

## Passivation Effect of Amorphous Silicon Oxide Thin Films Studied by Hydrogen Evolution

Kazuyoshi Nakada<sup>1</sup>, Shinsuke Miyajima<sup>1</sup> and Makoto Konagai<sup>1,2</sup>

<sup>1</sup> Department of Physical Electronics, Tokyo Institute of Technology  
2-12-1-NE-15, O-okayama, Meguro-ku, Tokyo 152-8552, Japan  
Tel. +81-3-5734-2662, FAX. +81-3-5734-2897, E-mail: nakada.k.aa@m.titech.ac.jp

<sup>2</sup> MEXT/JST FUTURE-PV Innovation Research Director  
2-12-1-NE-15, O-okayama, Meguro-ku, Tokyo 152-8552, Japan

### Abstract

Thermal desorption spectroscopy and effective lifetime measurements were carried on Si wafers passivated by a-Si:H and a-SiO:H thin films. It was found that denser passivation films have a higher passivation effect. Samples passivated by a-SiO:H showed effective lifetimes higher than the ones passivated by a-Si:H before and after annealing treatment, demonstrating the superior passivation quality of the former material. In addition, a shift on the hydrogen desorption peak temperature for high lifetime samples was found, indicating that bond strength of monohydride and/or dihydrides directly affects the passivation effect.

### 1. Introduction

The surface passivation of crystalline silicon is a crucial issue for fabrication of solar cells with thin substrates, as the effect of surface recombination velocity increases when the substrate thickness is reduced. The most common passivation technique for c-Si is the growth or deposition of dielectric films like SiO<sub>2</sub> or a-Si:H. The latter material is known to have a high passivation quality, with the advantage of fabrication by low temperature (<200°C) processes. However, the a-Si:H layer usually shows epitaxial growth when deposited at temperatures higher than 130°C [1]. The sensitivity of film quality to the deposition temperature narrows the window for optimum deposition, which could result in complications during the large-scale fabrication processes. An alternative to the conventional a-Si:H is the hydrogenated amorphous silicon oxide (a-SiO:H) [2]. Harmful epitaxial growth can be totally hindered even when this material is deposited at relatively high deposition temperatures (>180°C) [2]. Additionally, the passivation quality of a-SiO:H has been reported to be as high as the a-Si:H one [3]. Although the suppression of epitaxial growth has been attributed as one of the major factors for improvement of passivation quality with a-SiO:H films, understanding about the passivation mechanism has been lacking so far. One of the reasons for this is the difficulty on the evaluation of films with a thickness suitable for the passivation layer of heterojunction solar cells.

In this report, in order to gain insight about thin film passivation, we evaluated a-Si:H and a-SiO:H films by thermal desorption spectroscopy (TDS). TDS is a useful

method to obtain information about hydrogen content [4, 5]. It was found that samples with higher effective lifetime have denser passivation films and desorption peaks at higher temperatures.

### 2. Experimental

Intrinsic a-SiO:H and a-Si:H were deposited on the both sides of n-type FZ c-Si by VHF-PECVD method. The frequency was 60 MHz. A gas mixture of SiH<sub>4</sub>, H<sub>2</sub> and CO<sub>2</sub> was used for a-SiO:H deposition, while only SiH<sub>4</sub> was used for a-Si:H deposition. The heater temperature for a-SiO:H and a-Si:H were 210°C and 160°C, respectively. Lower heater temperature for a-Si:H was chosen in order to avoid epitaxial growth that usually occurs at relatively high temperatures [1]. Heterojunction solar cells with conversion efficiency over 20% have been achieved when the a-SiO:H reported here was applied as the passivation layer [6]. The thickness and resistivity of c-Si substrates were 280 μm and 3.0 Ωcm, respectively. The same wafer was used for both effective lifetime and TDS measurements. Prior to deposition of the films, the wafers were immersed in diluted HF to remove native oxide. The thickness and deposition rate of the films were measured by spectroscopic ellipsometry (SE). Minority carrier effective lifetime ( $\tau_{eff}$ ) was measured with a quasi-steady-state photoconductance (QSSPC) setup (Sinton Consulting, WCT-120) in the transient mode. All the samples were submitted to annealing treatment after the film deposition for improvement of passivation effect. Annealing was carried out in forming gas ambient at 210°C for 30 minutes. TDS measurements were performed with a heating rate of 20 K/min.

### 3. Results and Discussion

The  $\tau_{eff}$  for samples before and after thermal annealing are given on Table I. As it was expected, for all cases the  $\tau_{eff}$  improved after annealing treatment. This improvement is attributed to hydrogen diffusion from the film bulk to the film/c-Si interface, which terminates the surface dangling bonds. The highest  $\tau_{eff}$  were obtained for the samples passivated by a-SiO:H, demonstrating the superior passivation quality of this material when same thickness is applied. The samples deposited on (111) wafer showed higher  $\tau_{eff}$  than the samples with same structure deposited on (100) wafer. This can be attributed to the typical lower surface dangling

Table I Effective lifetime before and after thermal annealing

Sample	Passivation film	wafer type	$\tau_{eff}$ (ms)	
			as-depo	annealed
A	a-Si:H	(100)	0.045	1.5
B	a-Si:H	(111)	0.063	1.9
C	a-SiO:H	(100)	0.74	0.9
D	a-SiO:H	(100)	1.3	3.4
E	a-SiO:H	(100)	2.6	5.4
F	a-SiO:H	(111)	2.9	6.3

bong density of (111) wafers [7].

Figure 1 shows the hydrogen effusion spectra taken from samples passivated with different films. The spectra show two large peaks that can be deconvoluted into two Gaussian distributions. The lower temperature peak  $\beta_2$  is linked to the interconnected hydrogen-terminated internal voids and surfaces [7]. The hydrogen termination can be present in the dihydrides and/or clustered monohydrides forms. The higher temperature peak  $\beta_1$  is related as a parameter of denser material that is rich in isolated monohydrides. Figure 2 (a) shows the  $\beta_1/(\beta_1+\beta_2)$  peak intensity ratio, an indicative of film density, as a function of  $\tau_{eff}$ . Samples with high  $\tau_{eff}$  showed high  $\beta_1/(\beta_1+\beta_2)$  ratio, indicating that density of the films have a crucial effect on the passivation quality. Films with high defect density usually show a large concentration of voids, and consequently a low density. From the results above it was observed that the a-Si:H films have a lower density. As the passivation quality is also quite lower than the a-SiO:H one, is reasonable to assume that a-Si:H films have a larger density of voids and dangling bonds than the a-SiO:H material.

Another feature observed from TDS measurements is a trend where both  $\beta_1$  and  $\beta_2$  shift to higher temperatures when higher  $\tau_{eff}$  were obtained. The shift for  $\beta_2$  was nearly a linear function of  $\tau_{eff}$ . This suggests that weak bonding of

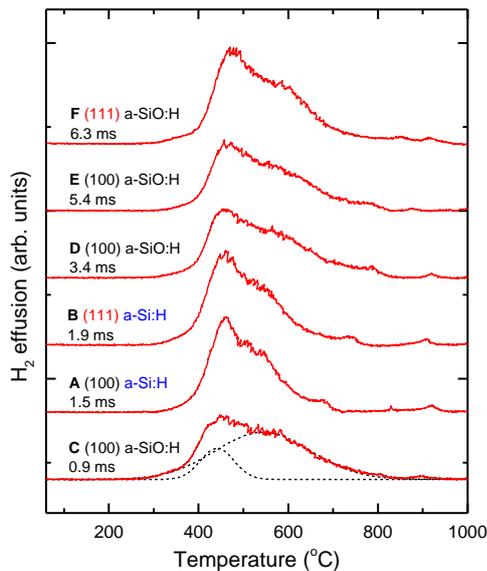


Fig. 1 TDS spectra of samples A~F. Two distinct peaks can be observed.

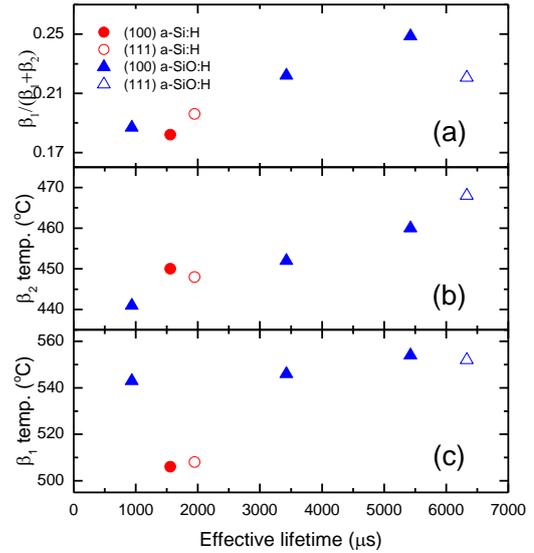


Fig. 2 Relation of effective lifetime and (a)  $\beta_1/(\beta_1+\beta_2)$  area deconvoluted into Gaussian functions, (b) low temperature desorption peak  $\beta_2$ , (c) high temperature desorption peak  $\beta_1$ .

clustered monohydride and/or dyhydride bonds can be considered as a direct indicator of low surface passivation. On the other hand, the  $\beta_1$  peak position for a-SiO:H samples were always higher than the a-Si:H one. This may have a partial contribution from the higher electronegativity of O atoms, making a stronger covalent bonding. The trend of higher peak temperature for samples with higher lifetime was also observed when comparing samples passivated with the same material.

#### 4. Conclusions

TDS and effective lifetime measurements were carried out on Si wafers passivated by a-Si:H and a-SiO:H. The higher  $\beta_1/(\beta_1+\beta_2)$  ratio of a-SiO:H films indicates a denser film structure with less voids. The higher density was reflected on the effective lifetime, which was higher than the a-Si:H samples before and after thermal annealing. The peak temperature shift is presumably attributed to bond strength, which may include an effect of O atom stronger electronegativity.

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