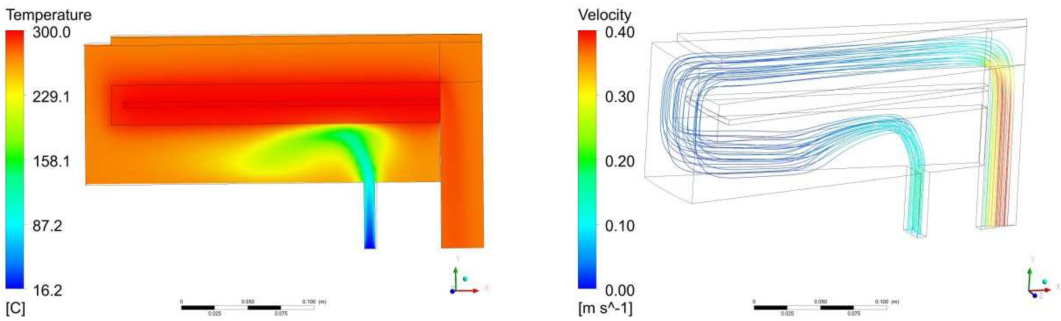

Figure 9. Results obtained for the adiabatic boundary condition: temperature distribution (left) and gasous streamlines (right) inside the CVD reactor.

Figure 10 shows the simulation results covering the distributions of temperature and gas pressure in the reactor chamber obtained for the convective boundary condition on the surfaces limiting the modeled structure with a typical values of the heat transfer coefficient of 10 W/cm^2K and the reference temperature of 25°C as well as the presence of radiative heat exchange inside the chamber with emissivity set to 0.2. The simulations performed with the convective boundary condition gave essentially different temperature distributions than previously. Now, the calculated value of the temperature T_1 on the susceptor is equal to 288°C and is much closer to the measured one. It confirms the suspicion that in the case of thermal processes in considered CVD reactor, the heat mass transfer connected with the gas flow is not the dominant path of heat transfer and the contribution of the heat exchange through the chamber walls must be taken into account.

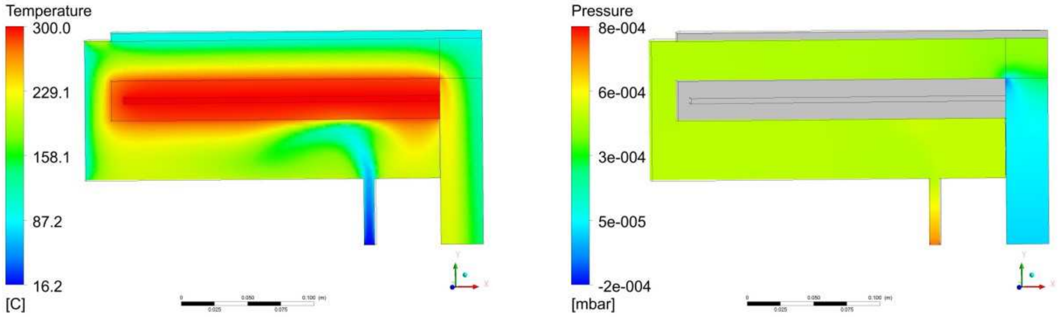

Figure 10. Results obtained for the convective boundary condition: temperature distribution (left) and gas relative pressure distribution (right) inside CVD reactor.

Taking the advantage of the CVD reactor measurement possibilities, an additional experiment has been carried out to confirm the correctness of the convective boundary condition. The temperature at the chosen point on the reactor side wall has been measurement using the thermocouple set-up and compared with the temperature at the same point evaluated numerically using adiabatic and convective boundary conditions. The comparison is shown in figure 11, which covers two curves representing the temperature distributions along the line covering the chosen check point (distance = 0 mm) taken from the 2-D distributions in figure 9 and figure 10, respectively. The black circle represents the thermocouple measurement. The measured value is about 10°C larger than that one evaluated numerically with the convective boundary condition being very far from the value estimated using the adiabatic boundary condition.

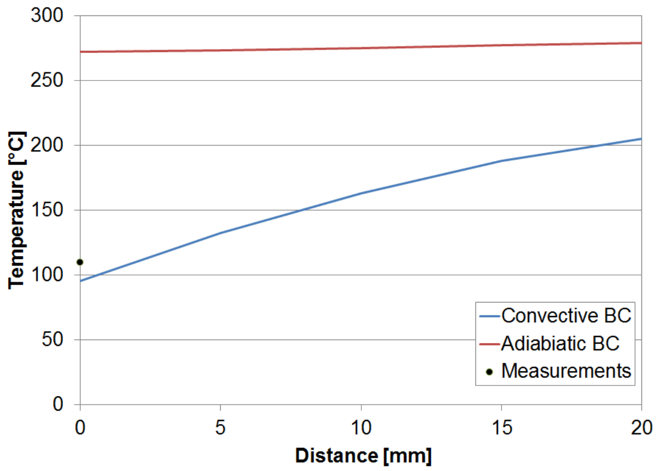

Figure 11. Temperature distributions at the wall of reactor chamber evaluated by the use of adiabatic and convective boundary condition and the temperature measured on the wall under the same operating conditions.

From the practical point of view, the main goal of any simulation is to evaluate the temperature in the processing area, i.e. in the susceptor area of CVD reactor. Therefore, the simulation results have been additionally compared with the temperature measurements along the line perpendicular to the susceptor plane, which begins at the check point T_1. In figure 12, the measured values are compared with the curves of temperature distribution extracted from figure 9 and figure 10 and the curves extracted from the simulations carried out for the same conditions but without the radiative heat exchange inside the chamber. The temperatures measured in the experiment were essentially lower than that one, obtained in the simulations not incorporating convection heat exchange with the surrounding and thermal radiation. The measured temperature T_1 on the susceptor surface was 281°C, whereas its value obtained in the simulation for the adiabatic boundary condition without radiation model was 299°C. This difference confirms that the heat removal by the gas flow is not the dominant process in the investigated reactor chamber also from the point of view of the evaluation of processing conditions.

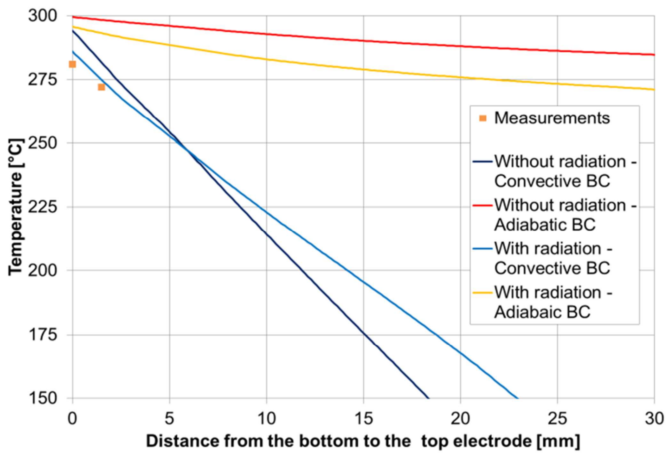

Figure 12. Temperature distribution along the line between electrodes located at point T1.

The results shown in figure 12 confirms that the heat removal from the CVD reactor chamber due to the convection phenomenon on the chamber walls is dominant but the participation of the radiation heat exchange can give also noticeable input to the final temperature distribution. It is rather small at the susceptor surface, and in the presented simulation it resulted in the difference of 8°C, but it increases in the area far from the susceptor, and at the top electrode the difference exceeds 45°C. This effect is clearly noticeable in figure 13, where the temperature distributions calculated for both the cases, with and without processes of radiative heat exchange, are presented.

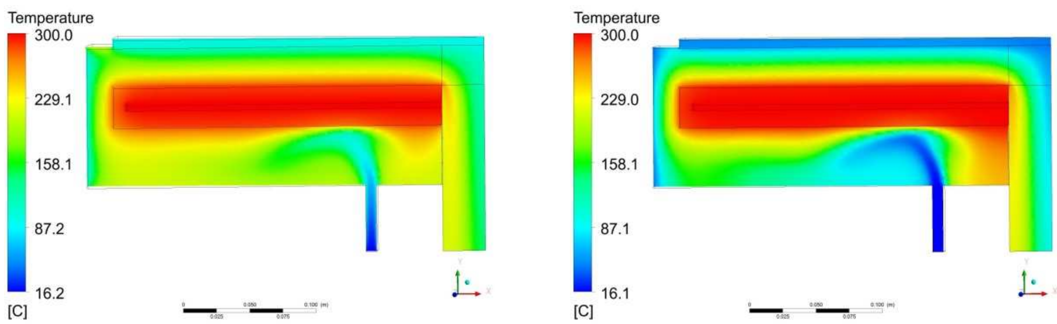

Figure 13. Temperature distributions in the CVD chamber obtained for the simulation with the radiative heat transport (left), and without the radiative heat transport (right).

The presented above results have been chosen and discussed as the representative one but they have been achieved for one set of parameters determining the work conditions i.e. the gas flow rate 1000 sccm, the pressure inside the chamber of 1 bar and the temperature of the heater 300°C. Their validity for the whole range of considered CVD reactor operating conditions has been confirmed also by many numerical and experimental investigations carried out for different set of these parameters.

Their results are gathered in a compact form in figure 14 and figure 15, for 1 bar and the lower pressure, respectively. The charts cover the comparison of temperatures in the check points T_1 and T_2 obtained experimentally and numerically using the convection boundary condition supported by the radiation heat exchange phenomenon. The difference between temperatures T_1 and T_2 in the numerical simulations is negligible, so only the single line has been plotted in the graphs.

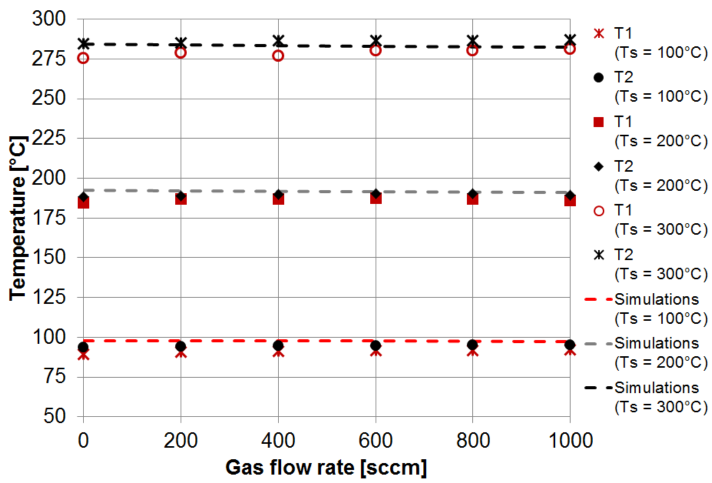

Figure 14. Comparison of simulations and measurement of the temperature dependence on the gas flow rate for the pressure inside the chamber of 1 bar.

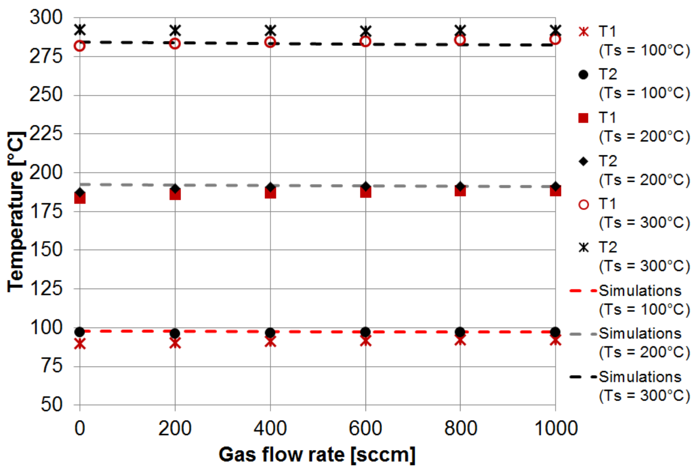

Figure 15. Comparison of simulations and measurement of the temperature dependence on the gas flow rate for the pressure inside the chamber of 7,6 mbar.

One can notice that the experimental points fit very well the curve obtained due to the numerical investigations in the whole range of considered operating parameters, which can be recognized as the prove of the correctness of used heat transfer models. In addition, the lack of noticeable influence of the gas flow velocity on the local temperature confirms the very small contribution of mass heat transfer in the investigated processes.

5. Conclusions

The paper deals with the evaluation of numerical approaches developed to create numerical models aimed at the simulation of the processes taking place in the CVD reactors chambers. Both experimental and numerical investigations have been employed with a specially adopted CVD reactor as the object of research. The rector has been adopted to work in the conditions typical for the film growth processes during semiconductors fabrication on the one hand and to create appropriate conditions for the necessary measurements, on the other hand.

The main goal of the carried out investigations was to develop and practically verify the numerical approaches allowing to design numerical models of heat and mass transfer taking place in the chambers of CVD reactors. Such numerical approaches has been created using ANSYS CFX commercial software and verified experimentally with the aid of the built-in thermocouple set up and IR measurements. The experiments proved that the developed numerical approaches allow credible modeling of the processes in CVD reactors. They indicated that the removal of heat dissipated in the susceptor heater takes place due to the convection heat exchange on the walls limited the reactor chamber with a little participation of the heat transfer connected with the gas flow. They also pointed out the role of the inner radiative heat exchange-in the total heat transfer inside the reactor chamber, which can result in significant changes in the temperature distribution far from the susceptor.

6. References

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Acknowledgments

This work has been financially supported by the EU project "GECCO" (Project No. 280694).