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Surface Passivation of c-Si by Nanoengineered AlO_x toward Low-Cost, High-Efficiency c-Si Solar Cells

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Abstract

This work investigated the influence of nano-scale interface engineering by post deposition annealing with remote nitrogen plasma on structures and interface properties, such as a negative fixed charge density and an interface trap density, of thin AlO_x passivation layers deposited on c-Si by O_3-based batch ALD at room temperature. We demonstrated that post deposition annealing with remote nitrogen plasma is effective technique to enhance interface properties of room temperature atomic layer deposited AlO_x layers as indicated by a largely reduced interface trap density of 4.8×10^{11} $eV^{-1}\cdot cm^{-2}$ and high negative fixed charge density of -3.6×10^{12} cm^{-2}. We also found that such excellent interface properties are owing to significantly improved chemical and structural properties of AlO_x passivation layers through nano-scale interface engineering by post deposition annealing with remote nitrogen plasma.

1. Introduction

The surface passivation employed to reduce surface recombination on crystalline silicon (c-Si) become increasingly more important to enhance the performance of solar cells as the wafer thickness progressively decreases due to the cost-driven reduction of the solar cell thickness. To improve the efficiency of thinner c-Si solar cells on p-type silicon, surface passivation by a suitable dielectric layer instead of a full Al-back surface field (Al-BSF) should be employed on the rear side of solar cells [1]. Recently, negatively charged, amorphous aluminum oxide (AlO_x) deposited by atomic layer deposition (ALD) provides an excellent surface passivation on both lowly and highly doped p-type c-Si. This feature is attributed to strong field effect passivation induced by a high negative fixed charge density (Q_f) up to $\sim10^{13}$ cm^{-2} in an AlO_x layer and moderate chemical passivation resulting in a low interface trap density (D_{it}) of $\sim10^{11}$ $eV^{-1}\cdot cm^{-2}$ at an ALD AlO_x/c-Si interface [2,3].

In the meantime, H_2O- and O_3-based batch ALD methods have been successfully used to deposit AlO_x layers for c-Si surface passivation, which is promising for mass production [4,5]. However, the optimal combination of the process conditions for ALD AlO_x passivation layers has been set to a deposition temperature (T_{dep}) $\geq$ 200 ℃ followed by post deposition annealing (PDA) in pure nitrogen at 400-450 ℃ for at least 10 min. Recently, we have reported that the fairly good quality surface passivation of c-Si by ~30-nm-thick AlO_x layers deposited by O_3-based batch ALD at room temperature (RT) can be obtained through nano-scale interface engineering of the AlO_x layers by PDA [6]. These justify the interest for a combination of room temperature ALD (RT-ALD) using O_3 as an oxygen precursor and decent PDA in order to reduce a thermal budget during preparation of AlO_x passivation layers. Meanwhile, only ultrathin AlO_x layers can be expected for the practical implementation into industrial solar cells due to the main drawback of ALD, i.e., the low deposition rate.

Therefore, in this contribution, we investigate the effect of nano-scale interface engineering by PDA with remote nitrogen plasma (RNP) on structures and interface properties, such as Q_f and D_{it}, of thin AlO_x passivation layers deposited on c-Si by O_3-based batch ALD at RT.

2. Experimental

About 10-nm-thick AlO_x passivation layers were deposited on both sides of a p-type (100) single c-Si substrate (MCZ, ρ = 15~30 Ω·cm, 770 μm) from TMA and O_3 by batch ALD process at RT. PDA with RNP at a RF power of 400 W was performed at temperatures ranging from 200 to 400 ℃ under a pressure of $\sim2.4\times10^{-3}$ Pa for 30 min. PDA in pure nitrogen was performed at 400 ℃ for 30 min to prepare control samples. Q_f and D_{it} were extracted from capacitance-voltage (C-V) measurements [7]. High resolution transmission electron microscopy (HRTEM) was employed to investigate AlO_x layer structures and interfacial structures formed at AlO_x/c-Si interfaces. Thickness and density of AlO_x layers were determined using X-ray reflectivity (XRR) and the results of XRR were calibrated by HRTEM and atomic force microscopy (AFM).

3. Results and discussion

We investigated the influence of PDA performed in pure nitrogen and with remote nitrogen plasma (RNP) on interface properties of ~10-nm-thick AlO_x layers deposited at RT by C-V measurements. As shown in Fig.1 very small positive or negative Q_f (Q_{eff}/q = $\sim\left|10^{10}\right|$ cm^{-2}) existed in as-deposited AlO_x layers but all annealed layers showed significantly increased negative Q_f regardless of PDA con-

ditions. In particular, AlO_x layers annealed with RNP at 400 ℃ show the best interface properties, i.e., the best surface passivation quality as indicated by the highest negative Q_{eff}/q of -3.6×10^{12} cm^{-2} and the lowest D_{it} of 4.8×10^{11} $eV^{-1}\cdot cm^{-2}$ among annealed AlO_x layers. They are similar to the results reported recently in our previous study, i.e., Q_{eff}/q of -4.2×10^{12} cm^{-2} and D_{it} of 1×10^{11} $eV^{-1}\cdot cm^{-2}$ for O_3-based batch ALD AlO_x layers deposited at 200 ℃ and annealed in pure nitrogen at the same temperature and time duration as those of PDA performed in this study [5]. Notably, however, such excellent values are achieved here by a combination of RT-ALD and PDA with RNP.

In Fig. 2 and Table I, HRTEM images and XRR results reveal that the significantly enhanced interface properties of AlO_x layers annealed with RNP at 400 ℃ seem to be owing to the better chemical and structural reorganization, i.e., the more pronounced extent of the densification and phase transformation of AlO_x interlayers compared to those of AlO_x layers annealed in pure nitrogen.

We previously reported that ~30-nm-thick O_3-based batch ALD AlO_x layers deposited at RT have a thick low-density interlayer including aluminum silicate with showing insignificant level of surface passivation in an as-deposited state. During PDA in pure nitrogen, thermal densification of the interlayer and phase transformation of aluminum silicate into mullite in the interlayer are induced by diffused oxygen and hydrogen from an AlO_x layer toward an AlO_x/c-Si interface. This nano-scale interface reorganization activates surface passivation of c-Si by RT-ALD AlO_x [6].

However, in case of thin AlO_x layers here, the chemical and structural reorganization of AlO_x interlayers by oxygen and hydrogen diffused from a thin AlO_x layer toward an AlO_x/c-Si interface is evidently incomplete after PDA in pure nitrogen as shown in Fig. 2 and Table I. By contrast, PDA with RNP can complete the chemical and structural reorganization of the interlayers as shown in Fig. 2 and Table I. The effect of PDA with RNP seems to be related to the formation and distribution of atomic hydrogen [8] as well as the passivation of oxygen vacancies (Vo) and formation of negative Q_f by atomic nitrogen incorporation into the thin AlO_x layers during PDA [9,10]. We will discuss the detailed mechanism of this nano-scale interface engineering by PDA with RNP and provide the deeper understanding of the role of atomic hydrogen and nitrogen to enhance chemical and field effect passivation by RT-ALD AlO_x in this presentation.

3. Conclusions

In this study, the influence of nano-scale interface engineering by PDA with RNP on interface properties of RT-ALD AlO_x passivation layers deposited on c-Si was investigated. We found that PDA with RNP can significantly improve interface properties, i.e., surface passivation quality of thin RT-ALD AlO_x layers by enhancing the chemical and structural reorganization of the AlO_x interlayer through nano-scale interface engineering. From the result, we can expect that PDA with RNP is promising technique to enhance the surface passivation of c-Si by RT-ALD AlO_x layers through nano-scale interface engineering toward fabrication of low-cost, high-efficiency c-Si solar cells.

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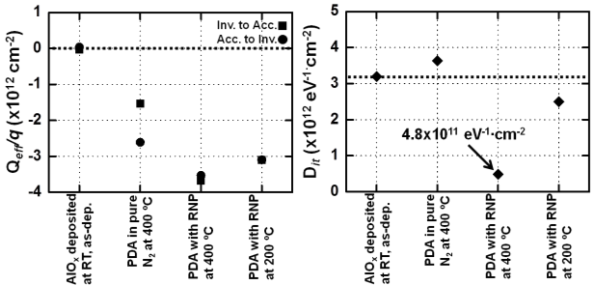

Fig.1 Q_{eff}/q and D_{it} of as-deposited and annealed AlO_x layers.

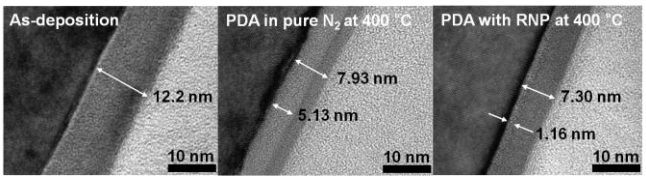

Fig. 2 HRTEM images of as-deposited and annealed AlO_x layers.

Table I. AlO_x thickness (t) and density (ρ) from HRTEM and XRR.

Samples	Total t_{AlOx} (nm)	$t_{TL/IL}$ (nm)	$\rho_{TL/IL}$(g/cm^3)
As-deposition	12.2	–	2.35
PDA in pure N_2	7.93	2.80/5.13	2.74/2.49
PDA with RNP	7.30	6.14/1.16	2.79/2.14

TL = top layer; IL = interlayer.