

Improvement of photoresponsivity of passivated BaSi₂ thin film layers by hydrogenated amorphous Si using radio-frequency H₂ plasma

Zhihao Xu¹, Kazuhiro Gotoh², Tianguo Deng¹, Takuma Sato¹, Kaoru Toko¹, Noritaka Usami² and Takashi Suemasu¹

¹ Univ. of Tsukuba
Institute of Applied physics
Ibaraki 305-8573, Japan

² Nagoya. Univ.
Graduate school of Engineering
Nagoya 464-8603, Japan

Phone: +81-29-8535-472 E-mail: suemasu@bk.tsukuba.ac.jp

Abstract

Hydrogenated amorphous silicon (a-Si:H) layers were formed on Si (111) substrates by an electron-beam evaporation of Si and subsequent supply of atomic hydrogen using a radio-frequency (RF) plasma generator. The hydrogen concentration was 10^{21} cm^{-3} by secondary ion mass spectrometry. The appearance of Si-H bonds was confirmed by Raman spectroscopy. Next, we studied the surface passivation effect of a-Si:H layers on 500-nm-thick BaSi₂. The internal quantum efficiency of the BaSi₂ films capped with a 3-nm-thick a-Si:H layers was improved by a factor of 4 compared to those capped with the pure a-Si layer.

1. Introduction

Semiconducting material BaSi₂ is regarded as a promising material for thin solar cell application, because of the suitable band gap (E_g) (ca. 1.3 eV), high absorption coefficient (α) $3 \times 10^4 \text{ cm}^{-1}$ at 1.5 eV, inactive boundaries, large minority carrier lifetime (τ) and diffusion length (L) [1]. In 2016, our group has achieved the conversion efficiency (η) approaching 10% by using of the structure of p-BaSi₂/n-Si heterojunction. On the top surface, the pure amorphous Si (a-Si) was applied to prevent oxidation of the BaSi₂ and act as a good path for hole transport [2]. According to CAICISS measurement and the first principle calculation, BaSi₂ epitaxial film is terminated by Si₄ tetrahedra and Si vacancies in Si₄ tetrahedra are more likely to exist as native point defects [3]. Besides that, a large amount of dangling bond exists in a-Si and work as defects. Both point defects and dangling bonds degrade the BaSi₂ solar cell performance. Thus, an alternative passivation layer should be investigated. From the viewpoint of surface passivation, the hydrogenated amorphous Si (a-Si:H) is preferable to passivate BaSi₂. The conventional method to fabricate a-Si:H layer is plasma enhanced chemical vapor deposition [4], where silane is decomposed by radio frequency (RF) plasma. In this work, a new and easy method was applied to form a-Si:H by molecular beam epitaxy (MBE) and RF plasma generator. Internal quantum efficiencies (IQE) of BaSi₂ were improved drastically by a factor of 4 compared to those capped with the pure a-Si.

2. General Instructions

We used an ion-pumped MBE system equipped with a standard Knudsen cell for Ba, an electron-beam gun for Si, and an RF plasma source for atomic hydrogen. Firstly, we tried to deposit 150-180-nm-thick a-Si:H on Si substrate covered by 200-nm-thick aluminum. The Al layer eliminates the signals associated with the Si substrate. In this work, the post-deposition (PD) method and the co-deposition (CD) method were applied. In the CD method, we deposited Si and H atoms simultaneously. On the other hand, in the PD method, H atoms were supplied after a-Si deposition. The same substrate temperature (T_s) was kept at 180 °C in both methods. For comparison, we also formed a pure a-Si layer on Al/c-Si substrate with the same T_s . Next, the a-Si and a-Si:H layers were applied to 500-nm-thick undoped BaSi₂ epitaxial films by MBE on a low-resistivity CZ-n⁺-Si(111) substrate ($\rho < 0.009 \Omega\text{cm}$) for photoresponse measurement. For one sample, a 3-nm-thick a-Si capping layer was deposited at 180 °C as a reference. For other sample, 3-nm-thick a-Si:H layers were formed at 180 °C by the CD and PD methods. After that, 80-nm-thick indium-tin-oxide (ITO) with a diameter of 1 mm and 150-nm-thick Al were sputtered on the front side and back side respectively as electrodes. Details of samples preparation are shown in Table I. Photoresponse spectra were evaluated by a lock-in technique using a xenon lamp with a 25-cm-focal-length single monochromator (Bunko Keiki, SM-1700A and RU-60N). The light intensity of the lamp was calibrated using a pyroelectric sensor (Melles Griot, 13PEM001=J). The depth profile of H atoms was characterized by secondary ion mass spectrometry (SIMS) by using Cs ions. Raman spectra were measured by Raman spectrometer (JASCO, NRS-5100) using a frequency doubled Nd: YAG laser (532 nm, 5.1 mW). The spectral resolution was not worse than 4.2 cm^{-1} . All measurements were performed at room temperature.

The Raman spectra of the substrate (Al/c-Si) and samples A-C are shown in Fig. 1. The transverse acoustic (TA) phonon and transverse optical (TO) phonon of Si-Si bonds in a-Si can be seen at around 180 cm^{-1} and 480 cm^{-1} respectively in all the samples except the substrate in the topmost of Fig. 1, meaning a-Si layers were formed [5]. The peak at around 2000 cm^{-1} caused by vibration of Si-H bonds was appeared in

samples B and C, indicating the Si-H bonds were formed by the irradiation of hydrogen plasma in both CD and PD methods. The peak at around 2090 cm^{-1} due to the stretching vibration of Si-H₂ bonds existed in sample B only, implying that the Si-H₂ bonds were formed by the CD method. Based on these results that the a-Si:H layers were formed by the MBE and RF plasma generator. Furthermore, the PD method is more favorable to passivate dangling bonds than the CD method, because, Si-H₂ bonds affect solar cell performance according to Nakamura *et al.* [6].

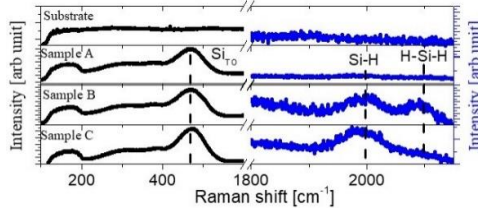


Fig. 1 Raman spectra of substrate, a-Si, and a-Si:H grown under the different fabrication methods and conditions.

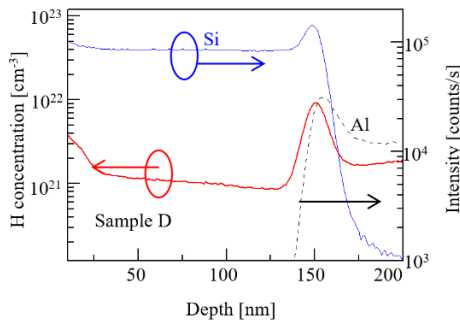


Fig. 2 Hydrogen depth profile of sample D

Figure 2 shows the SIMS depth profile of H atoms and secondary ions (Si, Al) intensities in sample D, formed by the PD method. The H concentration is approximately $1 \times 10^{21}\text{ cm}^{-3}$, distributing uniformly from 30 to 120 nm.

Figure 3 shows the *IQE* spectra of samples measured at $V_{\text{bias}} = -0.3\text{ V}$. The *IQE* is improved by capping with a-Si:H layers formed by the CD method and further improved for samples G and F capped with a-Si:H layers by the PD method in Fig. 3. These results provide a strong evidence that a-Si:H

is better than the pure a-Si for passivation of BaSi₂. As for the CD method, we speculate that hydrogen atoms stroke the BaSi₂ surface at the beginning of the forming of a-Si:H layers and hence *IQE* is suppressed compared to those formed by the PD method.

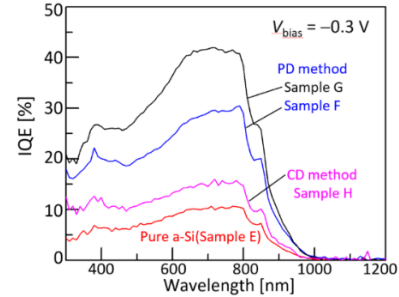


Fig. 3 *IQE* spectra of approximately 500-nm-thick BaSi₂ layers capped with approximately 3-nm-thick pure a-Si (Sample E) and a-Si:H (Sample F, G, and H) under the bias voltage of -0.3 V.

3. Conclusions

We have achieved to fabricate a-Si:H by the MBE and RF plasma generator. The formation of Si-H and Si-H₂ bonds were approved by the Raman spectroscopy. The H concentration is approximately 10^{21} cm^{-3} . By comparing *IQE* of BaSi₂ capped with different a-Si layers, the a-Si:H was a better passivation layer than the pure a-Si layer, due to the connection of H atoms and the dangling bonds in a-Si and interface of a-Si/BaSi₂.

References

- [1] T. Suemasu and N. Usami, J. Phys. D Appl. Phys **50** (2017) 023001.
- [2] S. Yachi, R. Takabe, H. Takeuchi, K. Toko, and T. Suemasu, Appl. Phys. Lett. **109** (2016) 072103.
- [3] S. Okasaka, O. Kubo, D. Tamba, T. Ohashi, H. Tabata, and M. Katayama, Surf. Sci. **635** (2015) 115.
- [4] R. C. Chittick, J. H. Alexander, and H. F. Sterling, J. Electrochem. Soc. **116** (1969) 77.
- [5] V. A. Volodin and D. I. Koshelev, J. Raman. Spectrosc. **44** (2013) 1760.
- [6] N. Nakamura, T. Takahama, M. Isomura, M. Nishikuni, K. Yoshida, S. Tsuda, S. Nakano, M. Ohnishi, and Y. Kuwano, Jpn. J. Appl. Phys. **28**, (1989) 1762.

Table I Samples preparation details

Sample	Structure	d _{a-Si} (nm)	Method	Time of H/Si (min)
A	a-Si/Al/c-Si	150	Deposition	0/180
B	a-Si:H/Al/c-Si	150	CD	180/180
C	a-Si:H/Al/c-Si	150	PD	180/180
D	a-Si:H/Al/c-Si	150	PD	60/180
E	a-Si/BaSi ₂ /c-Si	3	Deposition	0/3.5
F	a-Si:H/BaSi ₂ /c-Si	3	PD	1.75/3.5
G	a-Si:H/BaSi ₂ /c-Si	3	PD	5/3.5
H	a-Si:H/BaSi ₂ /c-Si	3	CD	3.5/3.5