Extended Abstracts of the 2015 International Conference on Solid State Devices and Materials, Sapporo, 2015, pp540-541

Investigation of the Optical Absorption in Si/SiO_2 Superlattice for the Application to Solar Cells

Shigeru Yamada[1], Makoto Konagai[1,2] and Shinsuke Miyajima[3]

[1] Japan Science and Technology Agency
FREA Main Bldg.,4F
2-2-9, Machiikedai, Koriyama, Fukushima 963-0215, Japan
Phone: +81-24-963-0837 E-mail: sigeru.yamada@pb.jst.jp
[2] Tokyo City Univ.
8-15-1, Todoroki, Setagaya-ku, Tokyo 158-0082, Japan
[3] Tokyo Institute of Technology
2-12-1-NE-17, O-okayama, Meguro-ku, Tokyo 152-8552, Japan

Abstract

The optical properties of Si/SiO_2 superlattices were investigated by optical absorption method. The optical bandgap shifted to higher energies by reducing Si-layer thickness. The annealing temperature also affects the optical bandgap. We found that the optical bandgap can be tuned from 1.1 eV to 2.1 eV by adjusting the annealing temperature and the Si-layer thickness.

1. Introduction

The conversion efficiency of 25.6 % has been achieved in a crystalline silicon (c-Si) solar cell [1]. To achieve Si-based solar cells with higher efficiency, a tandem structure using Si-based top and bottom cells needs to be developed. One of the promising materials as the top cell of the tandem cells is a nanostructured material such as quantum wells, quantum nanowires, and quantum dots using silicon related materials. The bandgaps of these materials are tunable based on quantum size effect [2]. A silicon/silicon dioxide superlattice (Si/SiO_2 SL) also has the potential for the absorber layer in the top cell.

Many researchers have estimated the optical bandgaps of SLs by photoluminescence (PL) method [3]. We also have reported the peak shift of PL spectrum [4]. However, it is difficult to precisely evaluate the optical bandgap of SLs by PL method due to the unintentional light emission from sub-oxide defects. In this study, the optical bandgap of the Si/SiO_2 SL was investigated by reflectance and transmittance measurements. The dependence of the absorption coefficient on the annealing temperature and the Si-layer thickness in a SL were investigated.

2. Experimental

Si/SiO_2 SLs were prepared by magnetron sputtering on Si substrates and quartz substrates. The Si/SiO_2 SL was prepared by sputtering of a Si-target in argon (Ar) and argon+oxygen ($Ar+O_2$). To investigate the dependence of the optical bandgap on the Si-layer thickness, the SLs with the thicknesses of 3.0 nm, 5.5 nm and 7.9 nm were prepared. The SiO_2-layer thicknesses of each sample were fixed at 2.2 nm. The deposition pressure, the deposition temperature, and the plasma power density were 1.0 Pa, 25 ºC, and 2.36 W/cm^2, respectively. The samples were annealed at 900 ºC, 1000 ºC, and 1100 ºC for 2 hours under forming gas (N_2:H_2=97 %:3 %) atmosphere. The crystallinity of the SL and the status of Si-O bonding were characterized by Raman scattering spectroscopy and Fourier transform infra-red (FT-IR) spectroscopy, respectively. The reflectance and transmittance of the SL were measured by ultraviolet-visible (UV-VIS) spectroscopy.

3. Results and Discussion

The absorption coefficient was calculated by the following equation:

$$\alpha = -\frac{1}{d}\ln\left(\frac{T}{1-R}\right) \qquad (1)$$

, where T, R, and d is the transmittance, the reflectance, and the thickness of a thin film. Under the assumptions that the density of states at the edges of the conduction band and the valence band can be approximated by parabolic shape, and k-selection rule is relieved in the nanostructures, the optical bandgap can be estimated by

$$\alpha h\nu = A\left(h\nu - E_g\right)^2 \qquad (2)$$

, which is known as Tauc model. Here, A, h, and ν are proportionality coefficient, Planck's constant and photon frequency, respectively.

Figure 1 shows the Tauc plots of the SLs, whose Si-layer thickness is 3.0 nm, for the annealing temperatures of 900 ºC, 1000 ºC and 1100 ºC, respectively. The absorption spectrum shifts to higher photon energies as the annealing temperature increases. FT-IR results indicated that sub-oxide phases in the sample decreased as the annealing temperature increased. These FT-IR results suggest that the sub-oxide phases, located near the Si/SiO_2 interface, changed to the stoichiometry phase. Additionally, the shape of the Tauc plot changes near the absorption edge with increasing annealing temperature. This thought to be related to the growth of nano-crystalline silicon. From the Raman spectra of the SLs for each annealing temperature, the TO-phonon peak centered between 510 cm^{-1} and 520 cm^{-1} originating from c-Si phase could not be found for the SL with the annealing temperature of 900 °C. On the other hand, the peak was observed for the SL with the annealing temperature of 1000 °C, which means that c-Si phase exists. The amount of c-Si phase increased more when the annealing temperature was 1100 °C. The dashed lines in Fig. 1 indicate the interpolation lines based on Eq. (2). For the as-deposited SL and the 900 °C-annealed SL, which mainly consist of amorphous phase, show only one slope at $(\alpha h\nu)^{1/2}$ from 150 to 600 $eV^{1/2}cm^{-1/2}$. On the other hand, for the 1000 °C-annealed and 1100 °C-annealed SLs, the two different slopes were observed in this $(\alpha h\nu)^{1/2}$ range. This change reflects the structural change observed by Raman measurements. The estimated bandgaps for each SL with the annealing temperatures of 900 °C, 1000 °C and 1100 °C were 1.83 eV, 1.83 eV, and 2.07 eV.

Figure 2 shows the Tauc plots of the SLs with the Si-layer thicknesses of 3.0 nm, 5.5 nm, and 7.9 nm, respectively, where the annealing temperature is 1100 °C. The estimated bandgaps for each Si-layer thickness and each annealing temperature are summarized in Table I. The bandgap shift was confirmed. Moreover, it was revealed that the bandgap between 1.1 eV and 2.1 eV can be realized in the Si/SiO_2 SL. As the Si-layer thickness decreased, the increase of the bandgap for higher annealing temperature was enhanced. This suggests that the existence of SiO_2-layers or Si/SiO_2 interface influences the bandgap. Therefore, we can conclude that the bandgap of Si/SiO_2 SL is influenced by the nano-crystalline silicon phase and the sub-oxide phase.

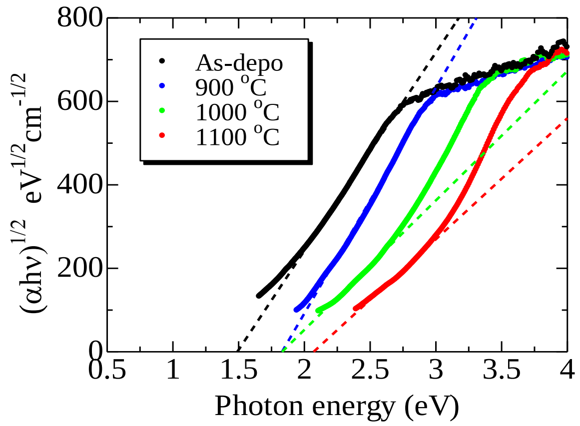

Fig. 1 Tauc plots of the Si/SiO_2 SLs with the Si-layer thickness of 3.0 nm for several annealing temperatures.

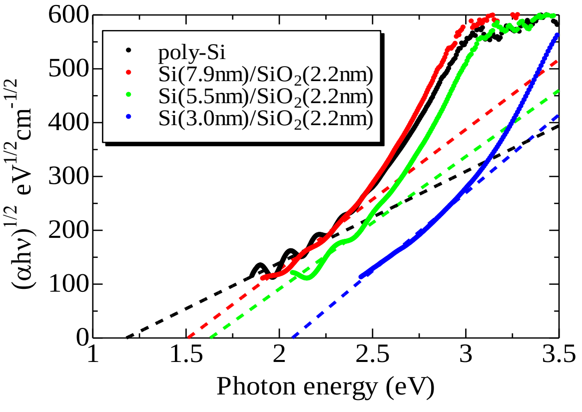

Fig. 2 Tauc plots of the Si/SiO_2 SLs with the Si-layer thicknesses of 3.0 nm, 5.5 nm and 7.7 nm for the annealing temperature of 1100 °C.

Table I Estimated bandgaps of the SLs for several annealing temperatures and several Si-layer thicknesses.

Si-thickness	1000 °C-annealed	1100 °C-annealed
poly-Si	1.17 eV	1.18 eV
7.9 nm	1.45 eV	1.51 eV
5.5 nm	1.54 eV	1.63 eV
3.0 nm	1.83 eV	2.07 eV

4. Conclusions

The optical bandgap of Si/SiO_2 was investigated using optical absorption method and Tauc model. The bandgap shift from 1.1 eV to 2.1 eV was confirmed. The bandgap is mainly influenced by the increase of nano-crystalline silicon phase and the decrease of sub-oxide phase.

Acknowledgements

This work was supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT), FUTURE-PV Innovation. We would like to express sincere thanks for their support.

References

[1] "Panasonic HIT® solar cell achieves world's highest energy conversion efficiency of 25.6% at research level", Public Reations Development Office, Panasonic Corp., Osaka, Japan, Apr. 2014.

[2] T. Tiedje, B. Abeles, D. Persans, B.G. Brooks, and G.D. Cody, "Bandgap and Resistivity of Amorphous Semiconductor Superlattices", *J. Non-Cryst. Solids* **66** (1984) 345-350.

[3] B. T. Sullivan, D. J. Lockwood, H. J. Labbe, and Z.-H. Lu, "Photoluminescence in amorphous Si/SiO_2 superlattice fabricated by magnetron sputtering", *Appl. Phys. Lett.* **69** (1996) 3149-3151.

[4] T. Higa, R. Ishikawa, S. Miyajima, and M. Konagai, "Properties of Si/SiO2 superlattice nanodisc array prepared by nanosphere lithography", *Proc. SPIE 9178 Next Generation Technologies for Solar Energy Conversion V* 91780P (2014).