

Ex-situ phosphorus-doped polycrystalline silicon passivating contacts for high efficiency solar cells by physical vapour deposition

Thien Truong¹, Di Kang¹, Er-Chien Wang¹, Pheng Phang¹, Daniel Macdonald¹,
and Josua Stuckelberger¹

¹ *The Australian National University, Canberra, ACT 2600, Australia*
thien.truong@anu.edu.au

Abstract

We present ex-situ phosphorus-doped polycrystalline silicon (poly-Si) passivating contacts fabricated by the physical vapour deposition method, specifically sputtering. This technique is currently of great interest to the photovoltaics (PV) community due to its low deposition temperature, small footprint, high throughput, and low-hazard solid targets and gases. We optimise the performance of the passivating contacts by adjusting various parameters from the sputtering of amorphous Si films to the formation of the poly-Si layers by a high-temperature thermal diffusion. A high iV_{oc} of ~720 mV together with a low J_0 of 2.6 fA/cm² after a hydrogenation treatment by atomic layer deposition (ALD) AlO_x and forming gas annealing (FGA), and a low contact resistivity ρ_c of less than 20 m Ω .cm² were achieved. Quokka3 simulations show that cell efficiencies as high as 24.7% are possible using the optimised passivating contacts. The results demonstrate the potential of these PVD poly-Si films as a promising candidate for future industrial solar cells.

Introduction

There are several methods for the deposition of the Si film to form poly-Si passivating contacts, such as low-pressure chemical vapour deposition (LPCVD), plasma-enhanced CVD (PECVD), or physical vapour deposition (PVD, specifically sputtering). The LPCVD method is currently the mainstream deposition technology in the industry due to its high throughput and low capital cost [1], [2]. One of the most significant disadvantages of this technology is the non-directional coating, which leads to the need for additional etching steps to remove unwanted depositions. Meanwhile, PECVD, with more directional deposition than LPCVD but less directional than PVD, has the capability of in-situ doping and is attracting more interest from the PV community. One drawback of this technology, similar to LPCVD, is the need for extra safety measures when dealing with toxic gaseous precursors such as silane or ammonia. On the other hand, sputtering, a PVD method, has recently attracted a lot of research interest, the deposition is directional and at low temperature. It requires low-hazard precursors or solid targets, and less safety requirements compared to LPCVD and PECVD. It is worth to note here that in-situ doping for n+ sputtered poly-Si films is difficult, as opposed to p+ sputtered poly-Si. Hence, the motivation is trying ex-situ n+ doping of the sputtered poly-Si films.

In this study, we focus on the development of *ex-situ* doped n+ poly-Si passivating contacts fabricated by sputtering, by varying the a-Si deposition conditions and the formation of the poly-Si layers by thermal phosphorus diffusion. The optimised contact parameters will be used as inputs for Quokka3 simulations to identify achievable cell efficiencies. Further processing is underway to fabricate Si solar cells featuring the sputtered poly-Si on the rear together with a boron diffused selective emitter structure on the front side.

Experimental details

Planar n-type Czochralski (Cz) wafers, 170 μ m thick with a resistivity of ~1 Ω .cm were used to prepare the lifetime samples and contact resistivity measurements. After a standard cleaning process, an ultrathin layer of chemical SiO_x (~1.3 nm) was grown onto the Si substrates. The samples were then transferred to a sputtering chamber and intrinsic amorphous Si (a-Si) layers were deposited on top of the oxidised samples. These samples were then subjected to a POCl₃ diffusion.

The samples were hydrogenated by depositing a 20 nm ALD AlO_x layer and annealing in FG at 425 °C for 30 minutes. The performance of the poly-Si passivating contacts was assessed via the implied open circuit voltage iV_{oc} , surface recombination J_0 and sheet resistance R_{sheet} parameters from photoconductance measurements. The Cox & Strack structure [3] was used to extract the contact resistivity of the poly-Si/ SiO_x stacks. After optimising the performance, the results are used as input parameters for simulations by Quokka3 to evaluate the potential solar cell efficiencies.

Results and discussion

First, we investigate the impact of sputtering conditions, such as deposition pressure and power on the performance of the poly-Si/ SiO_x passivating contacts for a specific diffusion recipe. Figure 1 shows the dependence of iV_{oc} and R_{sheet} as a function of deposition power and deposition pressure. As can be seen in figure 1A, increasing deposition power causes an increase in the iV_{oc} , with the best value of ~720 mV ($J_0 \sim 2.6 \text{ fA/cm}^2$) after hydrogenation for the sample with a deposition power of 230 W. This iV_{oc} is similar to an LPCVD poly-Si sample diffused in the same tube. Meanwhile, increasing the deposition pressure shows the reverse trend, with the highest iV_{oc} ~711 mV (after hydrogenation) at the lowest deposition pressure of 1.5 mTorr (Figure 1D). Note that different powers and pressures lead to a difference in thickness of the deposited films, hence, the performance after a given thermal diffusion step is different. The doping of the poly-Si/ SiO_x stacks can be assessed by the sheet resistance and doping profiles obtained by ECV. As can be seen in figure 1C, lower deposition power shows smaller doping concentration in the poly-Si films as well as in the c-Si substrates. The reverse trend is observed for the lower deposition pressure (figure 1F). Also, within the c-Si substrate, in both cases, the LPCVD samples show higher doping concentrations. Meanwhile, compared with the LPCVD samples, within the poly-Si layer, varying pressure shows a significant increment in the amount of phosphorus, but not the case for deposition power (figure 1C, 1F). It is interesting to note that, from figures 1B & 1E, the LPCVD samples have a smaller R_{sheet} (~100 Ω/sq). On the other hand, varying deposition pressure and power show less impact on the sheet resistance (with R_{sheet} ~200-300 Ω/sq).

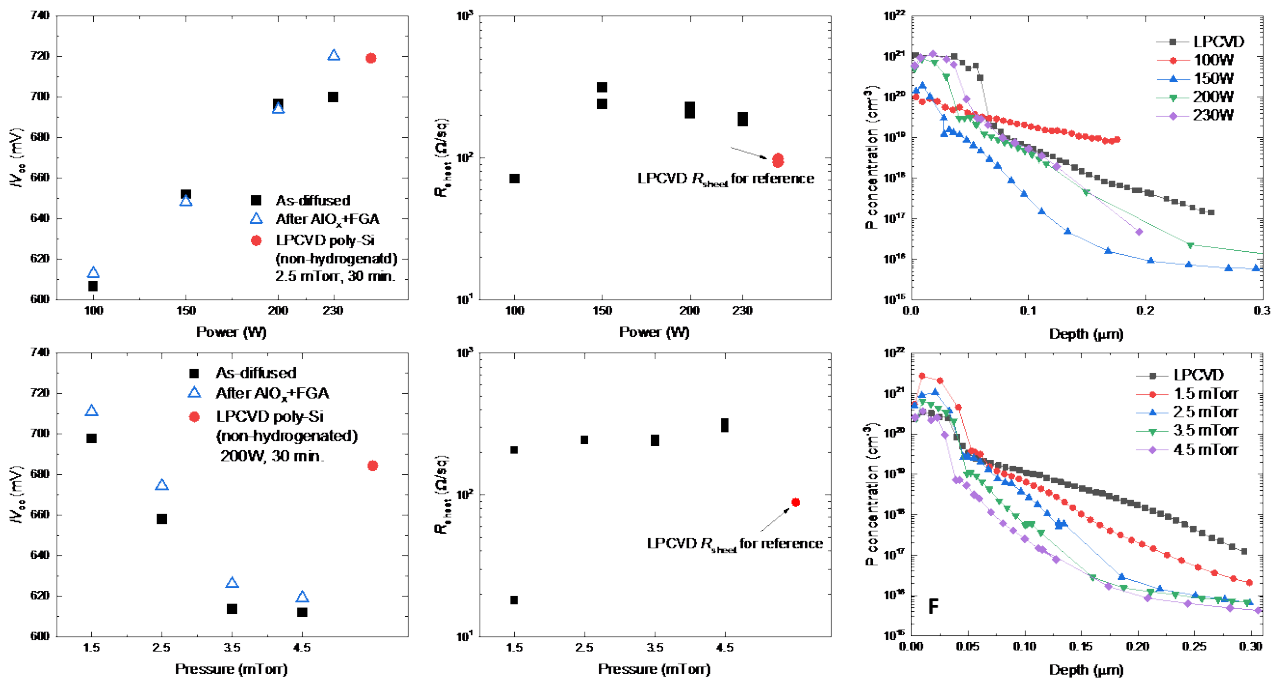


Figure 1. iV_{oc} , R_{sheet} and electrically active phosphorus (ECV) profiles as a function of deposition power (A-C) and pressure (D-F). A fixed pressure of 2.5 mTorr and a fixed power of 200 W with a same 30 minutes of deposition were used for the different power and different pressure recipes, respectively. The results are reported after a POCl_3 diffusion at 920 °C, with a deposition time of 25 minutes and a drive-in time of 30 minutes in N_2 environment.

Note here that, the LPCVD poly-Si samples in A-C and D-F are in different diffusions, hence the discrepancy in the performance and ECV profiles.

Secondly, using the Cox & Strack method, the dependence of the contact resistivity of the sputtered contacts on the deposition pressure and deposition power was studied (Figure 2). Generally, increasing the deposition power causes an increase in ρ_c except in the case of 200 W. As can be seen from the ECV profiles in Figure 1C, for the 100 W sample, the poly-Si film is too thin, and a large number of dopants penetrate into the c-Si substrate. This explains the low contact resistivity of the sample ($\sim 10 \text{ m}\Omega\cdot\text{cm}^2$, figure 2A). Meanwhile, with varying deposition pressure, the contact resistivity increases with pressure up to 3.5 mTorr, and then decreases. It is interesting to note that, when considering the sputtered samples with a similar thickness of poly-Si ($>200 \text{ W}$ or $<3.5 \text{ mTorr}$, with the same deposition time, from ECV profiles in figure 1), a low contact resistivity of less than $20 \text{ m}\Omega\cdot\text{cm}^2$ is achievable.

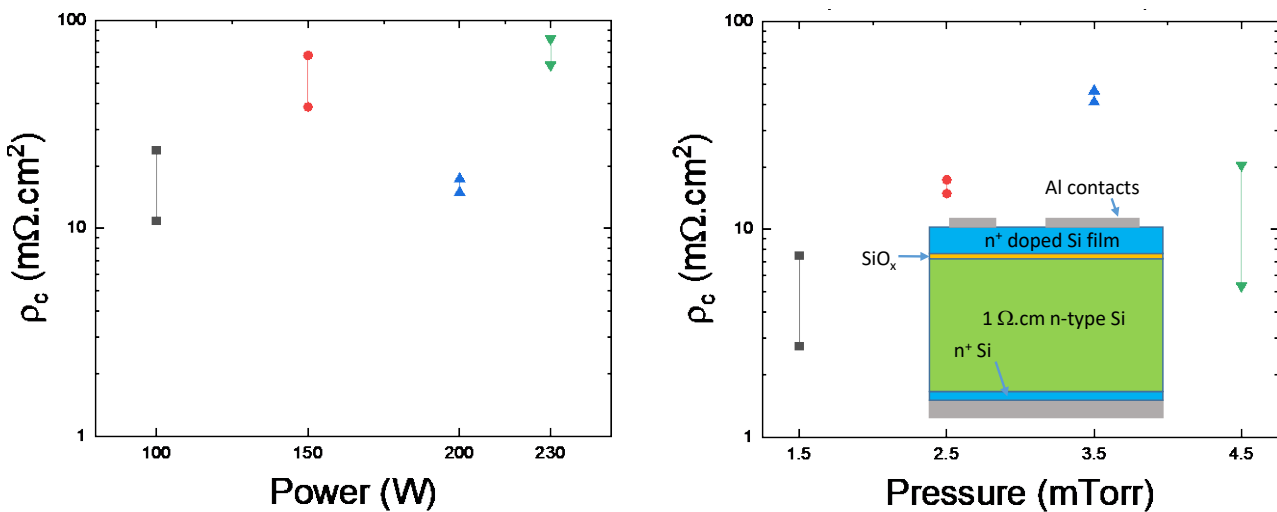


Figure 2. Dependence of contact resistivities ρ_c on power (A) and pressure (B) of the sputtered poly-Si contacts with the Cox & Strack method. The sputtering in figure A is at 2.5 mTorr and in figure B at 200 W with the same deposition time of 30 minutes. The POCl_3 diffusion is at $920 \text{ }^\circ\text{C}$ with a deposition time of 25 minutes and a drive-in time of 30 minutes.

The impact of different high-temperature thermal diffusion conditions, such as diffusion temperature, POCl_3 deposition time, and drive-in time on the performance of the passivating contacts fabricated with the same sputtered a-Si recipe was also studied. Firstly, we varied the diffusion temperature from $830 \text{ }^\circ\text{C}$ to $950 \text{ }^\circ\text{C}$ while fixing the POCl_3 deposition and drive-in time. It was found that $920 \text{ }^\circ\text{C}$ is the optimal diffusion temperature ($iV_{oc} \sim 705 \text{ mV}$ after FGA). Secondly, we fixed the diffusion temperature and drive-in time while testing different POCl_3 deposition times from 5 to 45 minutes. Increasing the deposition time caused an increase in iV_{oc} up to 35 minutes of deposition ($iV_{oc} \sim 685 \text{ mV}$ without hydrogenation). Lastly, we used different drive-in times from 5 to 60 minutes in an N_2 gas environment for samples with the same deposition time of 25 minutes and diffusion temperature of $920 \text{ }^\circ\text{C}$. It was found that 30 minutes of drive-in is the optimal condition ($iV_{oc} \sim 705 \text{ mV}$ after FGA). These results will be presented at the conference.

Finally, we use Quokka3 simulations [4] to predict solar cell efficiency potential based on the results achieved from the optimisation in the previous sections. Figure 3A shows the simulated current-voltage characteristics of an n-type silicon solar cell with a rear full area PVD deposited n+ poly-Si passivating contact, and front side boron-doped selective emitter. Also, the insets show the detailed schematic structure of the cell, and output electrical parameters from the simulation. Using best experimental values from cells fabricated previously in the ANU PV Lab, such as the passivated emitter recombination parameter $J_{0,e}$; metallised emitter recombination parameter $J_{0,\text{metal}}$; metallised

area percentage, front contact resistances, etc. [5], in combination with experimentally achieved values for the PVD deposited n+ poly-Si passivating contact from the test samples studied above, a conversion efficiency of 24.7% can be achieved. The contour plot in Figure 3B illustrates the dependence of the cell efficiency on J_0 of the rear n+ poly-Si contacts and J_0 on the front between the fingers, with the highlighted point (black star) representing the cell given in Figure 3A. The cell efficiency is limited by the front surface passivation between the fingers. It could increase to 25.3% by further improving the J_0 between fingers to below 5 fA/cm².

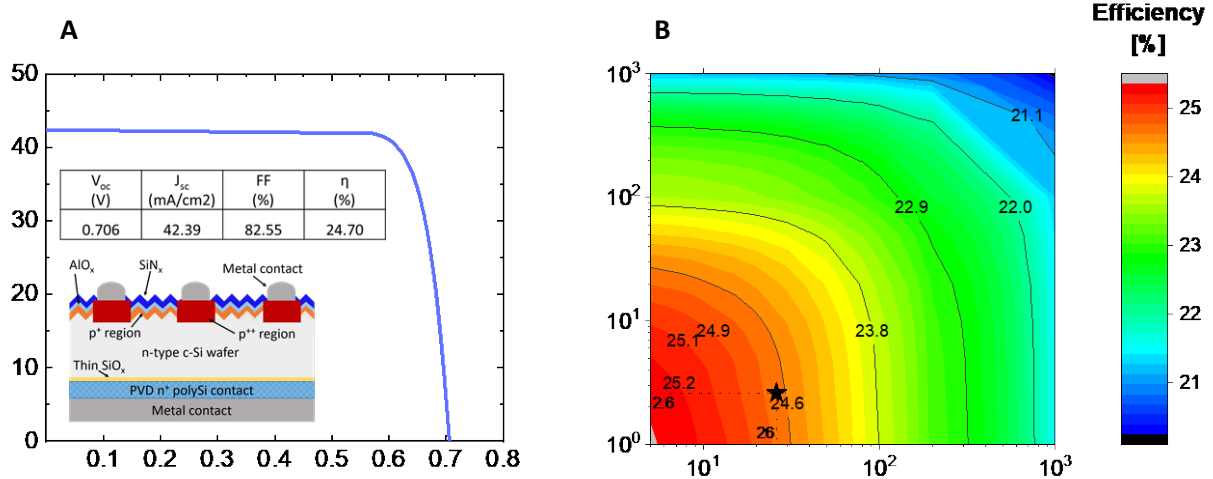


Figure 3. Quokka3 simulation results of solar cell performance with PVD deposited n+ poly-Si on the rear side using experimentally achieved input values.

Conclusion

In conclusion, we have demonstrated that, with the sputtering method, a high-quality *ex-situ* doped n+ poly-Si/SiO_x passivating contact can be achieved. With an iV_{oc} of ~720 mV, J_0 of ~2.6 fA/cm² together with a low contact resistivity of <20 mΩ.cm², the n+ PVD contact could potentially be featured in a full device with efficiency well above 24%, as simulated by Quokka3. These results show sputtering as a potential alternative to LPCVD or PECVD techniques in the fabrication of high efficiency Si solar cells based on poly-Si/SiO_x passivating contact structures. More work is underway to fabricate the full devices. Their performance will be reported at the conference.

References

- [1] M. Hermle, F. Feldmann, M. Bivour, J. C. Goldschmidt, and S. W. Glunz, "Passivating contacts and tandem concepts: Approaches for the highest silicon-based solar cell efficiencies," *Appl. Phys. Rev.*, vol. 7, no. 2, p. 021305, Jun. 2020, doi: 10.1063/1.5139202.
- [2] T. G. Allen, J. Bullock, X. Yang, A. Javey, and S. De Wolf, "Passivating contacts for crystalline silicon solar cells," *Nat. Energy*, vol. 4, no. 11, pp. 914–928, Nov. 2019, doi: 10.1038/s41560-019-0463-6.
- [3] R. H. Cox and H. Strack, "Ohmic contacts for GaAs devices," *Solid. State. Electron.*, vol. 10, no. 12, pp. 1213–1218, Dec. 1967, doi: 10.1016/0038-1101(67)90063-9.
- [4] A. Fell and P. P. Altermatt, "Detailed 3D full-cell modeling in Quokka3: Quantifying edge and solder-pad losses in an industrial PERC cell," *AIP Conf. Proc.*, vol. 1999, no. August, pp. 1–6, 2018, doi: 10.1063/1.5049246.
- [5] D. Yan, A. Cuevas, J. Bullock, Y. Wan, and C. Samundsett, "Phosphorus-diffused polysilicon contacts for solar cells," *Sol. Energy Mater. Sol. Cells*, vol. 142, pp. 75–82, 2015, doi: 10.1016/j.solmat.2015.06.001.