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Vacuum deposition of $CsPbI_3$ layers on textured Si for perovskite/Si tandem solar cells

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Abstract

We attempted the conformal deposition of Perovskite layers on textured crystalline Si (c-Si) surfaces, aiming at application to Perovskite/Si tandem solar cells. $CsPbI_3$ layers were deposited through vacuum deposition on several types of textured c-Si surfaces consisting of pyramids with different sizes. We confirmed the formation of uniform and good-coverage layers on the texture c-Si, which is, in principle, difficult to be realized by conventional solution process. We also confirmed a reduction in the optical reflectance on $CsPbI_3$ surfaces by ~10% (absolute) with respect to flat Si when the $CsPbI_3$ films were formed on textured Si. These results indicate the feasibility of Perovskite/c-Si tandem cells with textured c-Si, leading to low optical reflectivity and high photocurrent.

1. Introduction

Perovskite/Si tandem solar cells have a theoretical efficiency limit of 40.6%, and these are thus expected to become high-efficiency solar cells [1]. In the deposition of Perovskite layers on c-Si, flat Si wafers have been used in the conventional solution process such as spin coating [2]. This is because Perovskite films with good coverage cannot be formed on Si surfaces with antireflection texture structures.

In this study, vacuum deposition was applied for a new method to deposit $CsPbI_3$ perovskite layers on textured Si, instead of the conventional solution process. The formation of $CsPbI_3$ films with uniform thickness was realized by the vacuum deposition of PbI_2 and CsI on textured Si regardless of the size of pyramids on c-Si surfaces. Moreover, in order to verify the antireflection effect by the usage of textured c-Si wafers, we compared optical reflectance spectra after the formation of the $CsPbI_3$ films on flat and textured c-Si and estimated an increase in photocurrent.

2. Experimental procedures

We used 6-inch diameter 290-μm-thick mirror-polished floating-zone-grown n-type c-Si(100) wafers with a resistivity of 1–5 Ωcm. After cleaning the wafers in ozone water for 5 minutes, alkali anisotropic etching was performed on Si wafers using two types of etching solutions with different additives (SE-2000H, SUN-X 600) to form pyramid textures. The c-Si wafers were immersed in the etching solutions under the conditions shown in Table I. The textured wafers were then ultrasonically cleaned in deionized water for 15 minutes, followed by being cleaved into 2×2 cm^2 pieces. We observed the surfaces of the textured Si wafers by scanning electron microscopy (SEM) and evaluated the pyramidal-shaped texture sizes.

We next deposited 150-nm-thick PbI_2 and 80-nm-thick CsI in this order on the textured Si substrates by evaporation at deposition rates of 0.5 and 0.3 Å/s, respectively. These samples were then annealed at 350 °C for 1 minute on a hot plate to form $CsPbI_3$ layers. We also prepared $CsPbI_3$ layers on flat c-Si wafers in the same way for comparison. The coverage of $CsPbI_3$ layers on flat and textured c-Si wafers was confirmed from the cross-sectional SEM images. The details of the formation of $CsPbI_3$ by evaporation are summarized elsewhere [3].

We measured the reflectance spectra of the $CsPbI_3$/c-Si stacks using an ultraviolet-visible spectrophotometer (UV-vis), and compared a difference in the reflection loss between the samples with flat and textured wafers on which $CsPbI_3$ films were formed. Based on these results, we esti-

Table I Etching conditions and pyramid heights.

Etchant	SE-2000H			SUN-X 600		
Condition	90 °C, 15 min	90 °C, 30 min	90 °C, 60min	80 °C, 20 min	70 °C, 20 min	70 °C, 50 min
Height (μm)	2.21±0.52	2.46±0.75	1.47±0.23	1.23±0.27	2.90±0.84	7.25±1.68
	[M]		[S]			[L]

mated an increase in photocurrent under the assumption that all the absorbed photons generate carriers and all the carriers are collected as a current.

3. Results and discussion

Table I shows the heights of the pyramidal-shaped textures measured from the SEM images of the c-Si wafer surfaces after alkali etching. Textures with different sizes were obtained depending on etching solutions and conditions. We carried out the vacuum deposition of $CsPbI_3$ layers using three types of substrates indicated in the table: [S] size, [M] size and [L] size.

Fig. 1 shows the cross-sectional SEM images of $CsPbI_3$ layers deposited on the three types of textured wafers and on flat Si wafers. The conformal formation of $CsPbI_3$ layers can be seen for all the pyramidal-shaped c-Si surfaces. These results indicate that it is possible to form $CsPbI_3$ layers with good uniformity and coverage on textured Si wafers by vacuum evaporation, unlike in the case of conventional solution process. One can see protrusions in the $CsPbI_3$ films formed on textured c-Si particularly at the tips of the pyramids. Similar structures are seen also in the film formed on a flat c-Si wafer. These may originate from aggregated excess Cs [4].We think these protrusions could be eliminated by reducing the thickness of CsI and/or the co-evaporation of CsI and PbI_2.

Fig. 2 shows the optical reflectance spectra of three types of textured Si and flat Si with $CsPbI_3$ layers, and average reflectances (R_{AVE}) in a wavelength region of 300–1100 nm are summarized in Table II. All the $CsPbI_3$ films formed on textured Si showed R_{AVE} of ~10% (absolute) lower than that of $CsPbI_3$ films on the flat wafer. This suggests that reflection loss on the $CsPbI_3$ surface can be greatly reduced by using textured Si. We evaluated, from the reflectance (R) data, how much short-circuit current density (J_{SC}) increases in Perovskite/Si tandem solar cells by the utilization of textured c-Si using the following eq. (1).

$$J_{sc} = q \int_{300}^{1200} N_{Photon(AM1.5G)} \cdot (1 - R)\, d\lambda \qquad (1)$$

We assumed that all the unreflected photons are absorbed and produce photocurrent with 100% internal quantum efficiency, and the two sub-cells, $CsPbI_3$ and c-Si, produce the same current. J_{SC} for the flat and [M] size textured wafers were estimated to be 19.3 and 21.5 mA/cm^2, respectively. This means that J_{SC} can be improved by ~2 mA/cm^2 by using textured Si, which is a great benefit for the Perovskite/Si tandem cells.

4. Conclusions

The vacuum deposition of $CsPbI_3$ films can realize good coverage on pyramidal-shaped c-Si textures, which is difficult by the conventional liquid process. The conformal formation of $CsPbI_3$ films can be seen independent of pyramid size. The utilization of textured Si leads to an reduction in optical reflectance by ~10% (absolute), corresponding to an improvement in Jsc of ~2 mA/cm^2 in Perovskite/Si tandem cells. These demonstrate the possibility of realizing new fabrication processes for perovskite/Si tandem solar cells using textured Si.

References

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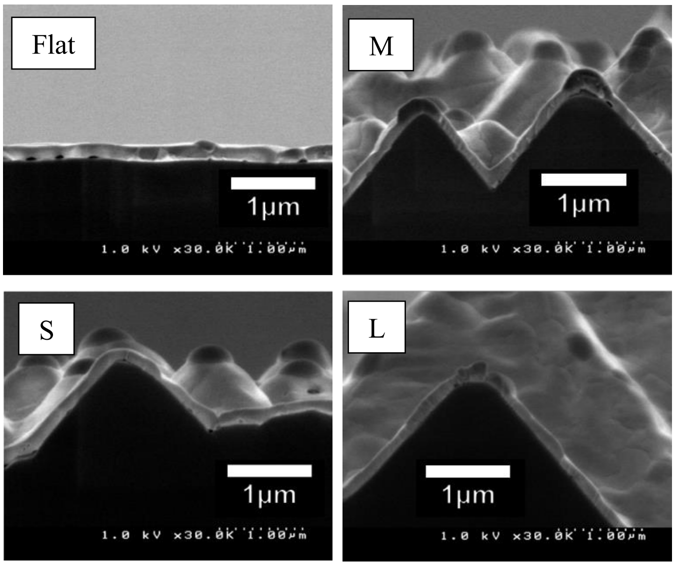

Fig. 1 Cross-sectional SEM images of $CsPbI_3$ films deposited on textured and flat Si.

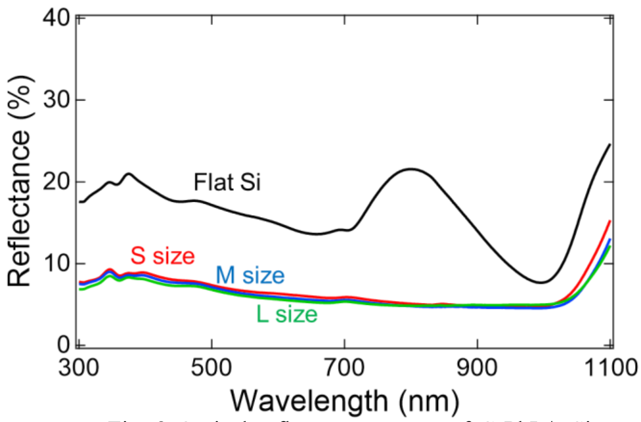

Fig. 2 Optical reflectance spectra of $CsPbI_3$/c-Si

Table II R_{AVE} on $CsPbI_3$ layers formed on flat and textured c-Si wafer in a wavelength region of 300–1100 nm.

	Flat wafer	S size	M size	L size
R_{AVE} (%)	16.16	6.60	6.20	6.09