

INFLUENCE OF AlO_x DEPOSITION TEMPERATURE ON THE PASSIVATION MECHANISM OF $\text{AlO}_x/\text{SiN}_y:\text{H}$ STACKS

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ABSTRACT: High efficiency solar cell concepts (e.g. passivated emitter, rear totally diffused (PERT) cells) rely on thin-film surface passivation layers, often deposited by chemical vapor deposition (CVD) due to the high parameter variability of the CVD. Many of these concepts use $\text{AlO}_x/\text{SiN}_y:\text{H}$ stacks which are investigated within this work. The passivation mechanism of these stacks after firing is analyzed depending on the deposition temperature of APCVD AlO_x layer. It is shown that annealed single layers show an opposite behavior in passivation quality depending on deposition temperature compared to the stacks. With corona charging, capacitance voltage (CV) measurements and secondary ion mass spectrometry (SIMS) it can be explained that this behavior can be attributed to the H diffusion kinetics through the AlO_x barrier layer. A higher deposition temperature leads to a layer with a higher mass density which suggests a slower diffusion of H through this layer. Fixed charges are shown to be more pronounced in single layers deposited at higher temperatures. However, the resulting stronger field effect for these layers is shown to be the subordinated passivation mechanism as compared to chemical passivation. The understanding of passivation mechanism enables further potential of optimization of CVD AlO_x .

Keywords: CVD based deposition, passivation, aluminum oxide

1 INTRODUCTION

High efficiency solar cell concepts (e.g. passivated emitter, rear totally diffused (PERT) cells) rely on thin-film surface passivation layers, often deposited by chemical vapor deposition (CVD) due to the high parameter variability of the CVD. Especially CVD AlO_x layers have shown to provide excellent surface passivation [1]. In this contribution, we investigate the passivation mechanism of atmospheric pressure (AP) CVD deposited AlO_x films based on trimethyl-aluminum and oxygen as precursors [2], which are a relevant alternative to coatings produced by plasma-enhanced (PE) CVD or atomic layer deposition [3], [4]. We aim at separating the effect of chemical passivation from the field effect by fixed charges in these layers, which enables the possibility to optimize the layer properties in production-relevant stacks like $\text{AlO}_x/\text{SiN}_y:\text{H}$.

2 EXPERIMENTAL

During sample preparation, the mono-crystalline Czochralski (Cz) Si wafers (n-type, $2\ \Omega\text{cm}$) are saw damage etched, cleaned and chemically polished using an HNO_3/HF solution. Float-Zone(FZ)-Si wafers (n-type, $200\ \Omega\text{cm}$; p-type, $200\ \Omega\text{cm}$) undergo a single HF etching step. AlO_x is deposited by an APCVD roller system at different set temperatures between $570\text{-}690^\circ\text{C}$ with constant layer thickness. Part of the wafers are subsequently coated with $\text{SiN}_y:\text{H}$ or $\text{SiN}_y:\text{H/D}$ (using ND_3 instead of NH_3) using a semi-remote CVD tool and fired at a sample peak temperature of 800°C . Reference wafers with single AlO_x layers are divided into two groups. One is fired in the same way as above and the other one is annealed for 30 min at 400°C . Both single layer groups show the same qualitative behavior, however, the passivation quality of the annealed group is higher and more comparable to the $\text{AlO}_x/\text{SiN}_y:\text{H}$ stacks and therefore shown in the following. The general process flow is schematically depicted in Fig. 1. The passivation quality is determined by applying photo conductance decay (PCD) measurements to determine the effective minority charge carrier lifetime τ_{eff} . For investigations of the passivation

mechanism, samples are measured applying the corona charging (CC) and capacitance voltage (CV) techniques.

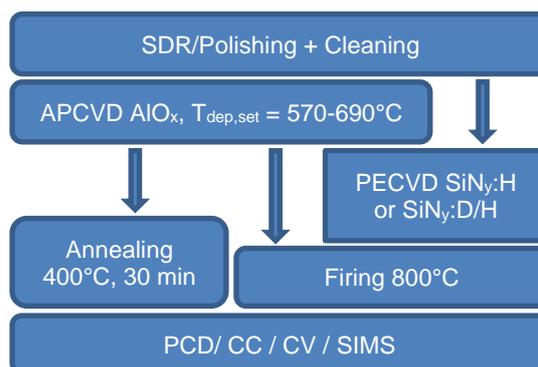


Figure 1: Schematic process flow of samples shown in the results section.

3 RESULTS AND DISCUSSION

Fig. 2 shows the effective surface recombination velocity S_{eff} of annealed AlO_x single layers and fired $\text{AlO}_x/\text{SiN}_y:\text{H}$ stacks. The calculation of S_{eff} is based on [5], [6]. For the single layers, S_{eff} decreases with increasing deposition temperature, while for the stacked layers S_{eff} increases. Thus, the additional $\text{SiN}_y:\text{H}$ layer seems to have a system-changing influence on the passivation quality, which can be attributed to a change in the passivation mechanism.

To separate chemical passivation and field effect passivation, CC is used. For this purpose, charges are gradually applied one-sidedly to the sample surface, which eliminates the field effect passivation on this side. Since the field effect of the other side may still be intact, this may not result in the pure chemical passivation, but an additional offset from field effect. The quality of chemical passivation for layers deposited at different temperatures can be compared via their respective maximum of S_{eff} or minimum of τ_{eff} reached when the amount of applied CC eliminates the field effect of the fixed charges.

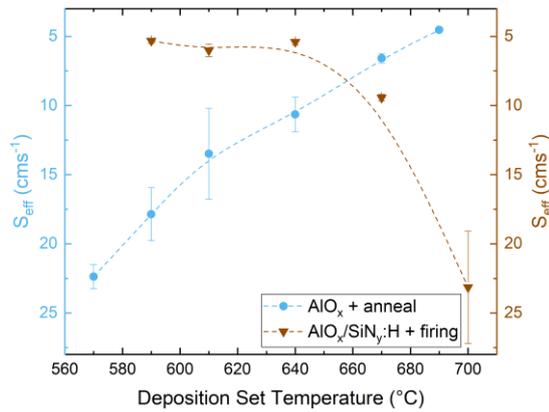


Figure 2: S_{eff} of annealed AlO_x (left axis) and of fired $\text{AlO}_x/\text{SiN}_y:\text{H}$ stacks (right axis) dependent on the APCVD deposition set temperature. Lines serve as guide to the eye.

Fig. 3 shows τ_{eff} as a function of the corona charging duration, for annealed AlO_x single layers and fired $\text{AlO}_x/\text{SiN}_y:\text{H}$ stacks. For the single layers, the height of the minimum of τ_{eff} increases with increasing deposition temperature. Accordingly, the chemical passivation of samples with a higher deposition temperature is more effective, meaning a likely higher density of passivated dangling bonds.

The fired stacks show in general a higher chemical passivation than the annealed single layers. This is likely to be attributed to a higher H content at the Si interface after firing with the additional H source on top. Nevertheless, the behavior of strength of chemical passivation for the stacks compared to the single layers is the other way around: the height of the minimum decreases slightly with increasing deposition temperature. This can be explained due to H diffusion through the AlO_x which is known to act as a barrier layer [7], and the barrier properties might be changed with changing deposition temperature.

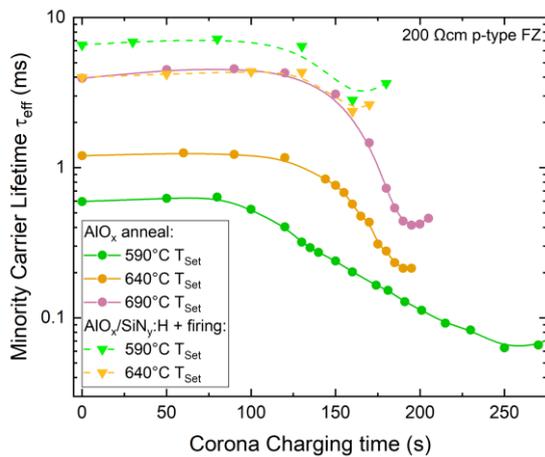


Figure 3: Measured τ_{eff} during application of Corona Charging dependent on the Corona Charging time for annealed AlO_x and fired $\text{AlO}_x/\text{SiN}_y:\text{H}$ stacks depending on the deposition set temperature.

To determine the amount of H diffusing from a $\text{SiN}_y:\text{H}$ layer through the AlO_x to the Si interface, a depth-resolved secondary ion mass spectrometry (SIMS) measurement is performed. $\text{AlO}_x/\text{SiN}_y:\text{H}/\text{D}$ stacks at different extreme

(one relatively cold, one hot) AlO_x deposition temperatures and a $\text{SiN}_y:\text{H}/\text{D}$ single layer are deposited. The $\text{SiN}_y:\text{H}/\text{D}$ is prepared using deuterated ammonia (ND_3) to distinguish the D from the $\text{SiN}_y:\text{H}/\text{D}$ from the H that originates from the AlO_x layer. Afterwards the samples have been fired.

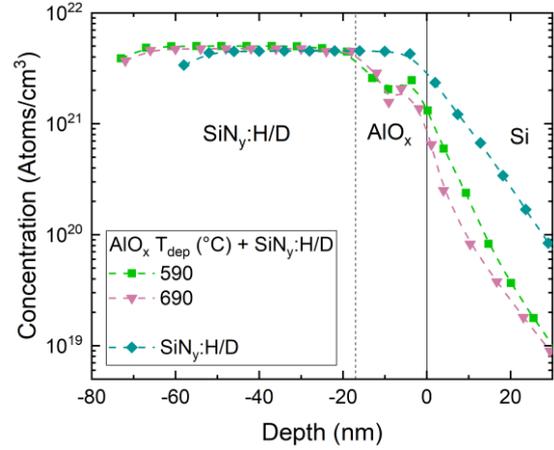


Figure 4: Concentration of D measured with SIMS in an $\text{AlO}_x/\text{SiN}_y:\text{H}/\text{D}$ stack dependent on the depth for different deposition set temperatures and a $\text{SiN}_y:\text{H}/\text{D}$ reference without AlO_x layer.

Fig. 4 shows the concentration of D with depth, as measured with SIMS. The signals are shifted so that the Si interface is located at zero depth in each case, calibrated with the Al signal (for samples with AlO_x) and by depth calibration (for the sample without AlO_x). The boundary of the AlO_x layer for the two samples with AlO_x layer is indicated by the dashed line. At the interface to Si, the D signal of the single $\text{SiN}_y:\text{H}/\text{D}$ layer shows the highest concentration.

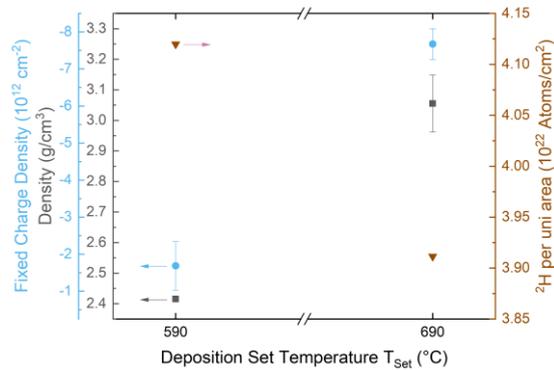


Figure 5: Density of AlO_x (left axis, grey), fixed charge density of annealed AlO_x (left axis, blue) and area concentration of D in AlO_x in an $\text{AlO}_x/\text{SiN}_y:\text{H}/\text{D}$ stack (right axis, brown) dependent on the APCVD deposition set temperature.

Fig. 5 shows the integral of the D concentration in the AlO_x layer plotted against the deposition set temperature (brown, right axis). Numerical integration was performed over the area attributed to the AlO_x layer in Fig. 4. The concentration of deuterium per unit area in the AlO_x layer decreases significantly with increasing deposition temperature. This suggests that with increasing deposition temperature, less D diffuses from the $\text{SiN}_y:\text{H}/\text{D}$ layer through the AlO_x layer to the interface and also into the Si.

Additionally, Fig. 5 shows the density of the AlO_x layer for the two different deposition temperatures (grey, left axis). The density increases with increasing deposition temperature. This can be an explanation for the fact that less H/D can diffuse from the $\text{SiN}_y\text{:D/H}$ layer through the AlO_x to the Si. Thus, the chemical passivation achieved by H saturation of interface defects may be lower for higher AlO_x deposition temperatures in fired $\text{AlO}_x/\text{SiN}_y\text{:H}$ stacks.

With a capacitance-voltage measurement, the fixed charge density Q_f in a layer can be determined and thus a prediction can be made about the field effect passivation. Fig. 5 shows Q_f for the two different deposition temperatures of annealed AlO_x single layers (blue, left axis). Q_f increases with increasing deposition temperature and thus the field effect passivation. Literature indicates [8] that this field effect can be weakened if fixed charges of the opposite polarization are added due to stacked layers, e.g. $\text{AlO}_x/\text{SiN}_y\text{:H}$. However, the negative charges at the interface seem to dominate the field effect compared to the additional positive fixed charges from the $\text{SiN}_y\text{:H}$, which means that the chemical passivation quality must be crucial to explain the behavior for the fired $\text{AlO}_x/\text{SiN}_y\text{:H}$ stacks regarding the higher passivation quality at lower AlO_x deposition temperatures.

4 CONCLUSION

In conclusion, the better passivation quality of a fired $\text{AlO}_x/\text{SiN}_y\text{:H}$ stack with AlO_x deposited at a lower temperature can be attributed to the lower density of the AlO_x layer. This allows more H to diffuse from the $\text{SiN}_y\text{:H}$ layer through the AlO_x to the interface. Despite the stronger charges in AlO_x layers deposited at higher temperatures, the chemical passivation by H is essential for the observed better passivation quality of $\text{AlO}_x/\text{SiN}_y\text{:H}$ stacks deposited at lower temperatures.

5 ACKNOWLEDGEMENTS

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