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Optical Absorption Enhancement by Mechanical Twins Grown Using Low Temperature Silicon Epitaxy

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Abstract

This paper presents the results of thin film silicon (Si) solar cells with *in-situ* doped epitaxial emitter deposited on Si substrate by rapid thermal chemical vapor deposition (CVD). High resolution transmission electron microscopy (HRTEM) images reveal that low temperature Si epitaxy growth induces mechanical twins at the junction interface. The presence of the twins alters the orientation of the crystal planes, increases the optical path length of light within the epitaxy film and improves the optical absorption. On the other hand, these twins appear to be the main cause for material-induced shunting at the *p-n* junction. Photoluminescence (PL) mapping indicate that lower growth temperature results in better interface quality.

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Keywords: Monocrystalline Si; Photoluminescence; Epitaxial; CVD

1. Introduction

In recent years, research has been focused on epitaxial thin film Si solar cells because it offers the potential in reduction of production cost and energy pay-back time [1-4]. Moreover, epitaxial emitter formation at high temperature by rapid thermal chemical vapor deposition (RTCVD) using trichlorosilane precursor is fast (e.g. ~1μm/ min) [5]. In addition, no chemical etching of the phosphorus silicate glass is needed due to *in-situ* doped Si epitaxy growth. More importantly, epitaxial emitter allows good control of emitter thickness and dopant profile for enhancement of the blue response of the solar cells. However, the outdiffusion of phosphorus (P) from Si at temperature over 1000°C has been observed in a previous study [6]. Therefore, a lower epitaxial growth temperature is favorable to minimize the dopant interdiffusion and form an abrupt *p-n* junction for wire array solar cells applications [7]. Furthermore, a good interfacial quality is critical to prevent performance degradation [8]. Therefore, in this study, we

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investigate the interfacial quality of epitaxial emitter grown on monocrystalline Si substrate, using lower thermal budget and dichlorosilane (DCS) as the gas precursor, and correlate it to its optical and electrical performance of the solar cells.

2. Experimental

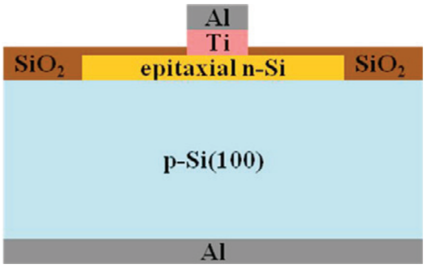

Fig. 1. Schematic of a solar cell with phosphorus-doped epitaxial emitter.

650 μm thick Czochralski Si substrates with a resistivity of 4-10 Ω.cm are first thermally oxidized. 1 cm × 1 cm Si windows, which act as a template for epitaxial growth, are then defined by photolithography and buffered oxide etch. The substrates are then cleaned with standard RCA clean to ensure a pristine growth interface prior to the epitaxial growth. Inside the RTCVD reactor, the substrates are heated *in-situ* in ultra pure H_2 at 1100°C to reduce the native surface oxides. Dichlorosilane (DCS) precursor and phosphine (PH_3) dopant gas are used for the *in-situ* phosphorus-doped epitaxial growth. Low temperature epitaxial growth is performed at 700°C and 900°C respectively, and the emitter thickness is fixed at ~600 nm. $POCl_3$ diffused (900°C) cell is also fabricated for comparison purpose. The epilayer is passivated with 10 nm thermal silicon dioxide (SiO_2) via rapid thermal oxidation. Front side contact with ~10 % optical shading are defined by photolithography and a bimetallic layer, consists of titanium (Ti) and aluminium (Al), is evaporated consecutively. Blanket Al is also evaporated on the wafer backside as contact. The cells are then subjected to forming gas anneal (FGA) at 400°C for 30 min. In order to avoid ambiguity introduced by process variations, surface texturization, antireflective coating, and back-surface field are excluded in the fabrication of the cells to allow investigation of the junction quality.

3. Results and Discussion

Table I. Solar cell parameters of 1 cm × 1 cm cells measured using a solar simulator at AM1.5G conditions at 300 K.

Process	V_{oc} (mV)	J_{sc} (mA/cm^2)	FF (%)	η (%)	FF_{pseudo} (%)	η_{pseudo} (%)	R_{shunt} (Ω)	R_{series} (Ω)
DCS 700°C	459	28.8	50.1	6.6	77.5	10.2	115	5.8
DCS 900°C	452	24.5	38.6	4.3	78.0	8.7	112	10.3

Table I presents the solar cell parameters measured using solar simulator for the 1 cm × 1 cm cells processed at different growth temperatures under AM1.5G conditions at 300 K. From Table I, we observe that both cells have low open-circuit voltage (V_{oc}) values, which can be attributed to insufficient surface passivation that leads to high surface recombination. This result correlates well to the low calculated shunt resistance (R_{shunt}) for both cells. In addition, DCS 700°C cell has higher V_{oc} than DCS 900°C cell, thus suggesting that the parasitic shunts may be material-induced and has a strong dependency on the growth temperature [8]. Aside from this, the V_{oc} value can be further improved if silicon substrate of 1 Ω.cm resistivity is used. Moreover, the low short-circuit current (J_{sc}) can be explained by the high line resistivity due to the thin top metallization (i.e. 800 nm), which corroborates well with the high calculated series resistance (R_{series}). Therefore, with the differences in *PCE*, V_{oc} and J_{sc},, DCS 700°C cell has ~50% higher efficiency than DCS 900°C cell. The highest *pseudo* efficiencies (η_{pseudo}) of these cells, predicted by the *pseudo-IV* analyses, are 10.2% and 8.7% for DCS 700°C cell and DCS 900°C cell, respectively.

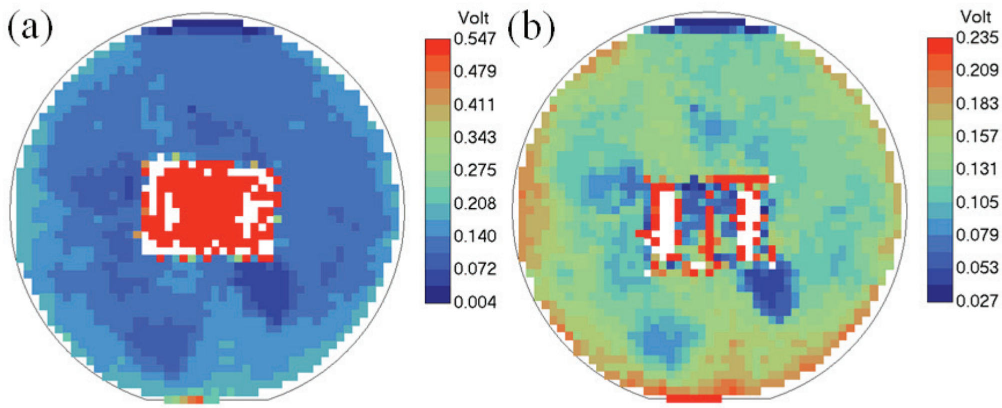

Fig. 2. Photoluminescence mapping of the solar cell with epitaxial emitter grown at (a) 700°C and (b) DCS 900°C

Photoluminescence (PL) mapping at 300 K was employed to detect the defects in the epilayer. The rectangular objects within the circle in Fig. 2 represent the cells. Fewer defects in the Si will result in more radiative recombination, and more emitted photons, and vice versa. We can see that DCS 700°C cell emits higher PL intensity as compared to the DCS 900°C cell, thus indicating that the epilayer is less defective in DCS 700°C cell.

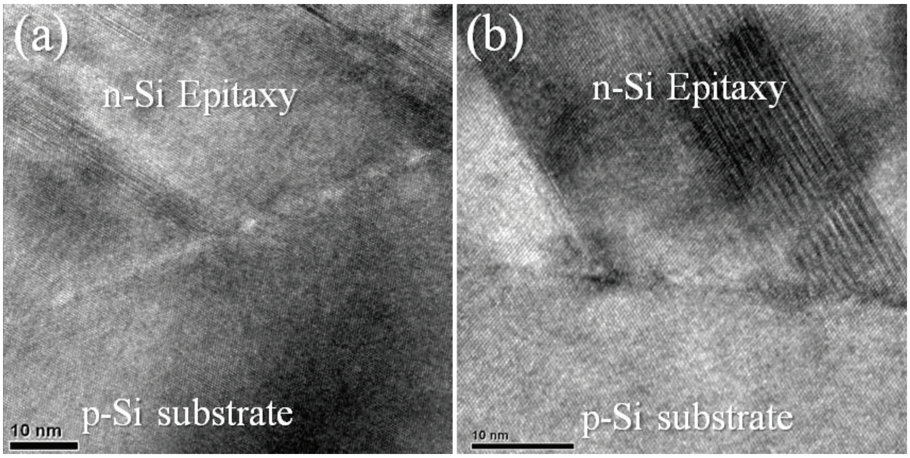

Fig. 3. Cross-sectional HRTEM images of (a) DCS 700°C cell, (b) DCS 900°C cell.

Cross-sectional high resolution transmission electron microscopy (HRTEM) analyses of the cells in Fig. 3) reveal mechanical twinning at the epitaxial emitter-substrate interface and also shows that the twinning is more severe in DCS 900°C cell. These mechanical twins may arise from the incomplete removal of oxide prior to epitaxial growth [9] and contribute to material-induced shunts due to strongly recombinative crystal defects [8], thus corresponding to the low calculated R_{shunt} values.

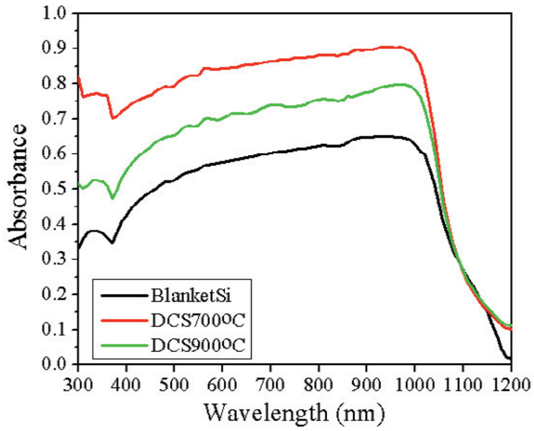

Fig. 4. Absorbance measurements of blanket p-Si substrate, DCS 700°C cell and DCS 900°C cell using UV-Vis spectroscopy.

Fig 4 shows the absorbance measurements obtained using Ultraviolet-Visible (UV-Vis) light spectroscopy. From Fig 4, we can calculate at least a ~15% reduction in light transmittance once the phosphorus-doped epitaxial emitter is grown on the p-Si substrate. This means that the presence of the mechanical twinning increases the optical path length of light due to changes in the crystallographic orientations, indirectly leading to an enhancement in optical absorption. It has been reported that high absorptance may be obtained by exposing the (111) equivalent crystallographic places in the inverted pyramids. These surface modifications can reduce reflection as well as increase the absorptance by trapping weakly absorbed light within the cell [10]. This suggests that the mechanical twins of (111) crystallographic orientation at the *p-n* interface may have led to the enhancement in optical absorption. The band-band absorption coefficient of Si at 300 K drops from 3.5 cm^{-1} at the bandgap of Si (1,103 nm) to 10^{-3} cm-1 at 1,250 nm [11]. However, in Fig. 4, the higher absorbance value at ~1200 nm wavelength for the cells with epitaxial emitters can be correlated to the presence of defects, within the epilayer, which can lead to formation of intermediate states within the bandgap.

4. Conclusion

Low temperature epitaxy growth induces mechanical twins within the Si film. Photoluminescence mapping suggests that lower temperature growth induces lesser material-induced shunts at the *p-n* junction. On the other hand, twinning alters the orientation of the crystal planes and increases the optical path length of light within the epitaxy film, thus improving optical absorption. More work is ongoing to optimize the competing effects between optical absorption enhancement and material-induced shunting before future integration of epitaxy emitter with wire array solar cells.

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