

## Investigation of interface state density and fixed charge of $\text{Sr}_x\text{SiO}_{x+2}$ on the $2 \times 1$ Sr-reconstructed Si substrate

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### Abstract

We investigated physical properties of Sr-silicate ( $\text{Sr}_x\text{SiO}_{x+2}$ ) films on Si substrates for interface state density ( $D_{it}$ ) and fixed charge (FC) state. The  $\text{Sr}_x\text{SiO}_{x+2}$  films were made from SrO layers by silicate reaction using Si atoms diffusing from the Si substrates. The SrO layers were deposited on  $2 \times 1$  Sr-reconstruction surface of the Si substrates. The  $D_{it}$  and the effective FC density ( $Q_{eff}$ ) of the  $\text{Sr}_x\text{SiO}_{x+2}/\text{Si}$  samples were measured for various thicknesses of the  $\text{Sr}_x\text{SiO}_{x+2}$  film by capacitance-voltage (C-V) measurements. For the samples on the  $2 \times 1$  Sr-reconstruction surface, the  $D_{it}$  was almost constant against the increase of the  $\text{Sr}_x\text{SiO}_{x+2}$  film thickness. (On the other hand, the  $D_{it}$  of the samples on H-terminated Si substrates, which were prepared by the conventional HF-etching, increases with increasing the thickness.) Furthermore, the  $Q_{eff}$  of  $\text{Sr}_x\text{SiO}_{x+2}$  films continuously increases with increasing the thickness. This result indicates that the  $2 \times 1$  Sr-reconstruction surface is quite effective to improve the  $D_{it}$  and FC state of the  $\text{Sr}_x\text{SiO}_{x+2}/\text{Si}$  structure.

### 1. Introduction

Recent solar cell industry has required to reduce the production cost of crystalline silicon (c-Si) solar cells. To achieve this request, it is necessary to reduce the usage of Si materials, because the cost accounts for a half of the cell cost. Then, use of thinner Si wafers (the estimated thickness from the viewpoint of the material cost is below  $100\mu\text{m}$ ) is one of the candidate of the cost reduction. To use the thin wafer, however, exposes a serious problem that the conversion efficiency of the solar cells was limited by surface recombination losses at the semiconductor interfaces due to the multiple reflection of sunlight. Hence, surface passivation becomes more important to improve the efficiency of the thin c-Si solar cell.

Field-effect passivation (FEP) is one of promising technique to solve the problem. [1] In the FEP, an internal electric field arising from presence of fixed charges (FCs) in the passivation layer repels the repulsive polarity of the minority carriers from the semiconductor interface. As a result, the carrier concentration decreases at the interface, and the surface recombination loss decrease. Recently, the FEP has been intensively studied for  $\text{AlO}_x$ . [2] However, the detail mechanism of the FEP and the origin of the FCs in passivation layers such as  $\text{AlO}_x$  were still unclear.

We have studied Sr-silicate (or  $\text{Sr}_x\text{SiO}_{x+2}$ ) as a candidate of the passivation layer materials, because the  $\text{Sr}_x\text{SiO}_{x+2}$  film fabricated on Si substrate has FCs of  $\sim 10^{12}\text{cm}^{-2}$ . Sr-silicate thin films can be fabricated on Si substrate

without interfacial  $\text{SiO}_x$  layer due to the reduction property of the Sr atoms to silicon. This means that the sample structure is simplified to single layer model as shown Fig.1 (In the  $\text{AlO}_x$  case,  $\text{SiO}_x$  layer is formed at the interface and the structure is more complicated.) Hence, we considered that the Sr-silicate is suitable for investigation of the detail mechanism of the FEP. There, however, exists a problem which is the interface state density ( $D_{it}$ ) of  $\text{Sr}_x\text{SiO}_{x+2}/\text{Si}$  structure increases with increasing the  $\text{Sr}_x\text{SiO}_{x+2}$  film thickness. We considered that the increase of  $D_{it}$  is caused by the initial surface state of the Si substrate.

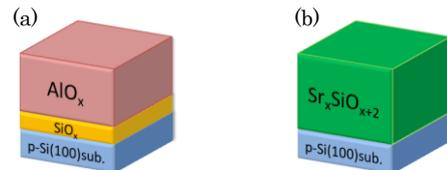


Fig. 1 Schematic illustrations of each interface structure for (a)  $\text{AlO}_x/\text{Si}$  interface and (b)  $\text{Sr}_x\text{SiO}_{x+2}/\text{Si}$  interface.

In this study, we demonstrated the use of  $2 \times 1$  Sr-reconstructed Si substrates and investigated the physical properties of  $\text{Sr}_x\text{SiO}_{x+2}$  films on the reconstructed-Si substrate for  $D_{it}$  and FC states. Sr-silicate films were fabricated by silicate reaction of SrO films with Si atom (diffusing from Si substrate) via post annealing treatment (PAT). The  $D_{it}$  and FC states of the  $\text{Sr}_x\text{SiO}_{x+2}$  films were characterized by capacitance-voltage (C-V) measurements. From the obtained data, we evaluated the effect of the  $2 \times 1$  Sr-reconstruction surface to improve the interface properties of the  $\text{Sr}_x\text{SiO}_{x+2}/\text{Si}$  structure.

### 2. Experiments

p-type c-Si(100) wafers (CZ,  $\rho=1-10\Omega\text{cm}$ ) were used as the substrates. All of the Si(100) wafers (size of  $0.8 \times 0.8\text{cm}^2$ ) were cleaned by the conventional RCA method. the  $2 \times 1$  Sr-reconstruction surface was fabricated by annealing at  $720^\circ\text{C}$  for 1min and an equivalent SrO layer thickness ( $\text{ML}_{eq}$ ) of 2.5  $\text{ML}_{eq}$ . [3] A reflective high-energy electron diffraction (RHEED) system with incident energy of 20 kV was used to monitor the structure of the sample surface during of fabrication of the  $2 \times 1$  Sr-reconstruction surface. Sr-silicate was fabricated by growing SrO layers on Si substrates and by annealing the SrO/Si structures. The SrO layers were grown on the Si substrates by PLD using a SrO single crystal target in a vacuum of  $< 1 \times 10^{-6}\text{Pa}$  at room temperature (RT). The thicknesses were from 2.5nm to 25nm. Post annealing treatments were done in oxygen atmosphere using a tube furnace. The annealing temperature was  $600^\circ\text{C}$  and annealing time was 360 min. Figure 2

shows the sample structure. Au thin films were deposited as the top electrodes with 400 $\mu$ m square using a metal etching mask at RT. C-V characteristics were measured using an LCR meter. XPS measurements were performed using an Al K $\alpha$  hv=1486.6 eV x-ray source in a vacuum below 10<sup>-7</sup> Pa at RT.

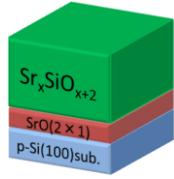


Fig. 2 sample structure

### 3. Result and discussion

Figure 3 shows the typical evolution of the RHEED pattern recorded along the [110] Si azimuth at each step during the fabrication of a SrO-buffered Si substrate. Figure 3 (a) shows the RHEED pattern of a clean Si (100) surface which was obtained after RCA cleaning. The diffraction pattern vanished after the SrO layer growth, as shown in Fig. 3 (b). This means that the SrO layer was grown in amorphous. After annealing the SrO/Si structure at 720 $^{\circ}$ C for 1 minute, the diffraction pattern recovered, as shown in Fig. 3 (c). Additional streaks appear half-way between the [00] and [01](or [0-1]) streaks, and this change indicates the formation of the 2 $\times$ 1 Sr-reconstruction surface.

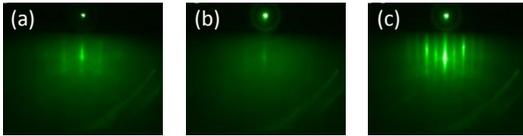


Fig. 3 (a)-(c) RHEED patterns recorded along Si[110] azimuth. (a) Si(100) substrate, (b) as-deposited surface of 2.5ML<sub>eq</sub> of SrO layer, and (c) after annealing at 720 $^{\circ}$ C for 1 min.

The interface structure of the annealed SrO(4 nm)/Si(100) samples was investigated by XPS. Figure 4 shows the Si 2p core-level spectra of the SrO/Si(100) sample and the SiO<sub>2</sub>/Si(100) sample prepared by thermal annealing. We have fitted the core-level spectra by Gaussian curves. For each spectrum, the experimental curves were well described by five components, Si<sup>0</sup>, Si<sup>1+</sup>, Si<sup>2+</sup>, Si<sup>3+</sup>, and Si<sup>4+</sup>, shown by each dashed line in Fig.2. The binding energies were in reference to Ref. 4. As seen by the significant doublet the substrate peaks of the Si substrates at 98.2 eV in both spectra, the overlayers were thin enough to obtain the spectra from the interface. The broad peaks located at higher binding energy side of the substrate peaks correspond to the over layer Si atoms, which are constructed of Si<sup>1+</sup> - Si<sup>4+</sup>. The Si<sup>4+</sup> peaks of the Sr<sub>x</sub>SiO<sub>x+2</sub>/Si(100) sample was detected at lower binding energy side comparing with that of the SiO<sub>2</sub>/Si(100) sample. It indicates that a silicate layer is formed in the sample and the SiO<sub>2</sub> layer absents at the interface. From this result, we could obtain Sr<sub>x</sub>SiO<sub>x+2</sub>/Si(100) structure at without interface SiO<sub>x</sub> layer. [4-5]

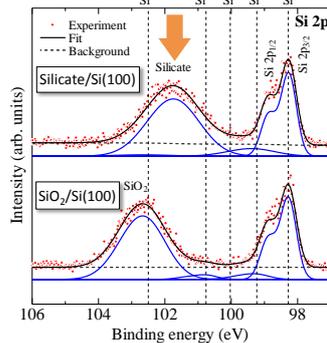


Fig. 4 Si2p core-level spectra for the Silicate/Si(100) and SiO<sub>2</sub>/Si(100).

We measured the C-V characteristics of the Sr<sub>x</sub>SiO<sub>x+2</sub>/Si samples. The D<sub>it</sub> and the effective FC density (Q<sub>eff</sub>) were estimated from the high-low method and the flat band shift voltage of the C-V curves. Figure 5 (a) and (b)

show the obtained C-V curves at the measurement frequency of 1MHz and the normalized C-V curve of the 25nm thick-samples with or without the 2 $\times$ 1 treatment, respectively. From fig.5 (b), in the case of the 2 $\times$ 1 treatment, the sharp slope and the small hysteresis width were observed in the C-V curve.

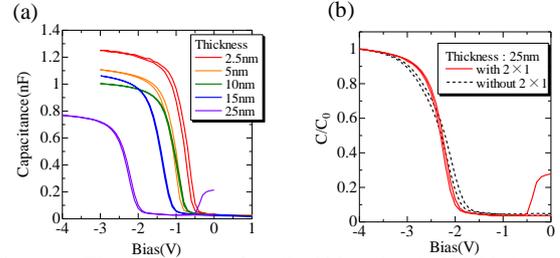


Fig. 5 (a) The C-V curve of Au/Sr<sub>x</sub>SiO<sub>x+2</sub>/2 $\times$ 1/p-Si(100)/Au sample of various Sr-silicate thicknesses. (b) C-V curve of Sr-silicate thickness 25nm at with 2 $\times$ 1 and without 2 $\times$ 1.

Figure 6 shows the D<sub>it</sub> values as a function of Sr<sub>x</sub>SiO<sub>x+2</sub> film thickness. The D<sub>it</sub> decrease with increasing the thickness up to 10nm, and it becomes constant above 10nm. We considered that the defect layer which exists around the interface region decreased due to the passivation effect of the 2 $\times$ 1 Sr-reconstructed structure. Figure 7 shows the Q<sub>eff</sub> values as a function of Sr<sub>x</sub>SiO<sub>x+2</sub> film thickness. The Q<sub>eff</sub> of the Sr<sub>x</sub>SiO<sub>x+2</sub> films with the 2 $\times$ 1 treatment slightly increases comparing with the without sample and proportionally increases above 15 nm. We considered that the Q<sub>eff</sub> increases arise from the decrease of the compensated charges due to the decrease of the defect layer. Hence, the 2 $\times$ 1 Sr-reconstructed treatment is effective to improve the D<sub>it</sub> and the FC states of Sr<sub>x</sub>SiO<sub>x+2</sub>/Si samples.

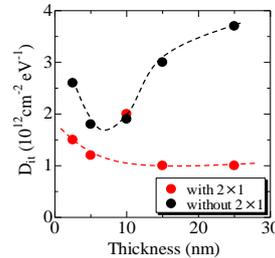


Fig.6 Thickness dependence of the D<sub>it</sub> of the Sr<sub>x</sub>SiO<sub>x+2</sub>/Si(100) structure.

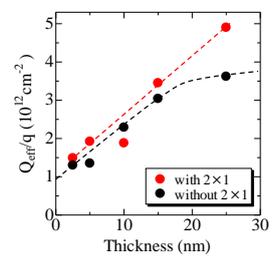


Fig.7 Thickness dependence of the Q<sub>eff</sub> of the Sr<sub>x</sub>SiO<sub>x+2</sub>/Si(100) structure.

### 4. Conclusions

We investigated D<sub>it</sub> and FC of Sr-silicate film on silicon substrate which was fabricated 2 $\times$ 1 Sr-reconstruction surface. By using the 2 $\times$ 1 Sr-reconstructed Si substrates, increase of D<sub>it</sub> was prevented, even increasing the Sr<sub>x</sub>SiO<sub>x+2</sub> thickness, and the Q<sub>eff</sub> continuously increases with increasing the thickness. This result indicates that 2 $\times$ 1 Sr-reconstruction surface is important for the Sr<sub>x</sub>SiO<sub>x+2</sub> passivation layers on Si surface to improve the D<sub>it</sub> and the FC states.

### References

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