Improvement of Electrical Properties of Silicon Quantum Dots Superlattice Solar Cells with a Dopant Diffusion Barrier Layer

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1. Introduction

Silicon quantum dots superlattice (Si-QDSL) solar cells are attracted as one of the noble concept solar cells [1]. Si-QDSL has the structure that the size-controlled silicon quantum dots (Si-QDs) are embedded in a wide bandgap material periodically. By controlling the size of Si-QDs, the bandgap of the Si-QDSL can be tuned [2].

The open-circuit voltage (V_{oc}) of 518 mV has been achieved in superstrate-type Si-QDSL solar cells [3]. However, the short circuit current density (J_{sc}) has been only 0.3 mA/cm². This small J_{sc} is probably due to the diffusion of phosphorus atoms from a doped layer into a Si-QDSL layer during high temperature thermal annealing to form Si-QDs in a Si-QDSL layer. It was reported that niobium doped titanium dioxide (TiO₂:Nb) has the diffusion barrier effect against phosphorus atoms [4]. In this study, the substrate-type solar cells with a TiO₂:Nb diffusion barrier layer between the Si-QDSL layer and the doped layer were fabricated. A high V_{oc} of 529 mV and high J_{sc} of 1.60 mA/cm² were achieved simultaneously.

2. Experimental

The structure of fabricated solar cell is shown in Fig. 1. This solar cell has substrate-type p-i-n structure using Si-QDSL as the absorption layer. The fabrication process of this structure is noted below. At the beginning, a phosphorus doped hydrogenated amorphous silicon (n-a-Si:H) was deposited on a quartz substrate by plasma enhanced chemical vapor deposition (PECVD). The n-a-Si:H layer was converted into the phosphorus doped poly-crystalline silicon (n^{++} -poly-Si:P) by thermal annealing at 900 °C for 30 min under forming gas atmosphere. A TiO₂:Nb layer was deposited on the n^{++} -poly-Si:P by radio frequency (RF) sputtering using a TiO2:Nb target (TiO2 92 wt%, Nb2O5 8 wt%). The flow rate and pressure of argon gas, deposition temperature, and power density were 10 sccm and 1.0 Pa, 25 °C, and 1.8 W/cm², respectively. The thickness was 2 nm. An amorphous superlattice which consisted of oxygen containing silicon rich hydrogenated amorphous silicon carbide (a-Si_{1+x}C:H:O) and oxygen containing stoichiometric hydrogenated amorphous silicon carbide (a-SiC:H:O) was deposited on the TiO₂:Nb layr by PECVD. The source gases were silane (SiH₄), monomethylsilane (MMS), hydrogen (H_2) , and carbon dioxide (CO_2) . The flow rates of SiH₄, MMS, H₂, and CO₂, deposition pressure,

temperature, frequency and plasma power density were 5 sccm, 2.5 sccm, 47 sccm, 0.5 sccm, 20 Pa, 193 °C, 60 MHz and 13 mW/cm² respectively. The flow rate of SiH₄ was controlled at 0 and 5 sccm alternately and periodically. The thicknesses of each a-Si_{1+x}C:H:O layer and each a-SiC:H:O layer were 5 nm and 2 nm, respectively. After the deposition, the sample was annealed at 900 °C for 30 min under forming gas atmosphere and 5-nm-Si-QDs were formed in the a-SiC:O matrix. Subsequently, the sample was exposed to hydrogen plasma for 2 hours to reduce the defects in the annealed Si-QDSLs. The flow rate of H₂, pressure, temperature, frequency and plasma power density were 200 sccm, 800 Pa, 320 °C, 60 MHz and 1.95 W/cm², respectively. A hydrogenated boron-doped amorphous silicon (p-a-Si:H) layer and an indium tin oxide (ITO) layer were deposited on the Si-QDSL layer by PECVD and RF sputtering, respectively. Finally, aluminum grid electrodes were evaporated on the sample. The thicknesses of each layer are shown in Fig. 1. For comparison, the solar cells without the TiO₂:Nb diffusion barrier layer was also fabricated. The solar cells were characterized by light I-V and quantum efficiencies measurements. The I-V measurements were performed under the AM1.5G illumination at a temperature of 25 °C.



Fig. 1 Structure of substrate-type Si-QDSL solar with TiO₂:Nb diffusion barrier layer.

3. Results and Discussion

Light *I-V* characteristics of solar cells without and with the TiO₂:Nb layer are shown in Fig. 2. The parameters of *I-V* characteristics are also summarized in Table I. The improvement of fill factor (*FF*) clearly indicates that the 2-nm-thick TiO₂:Nb phosphorus diffusion barrier layer does not block electron transport from the Si-QDSL to n^{++} -poly-Si:P layer. This is very important point for the device application of the TiO₂:Nb layer.

The insertion of the TiO2:Nb layer also improved the other solar cell parameters. A V_{oc} of 529 mV and a J_{sc} of 1.60 mA/cm² were achieved by using the TiO_2 :Nb layer. This improvement is due to the suppression of shrinking the thickness of the absorption layer by the diffusion of phosphorus atoms in a Si-QDSL layer. SIMS measurements revealed that the phosphorus concentration of a Si-ODSL layer of an annealed sample increased to around 4×10^{19} cm⁻³ without a TiO₂:Nb layer. This indicates that the Si-QDSL layer of the solar cell must be strongly n-type and near almost all electric field is applied the p-a-Si:H/Si-QDSL interface. This means that only carrier generated near the interface can contribute to photocurrent of the solar cell. On the other hand, when a 10-nm-thick TiO₂:Nb phosphorus diffusion barrier layer was inserted, the phosphorus concentration of a Si-ODSL layer of an annealed sample was found to be around 5×10^{16} cm⁻³. This suggests that 2-nm-thick TiO₂:Nb also has some diffusion barrier effect. If the TiO₂:Nb layer effectively prevents phosphorus diffusion and keep the Si-QDSL layer intrinsic, it is expected that electric field is applied in the whole Si-QDSL layer for the solar cell with the TiO₂:Nb layer.

Table I Parameters of the fabricated solar cells.

Parameters	Without TiO ₂ :Nb	With TiO ₂ :Nb
V_{oc} (mV)	328	529
J_{sc} (mA/cm ²)	0.18	1.60
FF	0.28	0.46
Eff. (%)	0.016	0.39



Fig. 2 Light I-V characteristics of the fabricated solar cells with and without TiO₂:Nb.



Fig. 3 Internal quantum efficiency of the fabricated solar cells with and without TiO₂:Nb.

This explanation is justified by internal quantum efficiency (*IQE*) measurements. Figure 3 shows the *IQEs* of the Si-QDSL solar cells with and without the TiO₂:Nb layer. The *IQE* of the solar cell with the TiO₂:Nb layer was improved in the whole visible wavelength region compared with that of the solar cell without TiO₂:Nb. It is clearly seen that the both *IQEs* decay to zero at a wavelength of around 700 nm. This wavelength corresponds to the bandgap of Si-QDSL [2], indicating that carriers generated in the n⁺⁺-poly-Si layer does not contribute to the photocurrent of the solar cells. Therefore, the improvement of J_{sc} is associated with the improvement of carrier collection properties in the Si-QDSL layer.

4. Conclusions

The J_{sc} of Si-QDSL solar cells was significantly improved by inserting a 2-nm-thick TiO₂:Nb layer which works as a phosphorus diffusion barrier. The V_{oc} and FF of the solar cells were also improved by the insertion. This results clearly indicates that TiO₂:Nb phosphorus diffusion barrier layer effectively suppresses phosphorus diffusion into Si-QDSL to n⁺⁺-poly-Si:P layer.

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