



# Influence of diffusion tube furnace ambient during emitter formation for a crystalline silicon solar cells

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**Abstract**— In this paper, we evaluate the throughput of a low pressure diffusion tube furnace in order to realize uniform phosphorous emitters p-type silicon solar cells. The doping profiles were measured using SIMS technique. The low-pressure tube furnace is designed to obtain emitter standard sheet resistances of about 40 ohm/sq range and a wafer uniformity of less than 3 %.

In other hand, Computational Fluid Dynamics models (CFD) are used to investigate heat transfer and fluid flows on the diffusion tube furnace. Comparisons among different CFD study and models from the literature and experiment are presented and compared to our results.

In the first part of this work a three dimensional mesh was created using GAMBIT™ Software. Some geometrical approximations of the real furnace and special approaches are used in order to solve the numerical difficulties. Afterwards, a 3D steady state modeling of the heat transfer during the formation of emitter is investigated. The somewhat complicated problem of coupled heat transfer by conduction, convection and radiation is studied with the FLUENT™ Simulation Code. Our CFD model is created to represent 3D modeling of heat flows and temperature distribution, and then their impact on solar cells characteristics is examined.

Next, Silvaco® Atlas Simulation Package was used to find and explain the strong relation between phosphorus diffusion conditions in emitter formation and electrical properties of silicon solar cells. Experimentally, low-pressure diffusion tube furnace conditions lead to a reduction of wafers arrangement without losses in sheet resistance uniformity, process time and throughput efficiency.

Overall, encouraging agreement was observed between CFD models and our simulation results. This suggests that CFD modeling can be used as a tool for improvement of diffusion tube furnace designs in photovoltaic industry and to develop heat transfer correlations.

**Keywords**— Silicon solar cells, phosphorus diffusion, emitter, diffusion tube furnace, CFD.

## I. INTRODUCTION

Industrial silicon solar cells emitters formed by POCl<sub>3</sub> diffusion is well known and largely used in the photovoltaic

industry. This process is performed into a diffusion tube furnace under special conditions of pressure, temperature, gases component rates and velocity flows.

During the diffusion process, POCl<sub>3</sub> reacts with oxygen to form the Phosphorus Silicate Glass (P<sub>2</sub>O<sub>5</sub>) which is deposited on the silicon surface and releases the phosphorus which can then diffuse deep in the silicon to form the p-n junction. This diffusion can be obtained in a conventional furnace under atmospheric pressure, but this technique present the difficulty to ensure the homogeneity of the formed emitter. However, another technique under low pressure allows an increase in the kinetic of gases and offers a better uniformity of dopant.

Several types of emitters can be obtained with the variation of the diffusion parameters: temperature, time and pressure. In our study, we are interested to the low sheet resistance emitter which is necessary for a good ohmic contact by screen printing method.

We start from a numerical simulation of the furnace by including all the equation of the problem, namely: mass and energy conservation equations and the momentum equation based on the k-ε model for the turbulence modeling. The method of finites volumes are used and solved by the SIMPLE algorithm.

The numerical simulation code FLUENT™ [1] is used to investigate the effects of the phosphorus diffusion parameters, especially the temperature distribution on the performances of the crystalline silicon solar cells obtained in the end of process.

## II. MODELING

Since the beginning of photovoltaic industry the quartz diffusion tube furnace are used during the emitter formation process by POCl<sub>3</sub> source in the solar cells manufacturing. One of the most important properties of quartz is its extremely low coefficient of expansion: 5.5x10<sup>-7</sup>mm°C (20-320°C). This makes the material particularly useful for critical applications which require minimum sensitivity to thermal changes.



However, some problems of homogeneity of the dopant appears on the wafers affecting consequently the formed junction, a simulation of this furnace is thus necessary to optimize the thermal diffusion process in order to increase the quality of the formed emitter and thus to obtain an efficiency improvement in the obtained solar cells.

Figure 1 show a schematic diffusion tube furnace conventionally employed in photovoltaic industry:

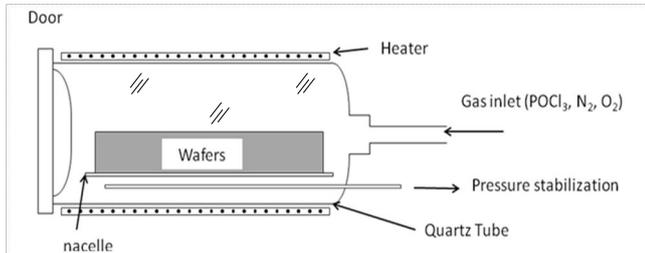


Fig. 1 Schematic description of a diffusion tube furnace

It is very important to know the temperature distribution during the diffusion process, to predict the dopant distribution and thus the emitter formed and the junction depth. In the first step we consider one quartz tube with three positions for the silicon wafers: at the inlet zone, in the middle zone of the tube and near the outlet zone, then to simplify the physical problem we consider only 3 silicon wafers positioned in each zone.

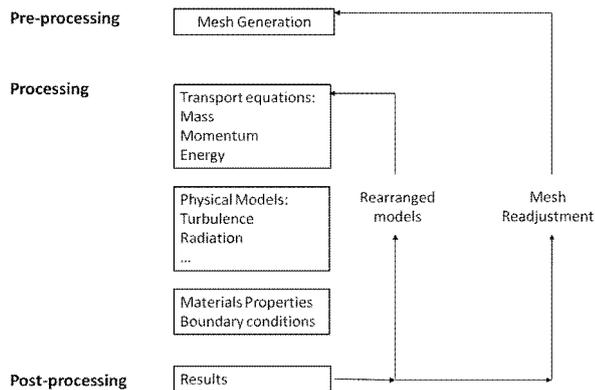


Fig. 2 Schematic CFD Modeling flow-chart

We start our simulation by built the mesh of our structure by using the GAMBIT<sup>TM</sup> mesh generator. A grid with about 685488 hexahedral cells and 1380570 nodes was created. The density of nodes is increased in the structure for a better computation of the thermal field (Fig. 3).

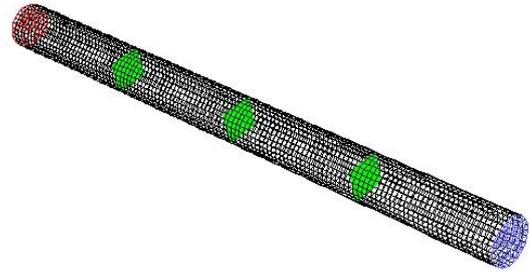


Fig. 3 Quartz tube furnace grid. Green color show the positioning of silicon wafers

Due to the high number of nodes and computational limitations, a laminar regime is used for the transient simulation. The heat transfer by conduction, convection and by radiation is calculated by using the FLUENT<sup>TM</sup> Code [1]. The radiative heat transfer is modeled by considering the "surface to surface" approach employed in FLUENT<sup>TM</sup> which is based on the calculus of radiation emitted from one zone to any other zone.

The diffusion of phosphorus in silicon is based on the Fick's laws, which stipulates that the diffusion profile follows initially a Complementary Error Function and a Gaussian distribution in a second stage [2]. We varied the diffusion parameters for a thorough study of the diffusion profiles.

The silicon wafers used are p-type with a 156x156 mm<sup>2</sup> surface. At a typical temperature between 800-900°C, the phosphorus atoms are released and the diffusion process is started.

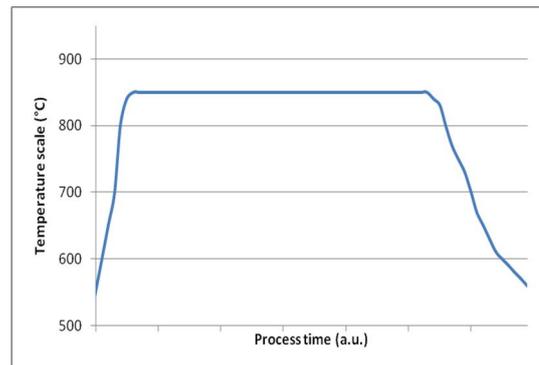


Fig. 4 Schematic single plateau temperature profile

The set of equations to be solved consists of the mass balance equation, the momentum balance or Navier-Stokes equation and the energy balance equation. The energy equation and radiation heat exchange equation are solved for the 3 dimensional geometry of the diffusion tube by using the volume finite element method provided by FLUENT<sup>TM</sup>. The solution procedure uses the Simple algorithm. The boundary



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conditions are imposed from the physical structure in such a way, that the temperature is imposed by the heating of the tube wall. The velocity is zero at the furnace wall, a specified mass flux at the inlet and a fixed pressure at the outlet was considered. We take into account a fixed value for the temperature at the furnace sides in the region where the heating element are placed and no heat flux through the walls outside this area. This supposition gives us adiabatic wall boundary conditions.

**III. RESULTS AND DISCUSSION**

Considering our boundary conditions, the convergence of problem is established at the 23rd range of algorithm solution. According to the figure 5, it was shown that the distribution of temperature is significantly reduced at the outlet zone, this give to our model better equability in temperature and thus an exact temperature profile.

In the other hand, the general flow characteristics within the tube furnace are dominated by the circulating gas at the inlet zone, this is the result of the large temperature gradient in this zone. This is confirmed by the contours of cells Reynolds Number (figure 6) which show the turbulence zones especially at the inlet zone and near the wall.

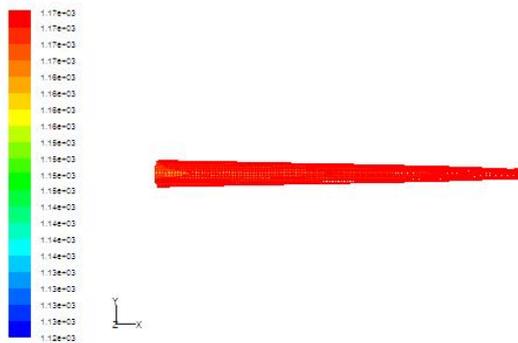


Fig. 5 Contour of relative total temperature in the tube furnace

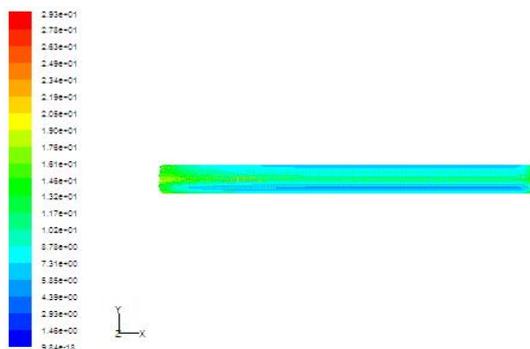


Fig. 6 Contour cell Reynolds number

This result leads us to optimize the placement of heating sources and the solar cells emplacement since the axis of the furnace is subjected to lower temperatures than near the wall. The observed non-uniformity in temperature distribution is caused by the density difference between hot and cold gas flows since the simulation was performed at high temperature at the inlet zone. This is confirmed by the contours of temperature showing how the cold gas flows along the center of the tube to the wafers.

It is well know that one of the disadvantages of the  $POCl_3$  tube furnace is the relatively low heating and cooling rate which increase the cycle time. [3] However, the temperature is the key parameter for the phosphorus diffusion in silicon. By the high temperature the diffusion phenomenon is started. In our case, a range of 800 to 850°C is allowed for acceptable sheet resistances in photovoltaic industry.

The processing time and heating flow were kept constant; the carrier gas flow rate was varied from 1 l/h to 15 l/h. In the other hand we have obtained different sheet resistance values with the variation of process temperature (figure 7).

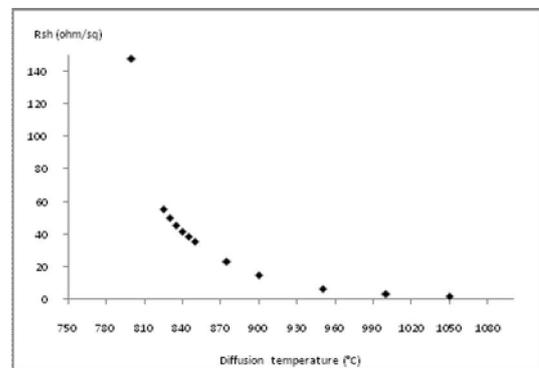


Fig. 7 Influence of the furnace temperature on the solar cell sheet resistance

The surface doping concentration and junction depth of the emitter are critical in order to provide the best yield. Panek et al. [4] obtained an emitter with 49 ohm/sq at a fixed carrier gas flow of 8 l/h, for the best output performance of solar cell. The influence of furnace temperature on the junction depth is showed in the figure 8. The temperature range 800-850°C is the ideal interval for an acceptable sheet resistance; this is confirmed by the values of manufacturing industry. [5]

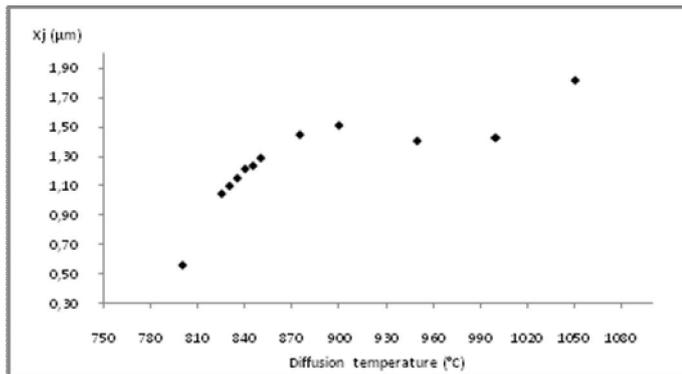


Fig. 8 Influence of the furnace temperature on the junction depth

#### IV. CONCLUSIONS

This paper presents a numerical study of heat transfer in a diffusion tube furnace designed for photovoltaic industry. Taking the advantage of the CFD tool, it is possible to predict and improve the behavior of gas flow into our specific structure, since the p-n junction formation is the most important step in crystalline silicon solar cells manufacturing. It's shown that, not only the temperature of the diffusion process is important but also the gases pressure and flow rate have to be controlled.

An optimum between the technological parameters during the emitter formation process by  $\text{POCl}_3$  diffusion is difficult to obtain if experiment attempts are only used. The numerical simulation and modeling in a 3 dimension steady state of heat transfer and fluid flows were performed taking into account

the main physical phenomena. These simulations are a valuable help in furnace optimization because they provide visual feedback on gas flow patterns and temperature distribution in the tube furnace and can predict the effects that different operating conditions have on temperature homogeneity across the silicon solar cells.

The quartz tube furnace volume, carrier gas flow rate, ambient gases flow rate, temperature etc. must be carefully monitored in order to fit compromise between designs for high efficiency silicon solar cells.

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