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Effect of oxygen annealing on spatial atomic layer deposited aluminum oxide/silicon interface and on passivated emitter and rear contact solar cell performance

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ABSTRACT

In this study, aluminum oxide (Al_2O_3) thin films are deposited via spatial atomic layer deposition on p-type silicon wafer. Then, a post-deposition annealing is performed in oxygen to activate the field-effect and chemical passivation. The annealing temperature is varied from 300 °C to 750 °C, and its effect on the structural properties and carrier lifetime of Al_2O_3/Si is investigated. The results show that at the annealing temperature of 600 °C, the highest minority carrier lifetime obtained is 446.5 μs and maximum surface recombination rate is 22.4 cm/s. Annealing temperatures higher than 600 °C lead to deteriorate surface passivation due to insufficient hydrogen passivation and structural change from AlO_4 to AlO_6 that cause low oxide fixed charge. Photovoltaic performance is simulated and compared with experimental results. The simulation shows that the p-type passivated emitter and rear contact (PERC) solar cell with the Al_2O_3 single layer annealed at 600 °C can have open-circuit voltage (V_{oc}) of 678 mV and conversion efficiency (η) of 21.96%, while the PERC solar cell with SiN_x:H/Al_2O_3 doubled layer can achieve V_{oc} of 679.7 mV and η of 22.03%, which is very close to the upper limit in the case of ideal rear passivation. The simulation is in a good agreement with the fabricated PERC solar cell showing V_{oc} = 679.2 mV and η = 21.6%.

1. Introduction

Passivated emitter and rear contact (PERC) solar cells have attracted a lot of attention in recent years. There has been continuous development to achieve cost-efficient processes such as wafer surface passivation [1,2], laser opening [3] and screen-printed aluminum local back surface field [4]. Aluminum oxide (Al_2O_3) grown by atomic layer deposition (ALD) has been reported to have excellent passivation quality on p-type silicon wafer as determined from carrier lifetime measurement [5]. Vacuum ALD can deposit high quality Al_2O_3 with a surface recombination rate of < 13 cm/s [6], but the process is time-consuming at a deposition rate of < 2 nm/min [7]. In contrast, spatial ALD recently shows great potential for Al_2O_3 deposition as its growth rate can be up to 70 nm/min [7], with an acceptable decrease in film quality. The fixed negative charge density within the Al_2O_3 layer induces an accumulation layer at the p-type silicon wafer surface that provides an effective field-effect passivation. A post deposition annealing is necessary to activate the field-effect passivation, as well as chemical passivation through formation of a high quality silicon oxide interfacial layer between Al_2O_3 and silicon wafer [8]. It has been reported that Al_2O_3 annealed in nitrogen or forming gas ambient at about 450 °C can have high level of passivation, and the reason is mostly related to the hydrogen atoms in the Al_2O_3 layer or provided by the ambient that diffuse into the silicon wafer surface to reduce the dangling bonds [9]. Higher temperature is not favorable due to dehydrogenation effect. Currently in industrial standard processes, the Al_2O_3 layer is annealed in the subsequent deposition process for hydrogenated silicon nitride (SiN_x:H) layer at 450 °C. However, effect of other annealing gas ambient that could possibly bring advantages on wafer passivation and PERC solar cell performance is seldom reported.

In this study, Al_2O_3 films are deposited in a spatial ALD system, and annealed in oxygen ambient with varying temperatures to investigate its effect on passivation. The relationship between the structural changes of Al_2O_3 and surface passivation is also presented. Finally,

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photovoltaic performance is simulated and compared with measurement.

2. Experiment

Six-inch (100) boron-doped p-type Czochralski silicon wafers with resistivity of 1 Ω-cm and thickness of 200 μm were used as substrates. The wafers were cleaned using a standard RCA process, and blow-dried with nitrogen. The last step of the RCA clean was in hydrogen fluoride, and native oxide on silicon was removed. Al_2O_3 thin films of 20 nm in thickness were deposited in a spatial ALD system. The spatial ALD was equipped with a multiple slit gas source head. The head had all the channels connected to it including precursors, inert gas, and the exhaust. Trimethylaluminum [$Al(CH_3)_3$] and H_2O were used as precursors to deposit Al_2O_3 films. Unlike conventional ALD in which the growth rate is limited by the cycle time of the precursor exposure sequence and purge time, in spatial ALD it is determined by the speed of the substrate that is continuously moving relative to the simultaneously delivered precursor sources. Nitrogen gas was used as a carrier gas as well as an inert separator gas. A spacing of about 350 μm was set between the movable substrate and the gas delivery head. The $Al(CH_3)_3$ and H_2O were kept at 17 °C and 35 °C, respectively. The gas delivery channels were kept at 70 °C to prevent the recondensation of the precursors. The substrate temperature was kept at 160 °C. A rotary pump was used for pumping waste gases. For minority carrier lifetime measurement, Al_2O_3 films were deposited on both sides of the wafers, followed by annealing in a furnace at 1.01×10^5 Pa for 20 min in a furnace with oxygen ambient. The annealing temperature was varied from 300 °C to 750 °C. To fabricate the PERC cells, the wafers were textured using alkaline solution to form pyramids and remove any marks on the wafer. To form a p-n junction, $POCl_3$ was diffused on the wafer in a standard tube thermal furnace and sheet resistance of the emitter was 75 Ω/square. Afterwards, a SiN_x:H anti-reflective layer of 100 nm thickness was deposited on the front of the wafer. The pyramids on the rear-side of the wafer were removed by KOH solution for 3 min to produce a flat surface. Then an Al_2O_3 layer of 20 nm in thickness was deposited using spatial ALD. On the top of Al_2O_3, a SiN_x:H of 120 nm in thickness was deposited. The rear-side local openings were created by laser scribing with a wavelength of 532 nm. The diameter and pitch of local contacts were 40 and 260 μm, respectively. The samples were then screen-printed with a Ag/Al paste and fired. The minority carrier lifetime of the wafer has been determined using Sinton WCT-120 lifetime tester at a specific carrier density of 1×10^{15} cm^{-3}. For capacitance-voltage (C-V) measurement, a standard metal-oxide-semiconductor (MOS) structure was used. The current density-voltage (J-V) characteristics were obtained using a solar simulator under one sun intensity (AM1.5G). The bonding configuration of the samples with different annealing temperatures was obtained using Fourier transformation infrared (FTIR) absorption spectroscopy (Tensor 27, Bruker Optics, Germany) in 400–1200 cm^{-1} with a resolution of 0.4 cm^{-1} at room temperature. The atomic depth profiles were obtained using secondary ion mass spectroscopy (SIMS, TOF-SIMS IV, Ion-ToF GmbH, Germany) with 5 keV Cs^+ as primary ions. The cross-sectional images of the samples were observed using a transmission electron microscope (TEM, JEM-3000F, JEOL, Japan) with an acceleration voltage of 300 kV. The elemental depth profiles were measured by using x-ray photoelectron spectroscopy (XPS, PHI Quantera SXM, ULVAC-PHI Inc., Japan) along with Al Kα monochromatic source and argon ion sputtering (2 keV, 10 pA) for the Al_2O_3/Si annealed at 450 °C and 600 °C. The binding energy scale of the XPS spectra was calibrated with the C 1 s peak located at 285 eV. The simulation of photovoltaic performance of PERC solar cells were carried out using PC1D computer software (version 5.9, University of New South Wales, Sydney, Australia).

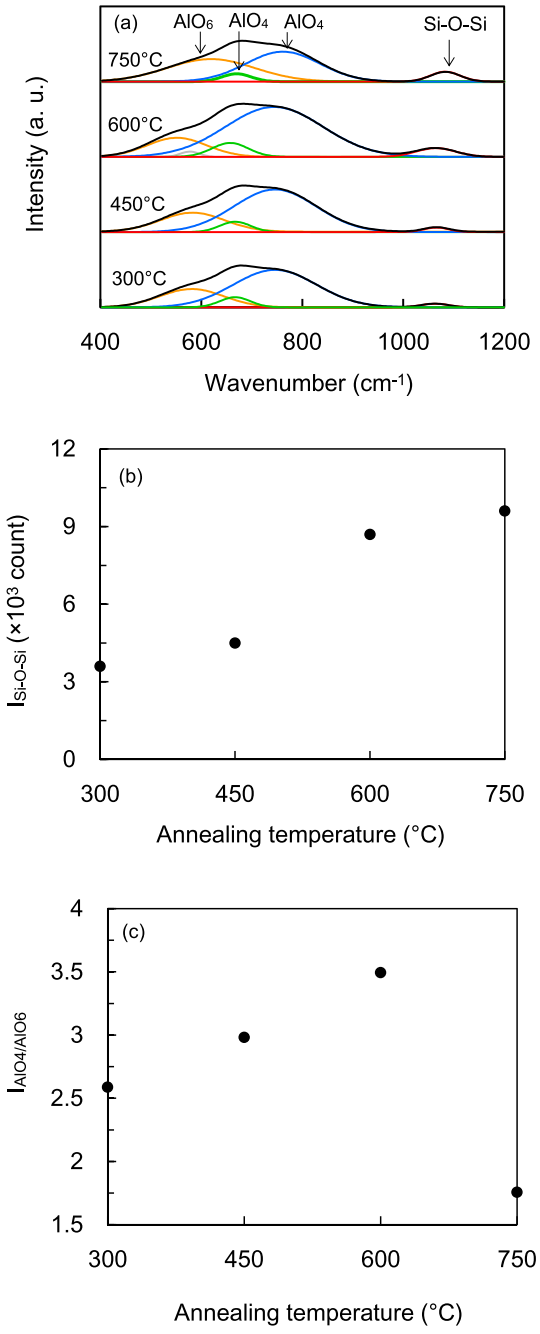

Fig. 1. (a) FTIR spectra, (b) Si—O peak intensity and (c) peak intensity ratio of AlO_4 to AlO_6 of the Al_2O_3 films annealed at different temperatures.

3. Results and discussion

Fig. 1(a) shows the FTIR spectra of the Al_2O_3 films annealed in oxygen ambient at different temperatures. In the wavenumbers of 400 to 1200 cm^{-1} the spectra can be deconvoluted into four Gaussian peaks. The peaks at 623 cm^{-1} can be assigned to the AlO_6 octahedral structure, while the peak at 667 and 774 cm^{-1} corresponds to the AlO_4 tetrahedral groups [9]. The AlO_6 and AlO_4 are the most dominant structure in Al_2O_3. The peak at around 1000–1080 cm^{-1} indicates the silicon oxide formation [10], which is usually grown as an interfacial layer between Al_2O_3 and Si wafer. A clear shift toward higher wavenumbers for Si—O peaks can be observed when the annealing temperature increase from 300 to 750 °C. This indicates that the structure of the interfacial silicon oxide is silicon-rich at low annealing