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COMPARISON BETWEEN EXPERIMENTAL RESULTS AND CFD MODEL CALCULATIONS FOR HIGH-THROUGHPUT CONTINUOUS SILICON CHEMICAL VAPOUR DEPOSITION EPITAXY

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ABSTRACT: Low-cost high-throughput epitaxy is one of the keystones for reducing the PV module cost to far below 50 €ct/Wp by new “kerfless” cell concepts. At Fraunhofer ISE the ProConCVD (Production Continuous Chemical Vapour Deposition) was developed to demonstrate feasibility of such a process. First long term experiments could proof the reliability and the reproducibility of the tool. 1300 multicrystaline silicon (mc-Si) wafers of 156 mm x 156 mm size were coated during 24 experiments in 4 weeks. With $SiCl_4$ as a precursor it was possible to deposit 9 µm thick epitaxial layers within 45 minutes. Thickness homogeneity higher than 90% was achieved over nearly 270 mm deposition width. Since at the edges of the reaction chamber a reduction of the deposited Si film can be observed, we investigated in Computational Fluid Dynamic (CFD) to identify the underlying reasons. The purpose of this work is to report the potential and the limitations of the current models. It could be shown that the gas inlet setup of the ProConCVD already uses 80 % of its theoretical potential in reference to the growth rate and the layer thickness homogeneity in transport direction is higher than 87 %.

Keywords: Epitaxy, Chemical Vapor Deposition (CVD), Computational Fluid Dynamic (CFD), high throughput, Silicon tetrachloride

1 INTRODUCTION

Today’s PV market is characterized by an ongoing challenge for decreasing manufacturing cost while keeping high solar cell efficiencies. New innovative cell concepts like the epitaxial solar cell with porous silicon bragg reflector [1] (“EpiCellPlus”), the Large-area module based on integrated interconnected recrystallized silicon on ceramic cells [2] (“IntegRex”) or the solar cells based on exfoliated porosified epitaxial silicon films [3] (“Lift-off”) can fulfill this requirement and lower the costs down to 45 €ct/Wp [4]. All these concepts demand a low-cost, high-throughput silicon deposition and epitaxy tool, which is still not available on the market. In 2007 Fraunhofer ISE started the construction of a high throughput chemical vapor deposition (CVD) epitaxy tool, the Production Continuous CVD (ProConCVD) [5].
The proper design of the most critical parts, the reaction chambers, is only possible with support by fluid dynamics and reaction kinetics. Based on smaller scaled reactors at Fraunhofer ISE, it was possible to build a Computational Fluid Dynamic (CFD) model including chemistry using Ansys Fluent. At present the first revision of the ProConCVD is completed and comparisons between model and real experiments are possible. This opens the door for a deeper understanding of the processes within the reaction chambers and determining the accuracy of the model. CFD plays a major role for defining future optimization potentials for the ProConCVD.

2 PROCONCVD - SETUP

The ProConCVD is based on smaller scaled reactors already running at Fraunhofer ISE, namely the RTCVD [6] and the CONCVD [7] reactors. While the deposition principle of these reactors is well established, we scaled up the continuous setup of the ConCVD by increasing the deposition area of the reaction chambers. Figure 1 shows the principle of one reaction chamber for the continuous setup.

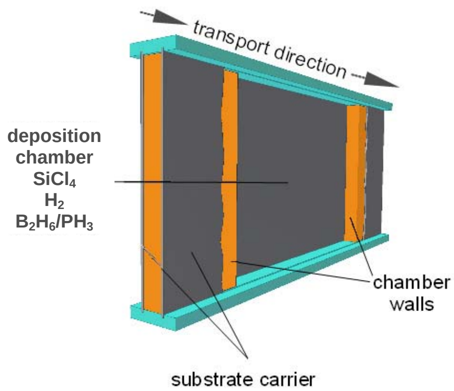

Figure 1: Schematic of the deposition chamber setup realized by the ProConCVD

Two parallel vertically mounted substrate carriers of approx. 500 mm height each form a “track” to transport the substrates (wafers of 156 mm x 156 mm) through the furnace, guided by top and bottom rails. The deposition chamber is formed by two separated graphite blocks with gas inlets and outlets in the hot zone of the furnace. Process gases like chlorosilanes as silicon precursor, hydrogen and dopant gases are injected by the inlet block and conducted by the outlet block (orange in figure 1). The substrate carriers are transported continuously along the side walls of the reaction chamber, thus the substrates will be continuously coated (in-line mode). Figure 2 shows the realized set up of three modular tracks with two sequential reaction chambers each.

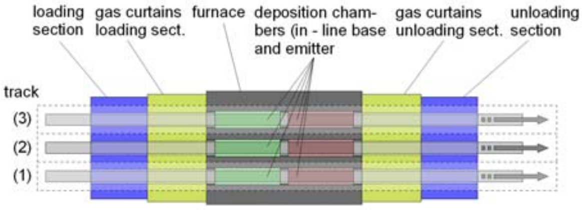

Figure 2: Schematic assembly of three substrate tracks of the ProConCVD [4]

The reaction chambers have a dimension of 1.4 m length for the first and 0.5 m for the second reaction chamber. The height of the reaction chambers is 0.5 m for all. Each chamber can be independently operated, which allows combinations of p- and n-type depositions. The first reaction chamber (green) is the main reaction chamber for bulk material and will be characterized in this paper. Compared to the smaller ConCVD reactor we scaled up the substrate area located in the reaction chamber by a factor 9 from 6 to 54 wafers.

Gas curtains at the loading and unloading sections separate the laboratory from the reaction chamber atmosphere. Figure 3 shows a simplified schematic sectional view from the top of one track with the gas curtains (green), the resistant heaters (red) and one reaction chamber (purple). The shown reaction chamber is modeled by CFD in this paper.

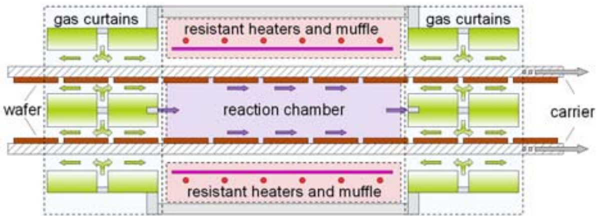

Figure 3: Simplified schematic sectional top view of one track of the ProConCVD

The 8 m long furnace is able to heat up the reaction chambers up to 1300 °C. Figure 4 shows the ProConCVD with a total length of 17 m at the SIMTEC laboratory of Fraunhofer ISE.

Figure 4: ProConCVD at SIMTEC laboratory of Fraunhofer ISE

3 EXPERIMENTAL AND SIMULATION SETUP

3.1 Experimental Setup

24 experiments were conducted in 4 campaigns with 6 experiments per week for each campaign. In this time approximately 1300 wafers were coated with silicon. In most experiments, multicrystalline silicon wafers 2nd grade were used for cost reasons. The main purposes of the experiments were to clean the reactor after construction phase, to show the long term stability of the process and to determine the vertical and horizontal deposition homogeneity.

For determining the deposition homogeneity 11 continuous experiments with a transport carrier speed of 2.1 m/h were done. The Cl/H ratio was set to 0.04 with $SiCl_4$ as precursor. Process temperatures higher than 1000 °C guaranteed epitaxially grown layers on multicrystalline silicon substrates. Thickness maps of the wafers were measured with a CYBER CT250T white light interferometer. Typically 3 wafers per carrier were analyzed by thickness measurement (see figure 5).

3.2 Simulation Setup

All CFD calculations reported in this paper were done with Ansys Fluent 13.0. Turbulence is taken into account via the k - ε - model [8]. The chemical reaction of $SiCl_4$ to solid Si (see equation 3.1) is considered to follow the Arrhenius equation 3.2 (forward equation) and 3.3 (backward equation) [9] [10].

$$SiCl_4 + 2H_2 \Leftrightarrow Si(s) + 4HCl \qquad \text{3-1}$$

$$R_1 = A_1 T^{\beta_1} e^{-E_1/RT} \left(C_{SiCl_4}^{\eta'_{SiCl_4}} \cdot C_{H_2}^{\eta'_{H_2}} \right) \qquad \text{3-2}$$

$$R_2 = A_2 T^{\beta_2} e^{-E_2/RT}\ C_{HCl}^{\eta'_{HCl}} \qquad \text{3-3}$$

The symbols are defined as follows: R_1 - forward reaction rate, R_2 - backward reaction rate, A - pre exponential factor, T - temperature, β - temperature exponential factor, E - activation energy, R - gas constant, C - concentration at the surface and η' - concentration exponential factor.

The boundary conditions for the simulations are the same as in the experimental setup with two differences:

1. For the model “Sim-1” the inlet parameters for hydrogen are idealized (homogeneous flow field over the gas inlet) while the model “Sim-2” represents the real geometry.
2. The temperatures are set as constant in both models.

Moreover, it is important to mention, that the models Sim-1 and Sim-2 include the main reaction chamber 1 with the influence of the left and right bordering gas showers as shown in figure 3.

4 RESULTS AND DISCUSSION

Figure 5 shows exemplarily one of the ProConCVD carriers with nine 156 mm x 156 mm epitaxially coated multicrystalline silicon substrates. The wafers which usually were thickness measured are highlighted in the middle row.

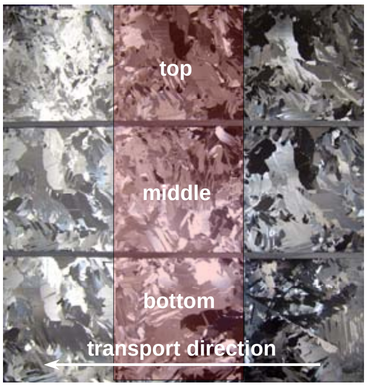

Figure 5: ProConCVD carrier with nine 156 mm x 156 mm epitaxially grown layers on mc-Si substrates. Red marked substrates were characterized by thickness measurement.

The substrates show shiny epitaxial layers, and by naked eye no major growth defects like polycrystalline areas are detectable. A closer look to the homogeneity analysis and the CFD model predictions is given in figure 6. In the diagram the homogeneity is plotted over the reaction chamber height. The homogeneity is calculated from the maximum thickness value in % by averaging the top, middle and bottom wafers from four carriers (experimental data only). The thickness of the wafers of each group does not deviate more than +/- 10 % from the average value.

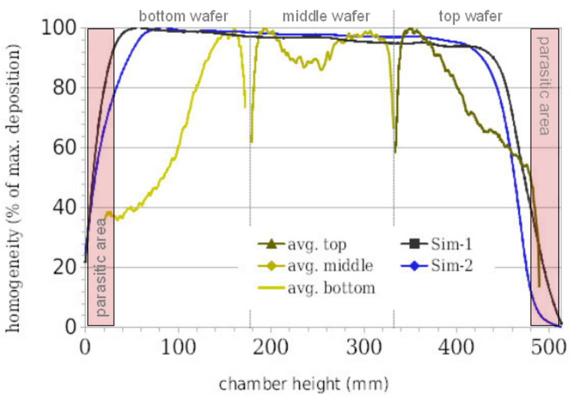

Figure 6: Average vertical homogeneity distribution of 12 epitaxially coated wafers (each 4 per position) (green), CFD prediction with ideal gas inlets (Sim-1, blue) and real gas inlets (Sim-2, grey)

As sketched in Figure 6 the reaction chamber is divided into two parts: the parasitic area where no substrates cover the carriers (red) and the area for the bottom, middle and top wafers. In vertical direction the reaction chamber reaches homogeneity higher than 90 % over a width of 270 mm, starting from 120 mm. This area is covered by the middle wafers and a part of the bottom and top wafers. The profiles for higher and lower heights are very pronounced. The homogeneity decreases down to ~ 40 % for the bottom wafers and ~ 55 % for the top wafers. The homogeneity loss for the top wafers can be well simulated by the CFD model Sim-2. It predicts a vertical homogeneity loss from 95 % down to 20 % for the top wafers. Based on the simulation gravity is responsible for this homogeneity reduction. The heavy precursor de-mixes towards the bottom over the reaction chamber length due to the low average velocity in the reaction chamber. This effect can be reduced by higher gas fluxes. On the other side the homogeneity loss for the bottom wafer can not be explained by the CFD model. A small loss is related to fluid dynamic boarder effects as can be seen in figure 6, but not as strong as observed in the experiment. One possible explanation can be a temperature gradient present in the experiment but assumed as constant for the model.

The comparison between the theoretical homogeneous inlet flows of model Sim-1 (figure 6) with the real inlet flows of model Sim-2 shows no significant differences. This indicates the closeness of the realized inlets to ideal conditions in reference to vertical homogeneity.

Compared to the vertical homogeneity the horizontal homogeneity (in transport direction) reaches values higher than 89 % for the bottom wafer, 87 % for the middle wafer and 90 % for the top wafer as can be calculated from the thickness mapping in figure 7. The thickness mapping resolves the different growth rates on different crystal grains, as well as varying rates due to surface structures present on the 2[nd] grade wafers (e.g. saw marks), thus increasing error margins for evaluation of the thickness homogeneity values.

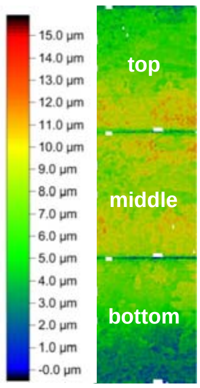

Figure 7: Layer thickness mapping of one bottom, middle and top wafer.

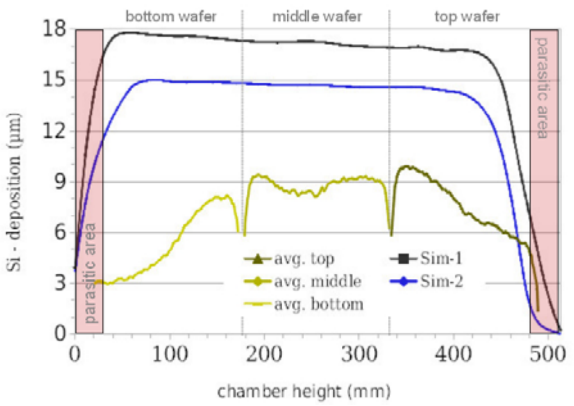

Figure 8: Average thickness of 12 epitaxially coated wafers (each 4 per position) (green), CFD prediction with ideal gas inlets (Sim-1, blue) and real gas inlets (Sim-2, grey)

Figure 8 shows the average epitaxial layer thickness of the experiment compared to the model predictions. The epitaxial layer thickness for the middle wafers reaches 9 µm, while the minimum layer thickness for the wafers at the top and the bottom reaches 5 µm and 3 µm respectively. The CFD model Sim-2 overestimates the layer thickness for the middle wafers by a factor of 1.6 (6 µm absolute) compared to the experiment. Consequently, for the next model release the used Arrhenius parameters have to be adjusted. Figure 8 also shows, that model Sim-1 (idealized gas inlets) predicts an only 20% increased deposition thickness compared to model Sim-2. The real gas inlet geometry of Sim-2 accordingly already uses 80 % of its theoretical potential.

5 CONCLUSION

Practical ProConCVD experiments with over 1000 wafers were done to clean the reaction chamber after the construction, to show the long term stability of the process and to determine its deposition homogeneity. It was possible to deposit 9 µm thick homogeneous epitaxial layers on 156 mm x 156 mm wafers within 45 minutes. The homogeneity for the reaction chamber middle in these experiments reaches 90 %. For the reaction chamber top and bottom, with homogeneities > 89 % in transport direction, drastically lower values were observed for the vertical homogeneity. CFD models found the gravity effect of the heavy precursor as one possible reason for the homogeneity loss of the top wafer. On the other side no fluid dynamic explanation could be found for the vertical homogeneity reduction at the reaction chamber bottom. The existence of temperature gradients is under discussion and will be tested by further experiments and simulations. Furthermore the CFD analysis shows the closeness of the realized gas inlet geometry to the theoretical ideal homogeneous inlet flow. Because of the CFD model overestimates the layer thickness by the factor 1.6, the Arrhenius parameters have to be adjusted for further calculations.

6 ACKNOWLEDGEMENT

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