

Effect of hot-wire passivation on the properties of hydrogenated microcrystalline silicon films to reduce post-deposition oxidation

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Abstract

Hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) films have a large number of grain boundaries that oxidize after deposition, leading to deterioration of device performance. In this study, post-treatment of $\mu\text{c-Si:H}$ thin films was carried out with methane-related radicals generated by a hot wire. The effect of the hot-wire passivation on the properties of the $\mu\text{c-Si:H}$ thin films was investigated using Fourier-transform infrared (FT-IR) transmission spectroscopy. Through post-treatment, hydrogen on the silicon-crystallite surface was substituted with hydrocarbon. Further, an increase in filament temperature (T_{fil}) was found to enhance passivation. For films treated at T_{fil} above 1700 °C, post-oxidation and nitridation hardly occurred, whereas films treated at T_{fil} below 1400 °C were oxidized and nitrided even after post-treatment.

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1. Introduction

Hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) films have advantages of being cheaper and possessing a larger deposition area than crystalline and polycrystalline silicon. However, $\mu\text{c-Si:H}$ deposited at a high deposition rate has been shown to have a large number of voids at grain boundaries [1]. This leads to deterioration of device performance that include increases in dark conductivity and reductions in activation energy [2,3]. Post-treatment is a useful method to improve grain boundaries [4]. Further, as a hot wire is a good catalyst for decomposing feedstock gas [5], we investigated the effect of hot-wire passivation on the properties of $\mu\text{c-Si:H}$ thin films.

Hydrogen is generally used for post-treatment [4], however, in this study post-treatment was carried out in a methane atmosphere. Methane was chosen instead of hydrogen because: (1) with $\mu\text{c-Si:H}$, light-induced degradation rarely occurs as it does with amorphous silicon [6], but an increase in hydrogen content has the possibility of bringing about light-induced degradation even for $\mu\text{c-Si:H}$ [7,8], (2) the Si–H bond energy is lower than that of the Si–C bond [9], (3) the size of the methyl radical is almost the same as that of the silicon atom [10], so much so that the film becomes denser, and (4) the incorporation of a small amount of carbon atoms in silicon films leads to increases in photoconductivity and photosensitivity [11].

2. Experiment

$\mu\text{c-Si:H}$ thin films were deposited on silicon wafers ($10 \times 10 \text{ mm}^2$) by a hot-wire chemical vapor deposition

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system, as detailed elsewhere [12]. Tungsten wires of 0.5 mm diameter were used as a filament. The distance between the substrate and the filament was 26 mm. The gas flow rates of hydrogen and silane were 4 and 2 sccm, respectively, and total gas pressure was 133 Pa. The temperatures of the filament and substrate holder were 1700 and 250 °C, respectively. Film thickness, crystalline volume fraction and mean crystalline size of the resulting $\mu\text{-Si:H}$ films were about 600 nm, 65% and 15 nm, respectively [12]. Right after deposition, passivation was carried out in a methane atmosphere in the same film-deposition chamber. The gas flow rate of methane was 20 sccm, and gas pressure was 133 Pa. Temperatures of the substrate holder were 250 °C. Filament temperature (T_{ft}) was varied between 1000 and 2000 °C. Post-treatment time was 30 min.

Fourier-transform infrared (FT-IR) transmission spectra were measured using an FT-IR spectrometer (Spectrum 2000, Perkin Elmer) over a range of 400–3000 cm^{-1} , with a resolution of 1 cm^{-1} . The IR absorption coefficient was estimated using the procedure described by Guivarc'h et al. [13]. For each mode, integrated absorption intensity I , given by a formula

$$I = \int \frac{\alpha(\omega)}{\omega} d\omega, \quad (1)$$

where $\alpha(\omega)$ is the infrared absorption coefficient at wave-number ω , was evaluated.

3. Results

For as-treated films, IR spectra in the wavenumber region between 400 and 1400 cm^{-1} were composed of four fundamental peaks: Si–H wagging (630 cm^{-1}) [14,15], Si–C stretching (780 cm^{-1}) [14,15], Si–O stretching ($\sim 1050 \text{ cm}^{-1}$) [16] or Si–CH_{*n*} wagging ($\sim 980 \text{ cm}^{-1}$) [14,15], and Si–CH₃ bending (1240 cm^{-1}) [14,15] modes (Fig. 1). For aging films on the other hand, in addition to the peaks noted above, peaks due to Si–N stretching ($\sim 873 \text{ cm}^{-1}$)

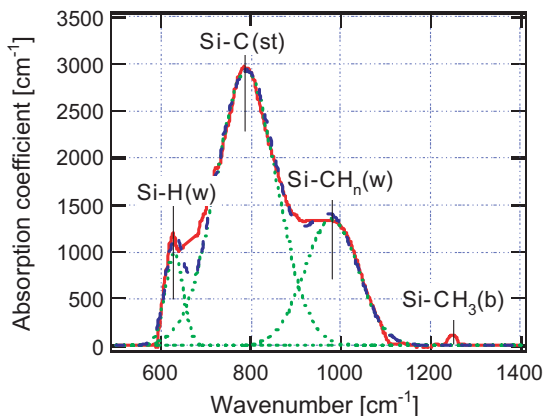


Fig. 1. IR absorption spectrum for film treated at $T_{\text{ft}} = 2000 \text{ °C}$, the measured spectrum (500–1200 cm^{-1}) (solid curve) is fitted by the sum of three Gaussian peaks with peak wavenumbers of 630, 790 and 980 cm^{-1} .

[17,18] and Si–O stretching (1064 cm^{-1} and 1148 cm^{-1}) modes were observed [16] (not shown).

Fig. 2 shows the T_{ft} -dependence of the integrated absorption intensity, $I_{\text{Si-C}}$, of the Si–C(st) mode of post-treated $\mu\text{-Si:H}$ films, together with that of untreated films. As shown in Fig. 2, for the films treated at T_{ft} below 1200 °C, $I_{\text{Si-C}}$ was the same as that of untreated films. $I_{\text{Si-C}}$ increased with increasing T_{ft} from 1200 to 1400 °C, indicating that methane decomposed on the tungsten-filament surface heated at $T_{\text{ft}} = 1400 \text{ °C}$ [19]. At T_{ft} above 1400 °C, $I_{\text{Si-C}}$ increased with increasing T_{ft} , indicating that the intake of carbon atoms into the films increased. $I_{\text{Si-C}}$ remained unchanged with time for all films, indicating that carbon atoms were not incorporated into the films after deposition and post-treatment.

Fig. 3 shows the T_{ft} -dependence of the integrated absorption intensity, $I_{\text{Si-O}}$, of the Si–O(st) mode. It is difficult to distinguish the peaks of the Si–CH_{*n*}(w) and Si–O(st) modes of the as-treated films because the peak positions are close to each other. Therefore, $I_{\text{Si-O}}$ includes the integrated absorption intensity of the Si–CH_{*n*}(w) mode. Fig. 4 shows

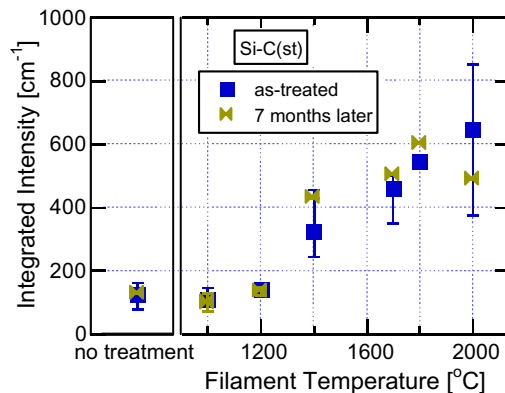


Fig. 2. T_{ft} -dependence of the integrated absorption intensity, $I_{\text{Si-C}}$, of the Si–C(st) mode of post-treated $\mu\text{-Si:H}$ films together with that of untreated films.

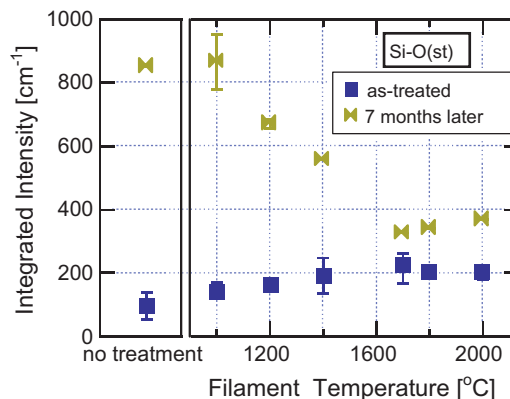


Fig. 3. T_{ft} -dependence of the integrated absorption intensity, $I_{\text{Si-O}}$, of the Si–O(st) mode of post-treated $\mu\text{-Si:H}$ films together with that of untreated films.

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