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THERMAL PROFILE EVALUATION OF A SILICON WAFER IN THE APPARATUS FOR RAPID THERMAL CHEMICAL VAPOUR DEPOSITION

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Rapid Thermal Processing (RTP) is currently a very popular technology. It is widely used for many applications in semiconductor manufacturing processes including annealing (Rapid Thermal Annealing, RTA), oxidation (Rapid Thermal Oxidation, RTO) and chemical vapour deposition (Rapid Thermal Chemical vapour Deposition, RTCVD). RTP systems are single-wafer, cold wall chambers that utilize radiant heat sources to rapidly heat up the semiconductor substrate at high temperature and maintain it for a short length of time. One of the main technological hurdles that RTP must overcome is that of heating the wafer uniformly. The aim of this contribution is to evaluate the different ways used for the simulation of the heating of a silicon wafer by infrared lamps in a RTCVD system. The simulation results obtained, especially the temperature profiles of the wafer, are compared with experimental data. The reactor of the RTCVD system used is cylindrical. The heating is performed with two banks of twelve tungsten-halogen lamps located above a quartz window on top of the reactor. Numerical calculations are carried out through a computational fluid dynamics code CFD’ACE+ by using both discrete ordinate method (DOM) or Monte-Carlo method (MCM) of the radiation module. Experimental results are obtained by heating a silicon wafer having thermocouples embedded along a wafer diameter. Finally, we conclude by a comparison between both the approaches.

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Keywords: RTCVD, Computer simulation, Heat transfer, Discrete ordinate method, Monte-Carlo method

1. Introduction

Rapid thermal processing (RTP) is an attractive technology to replace conventional batch processes in the microelectronic industry [1-3]. RTP using a series of lamps for radiative heat transfer has advanced after earlier studies [4,5] and it is widely used in applications in rapid thermal annealing (RTA) [6] or rapid thermal oxidation (RTO) [7] processes. RTP systems are single-wafer, cold-wall chambers that utilize radiant heat sources to rapidly heat up the silicon substrate at high temperature.

In our case, RTP is used for the applications in semiconductor manufacturing including chemical vapour deposition (CVD) on silicon substrates (wafers).

Chemical vapour deposition involves complex and strongly coupled phenomena occurring at multiple length and time scales. In order to obtain uniform thickness of film on silicon substrate, the uniformity of the substrate temperature is the key subject to be studied [8].

In the past, design optimization of technical systems was usually based on the experience of the designer, who analysed the system performances and modified individual system parameters. This kind of optimization becomes more and more difficult with an increasing number of design parameters. That is why the use of numerical methods for parameter optimization combined with simulation is a promising approach to overcome this problem.

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Numerous numerical models have been developed to simulate the CVD process and a variety of specialized tools is available: ANSYS, FEMLAB, MATLAB, FLUENT, CFD-ACE+.

Predicting the microstructure and properties of materials is a tremendous scientific and economic challenge and in consequence the literature on the subject is becoming abundant. However, only a few reviews have focused on modelling of thin film growth by vapour deposition technique.

In this paper, we are presenting the simulation results of a RTCVD reactor type JETSTAR 200 developed at Qualiflow – Montpellier [9], using the program CFD-ACE+ [10].

The aim of this work is to validate the model by comparing the simulation results to the experimental ones. Following this study, our near-future research work will be focused on the determination of suitable deposition parameters and reactor geometry to obtain a flat temperature profile of the wafer.

2. Experimental

The simplified schematic diagram of the RTCVD reactor is presented in Fig. 1.

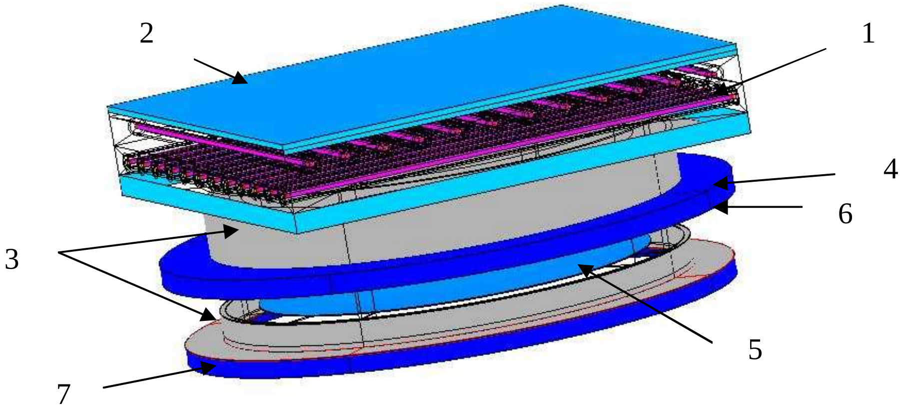


Fig. 1. Simplified schematic diagram of the RTCVD reactor: 1- lamps, 2- reflector wall, 3-reactor walls (stainless steel), 4-quartz window, 5-wafer, 6- inlet, 7-outlet.

Tungsten-halogen lamps, for which power can be manipulated in groups, are used as radiation sources to heat the wafer. To avoid the deposition on the reactor walls, the latter are kept at a low temperature using a cool water flow. The substrate is a silicon wafer having a diameter of 200 mm and a thickness of 775 µm.

The experimental measurements of substrate temperature have been realized, using five K-type thermocouples embedded in the backside of the silicon wafer, linearly arranged from the centre to the edge of the silicon substrate, as shown in Fig. 2. The temperature profile is measured in nitrogen ambient at reduced pressure.

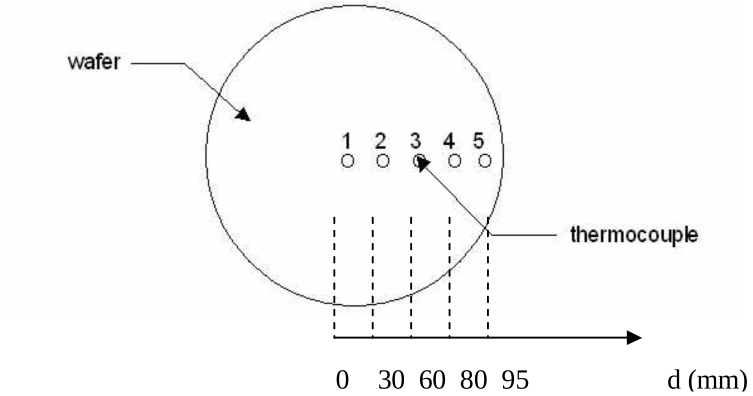


Fig. 2. Thermocouples position measured from wafer centre.

3. Simulation

3.1. Theory

Numerical integration of the partial differential equations was performed using the commercial software CFD-ACE. Input parameters of the simulation program are material ones such as thermal conductivities, specific heats, etc

Governing equations required for the simulations are the conservation of mass (continuity equation), momentum (Navier–Stokes equation) and energy. Most of the equations can be expressed in the form of a generalized transport equation (generic conservation equation) with respectively the transient term, the convective term, the diffusion term and the source term:

$$\frac{\partial \rho\phi}{\partial t} + \nabla \cdot \left(\rho\vec{V}\phi\right) = \nabla \cdot \left(\Gamma\nabla\phi\right) + S_{\phi}$$

where ρ is the density, t is the time, ϕ is the general flow variable, Γ is the diffusion coefficient.

The numerical calculations are made using the finite volume method in which the conservation equations are integrated over each domain cell of the geometry. More details concerning the mathematical background can be found in [11].

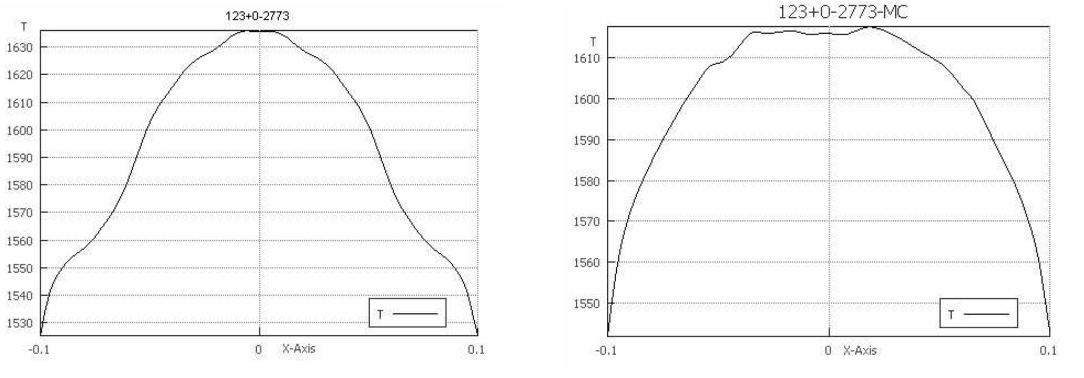
A two dimensional geometry of the machine was done. Since the furnace has got two perpendicular banks of tungsten-halogen infrared lamps, in the lower bank the sections of the lamps are represented whereas in the upper one, a full-length lamp can be seen. The grid is structured and most of the cells have a rectangular shape, which makes the calculations easier.

Also, 3D simulations were performed to show that the results made in the 2D case give similar results for the real 3D case.

Black body radiation is calculated by the Stefan-Boltzmann law. Two radiation models were used: 1) the Discrete Ordinate Method (DOM), in which the radiative heat transfer equation is replaced by a discrete set of equations for a finite (specified) number of ordinate directions, and 2) the Monte Carlo Method (MCM), where the radiative heat transfer equation is puzzled out by tracing the ways of a representative number of rays.

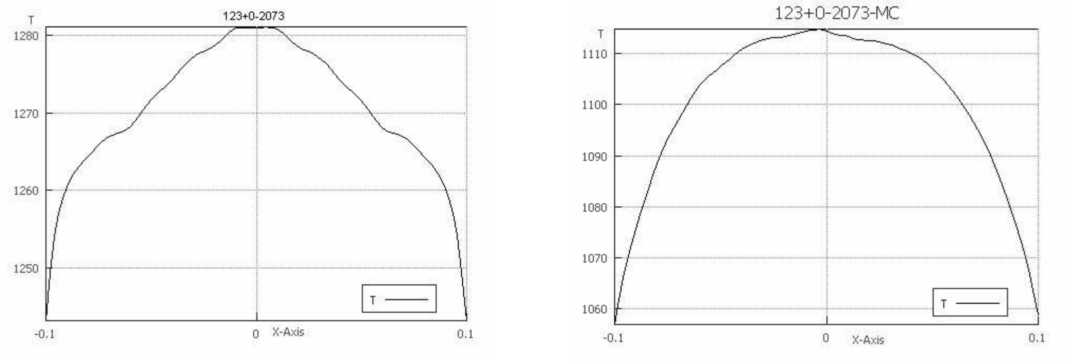
3.2. Results

As our aim is not to obtain a flat temperature profile but rather to validate the numerical simulation, all the simulations are performed by imposing the same temperature to all the lamps defined as “wall” at constant temperatures and in the experiments the IR lamps are supplied with the same powers. Comparison between the simulation results by the two methods DOM and MCM (Fig. 3, 4) has shown that the Monte Carlo method leads to temperature profiles of the wafer in better agreement with the experimental ones.



$\Delta T \approx 110K$, DOM $\Delta T \approx 80K$, MCM

Fig. 3. Temperature profile along the wafer diameter, determined by DOM and MCM methods for a temperature of lamps of 2773 K. ΔT is the temperature difference between the centre and the edge of the wafer.



ΔT ≈ 40 DOM

ΔT ≈ 55 MCM

Fig. 4. Temperature profile along the wafer diameter, determined by DOM and MCM methods for a temperature of lamps of 2073 K. ΔT is the temperature difference between the centre and the edge of the wafer.

The simulation profiles obtained by MCM are closer to the real ones than those obtained using DOM. This is because of the MCM ability to treat all directions of heat transfer in a continuous fashion (rather than along discrete directions as in the Discrete Ordinate Method) and its ability to account for strong oscillations in the spectral radiative properties. In addition, this is the only method that can treat non-diffuse reflection from walls. Thus, its strength is best realized for Rapid Thermal processing and Rapid Thermal Chemical Vapour Deposition applications [11,12]. Consequently, only the results obtained by using MCM are presented below.

4. Validation

The simulations were verified by superposing the experimental profiles to the simulated ones for a different power applied to the furnace lamps. These results are displayed in Fig. 5 for a 50%, 65% and 80% power supplied.

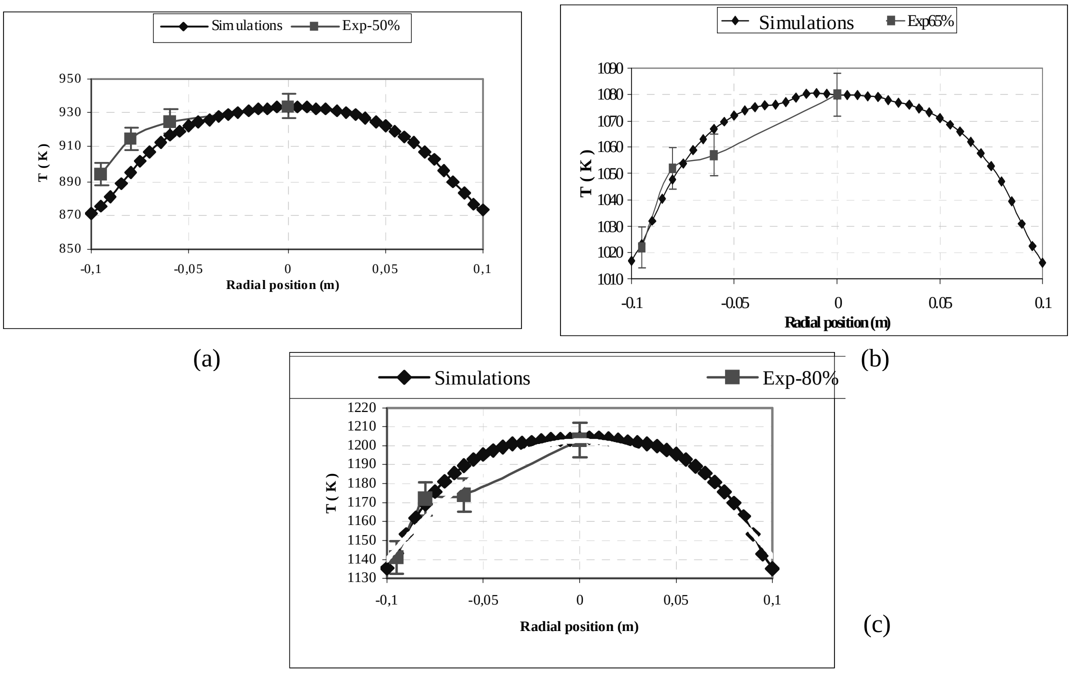


Fig. 5. Comparison between the simulation results and experimental data. The supplied power of the lamps is a) 50% - the lamps are at 1748 K, b) 65% - the lamps are at 1943 K, c) 80% - the lamps are at 2118 K.

6. Discussion

As can be seen, the calculated profiles are consistent with the experimental data.

In the end, we must prove the coherence of the results: first between different simulation results and second between the simulation results and the experimental ones.

Fig. 6 and Fig. 7 show the plot of the temperature on the wafer centre in function of the temperature of the lamps and that of the temperature of the lamps in function of the power supplied during the experience, respectively.

In Table 1 we presented the measured and calculated difference between the temperature on the wafer centre and on the edge. The error is less than 2.1% and we can conclude that the model is validated.

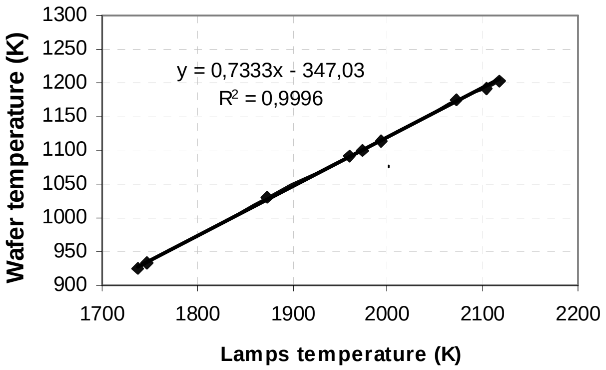


Fig. 6. Plot of the temperature on the centre of the wafer in function of the temperature of the lamps.

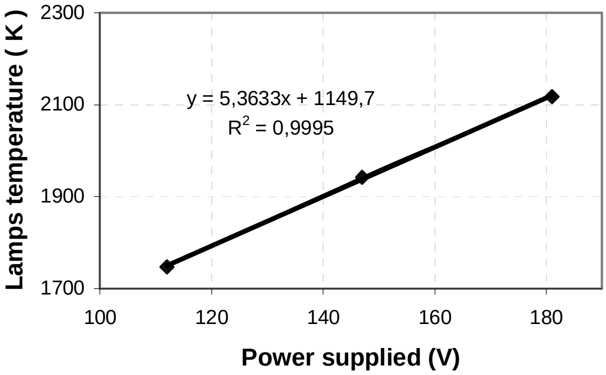


Fig. 7. Plot of the temperature of the lamps as a function of the power supplied during the experience.

Table 1. The measured and calculated difference between the temperature on the wafer centre and on the edge for the powers supplied by the three lamps.

Power lamps	ΔT_{exp}	ΔT_{simul}	Error	% Error
50%	40	58.5	18.5	2.03
65%	58	57	-1	0.1
80%	62	60.4	1.6	0.14

7. Conclusions

Using simulations to investigate how several parameters influence the temperature inside a RTCVD reactor a better understanding of the heating process has been achieved. Most of the simulations were made for a 2D case but the results obtained for the real 3D case are similar. Up to day, a flat temperature profile can be obtained by trial and error method but it should be more rational to predict the power to supply to each lamp group according to the process. As the model used is validated, the new knowledge and future simulations could be used as a tool for reactor optimization.

References

[1] S. Poscher, T. Theiler, Materials Science in Semiconductor Processing **1**(3-4), 201 (1998).
[2] A. Mrwa, G. Ebest, M. Rennau, A. Beyer, Solar Energy Materials and Solar Cells **61**(2), 127 (2000).
[3] A. Kersch, T. Schafbauer, Thin Solid Films **365**(2), 307 (2000).
[4] J. M. Fairfield, G. H. Schwuttke, Solid-State Electron. **11**, 1175 (1968).
[5] R. Iscof, Semicond. Int. **8**, 78 (1985).
[6] S. Metha, D. Hotul, Mater. Res. Soc. Symp. Proc. **92**, 95 (1987).
[7] S. R. Wilson, R. B. Gregory, W. M. Paulson, Mater. Res. Soc. Symp. Proc. **52**, 181 (1986).
[8] F. Roozeboom, Mater. Res. Soc. Symp. Proc. **303**, 149 (1993).
[9] http://www.qualiflow.com
[10] http://www.cfdrc.com
[11] CFD Research Corporation, CFD'ACE (U) User Manual, Version 6.6. 2002.
[12] CFD Research Corporation, CFD'ACE (U) Module Manual, Version 6.6. 2002.