Characterization and FDTD simulation analysis on light trapping structures of amorphous silicon thin films by laser irradiation

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ABSTRACT

The effect of laser energy density on the light-trapping structures of amorphous silicon (α -Si) thin films is studied both theoretically and experimentally. The thin films are irradiated by a frequency-doubled ($\lambda=532$ nm) Nd:YAG pulsed nanosecond laser. An effective finite difference time domain (FDTD) model is built to find the optimized laser energy density (E_L) for the light trapping structures of α -Si. Based on the simulation analysis, it shows the variation of reflection spectra with laser energy density. The optimized reflection spectra at $E_L=1000$ mJ/cm² measured by UV-visible

spectroscopy confirms to agree well with that corresponding to the depth to diameter ratio (h/D) in the FDTD simulation. The surface morphology characterization by optical microscope (OM) and scanning electron microscope (SEM) accords fairly well to of light-trapping modeling in the simulation.

Keywords: light trapping; amorphous silicon; finite difference time domain; laser irradiation

1. INTRODUCTION

In the last years, amorphous silicon (α -Si) films on glass substrates have attracted a great deal of attention in photovoltaics, microelectronics and display technologies because of its potential applications for electronic devices, especially thin film solar cells [1-3]. **Efficient light-trapping structures of thin films must satisfy two kinds of requirements: both strongly optical absorption and effectively electrical transportation.**

To improve collection of photogenerated carriers, various crystallization techniques of hydrogenated amorphous silicon (a-Si:H) films can be performed to prepare polycrystalline silicon (poly-Si) films, such as laser induced crystallization (LIC)[4-6], metal induced crystallization (MIC)[7-9], solid phase crystallization (SPC)[10-12].

Due to the minimum thermal damage to the underlying substrates, laser induced crystallization has been extensively used to produce good quality poly-Si films [13].

With these requirements, laser technology not only improves electrical transportation effectively, but also enhances optical absorption strongly. **The light-trapping structures**

of thin films have been widely used in manufacturing process of conventional

crystalline solar cells (c-Si) to benefit optical absorption, such as pyramids in monocrystalline silicon [14] and etching pits in poly-Si [15]. However, it is worth discussing how to decrease optical reflection of α -Si thin film through light-trapping structures [16-19]. Compared to the radial pin junction upon Si nanowire forest [20, 21], the laser texturing is more suitable to be used in manufacture both crystalline silicon and thin film solar cells of the mass production. Because the extent of laser texturing can be controlled accurately, the average reflectance can be adjusted by laser energy density. But the radial pin junction upon Si nanowire forest can only be used in preparing thin film solar cell. And the most of Si nanowire must be prepared by chemical reaction. So Si nanowire technology is harder to control the uniformity of texturing than laser technology.

In this paper, we present theoretical and experimental study of optical properties of α -Si thin film including light-trapping structures. The finite difference time domain (FDTD) method is used to study the light-modulated characteristics of light-trapping structures. Reflection spectra of crystalline silicon with different depth to diameter ratio of pits are simulated by FDTD method. This experimental work aims to focus on the correlation between reflection spectra and laser energy density. Surface characterization and FDTD simulation analysis of light trapping structures after laser irradiation are investigated.

2. EXPERIMENTAL DETAILS

Intrinsic α -Si thin films are prepared by the following procedure. First, above

67 600 nm-thick α -Si:H films as a layer is deposited on the glass substrates using plasma
68 enhanced chemical vapor deposition (PECVD) by silane (SiH_4) with hydrogen (H_2).
69 The experimental parameters of deposited α -Si:H thin films are shown in Table.1. The
70 PECVD system is HLF-400 made in Beijing Beiyi Innovation Vacuum Technology
71 Co., Ltd. Before the thin films are deposited on glass substrate, heat-resistant tape has
72 been adhered to the corner of glass substrate. After we finish depositing α -Si:H thin
73 films and uncover tape from the substrate, the thickness of thin film is measured on
74 the step between glass substrate and thin films by stylus profiler. Thickness
75 measurement of stylus profiler is Veeco Dektak 150. Then light-trapping structures
76 are formed on the surface of α -Si:H samples using a frequency-doubled Nd:YAG laser.
77 All of samples were dehydrogenated at $E_L=100 \text{ mJ/cm}^2$ prior to the laser irradiation.

78 The hydrogenated amorphous silicon thin films are irradiated by a
79 frequency-doubled ($\lambda=532 \text{ nm}$) Nd:YAG pulsed nanosecond laser with laser beam
80 shaping system introduced by a fly-eye lens array. The beam shaping system,
81 including fly-eye lens array, transformed the incoming Gaussian laser beam into a
82 flattop one. A wave-front analyzer was used to examine the intensity uniformity on
83 the image plane [22]. The laser can operate at a repetition frequency of 30 Hz and
84 pulse duration of 10 ns. The laser beam by shaping system is homogenized to a spot
85 of $4 \text{ mm} \times 4 \text{ mm}$. The Nd:YAG laser is supported by Shanghai Institute of Optics and
86 Fine Mechanics.

87 Raman spectra are measured by Jobin Yvon LabHR Raman spectrometer at
88 room temperature using the 514.5 nm line of an Ar^+ laser. The surface morphology of

films is determined by optical microscope (OM). The Scanning Electron Microscope (SEM) made by Japan Hitachi SU1510 is used to measure diameter and depth of etching pits. UV-visible reflection spectra are measured by Hitachi U-2910 spectrophotometer.

3. RESULTS AND DISCUSSION

3.1 Structural modeling

In this paper, the software of FDTD Solution is used as analysis for simulating light-trapping structures of α -Si thin film. The size of rectangular model is that the length, width and height are 2.5 cm, 2.5 cm and 1 mm respectively. The physical and optical values of silicon materials are used as parameters in the simulation. In the regions of pits, the a-Si has been crystallized from amorphous phase to polycrystalline phase by laser irradiation. Except for these regions, the other regions still remain amorphous phase after laser irradiation. The materials in the regions of pits and others have been selected to simulate by poly-Si and a-Si respectively. Different depth to diameter ratio of pits is selected to simulate the properties of optical reflection. The optimal results can be analyzed to obtain the lowest reflectivity in the wavelength of visible light. There are five kinds of patterns varying the depth to diameter ratio of pits as shown in Tab. 1. The planar and cross-section modeling of light-trapping structures after laser irradiation has been shown in Fig.1. The basic planar light-trapping structure of α -Si thin film on substrate has demonstrated in Fig.1 (A). The Fig.1 (B) shows the cross-section of light-trapping structures after laser

111 irradiation, where D represents diameter of pits and h represents depth of pits.

112 The surface morphology of light-trapping structure irradiated by laser energy
113 density (E_L) at 1000 mJ/cm^2 characterized by OM has been obtained in Fig.2 (A). It
114 exhibits that cross-section morphology of light-trapped structure is characterized by
115 SEM in Fig. 2 (B). There are several pits in the profile of red line corresponding to
116 planar structural characterization. These pits are formed by high energy laser in the
117 very short time. It is found that $E_L=1000 \text{ mJ/cm}^2$ is the best laser energy density to
118 form optimal light-trapping structure on the surface of α -Si thin film, because it owns
119 uniform size of pits and the highest depth to diameter ratio. Therefore the structural
120 modeling simulated by FDTD method in Fig. 1 accords very well to the experimental
121 result characterized by OM and SEM in Fig. 2.

122 3.2 Surface morphology

123 We select five kinds of samples irradiated by laser at original (untreated),
124 $E_L=600 \text{ mJ/cm}^2$, 800 mJ/cm^2 , 1000 mJ/cm^2 , 1200 mJ/cm^2 , respectively to investigate
125 the surface morphology of thin films. The related experimental and simulative
126 parameters of samples have been listed in Tab. 1.

127 The characterization of Raman spectroscopy is also displayed in Fig.3. In the
128 picture, α -Si and poly-Si phase can be obtained through different Raman shift. The
129 α -Si exhibits a broad peak at $\sim 480 \text{ cm}^{-1}$ (Fig.3A). Because α -Si:H thin films irradiated
130 by low energy laser still includes parts of amorphous phase, the broad Raman peak at
131 $\sim 480 \text{ cm}^{-1}$ demonstrates amorphous phase. Exposing the α -Si:H thin films to poly-Si
132 by laser irradiation, a new peak of crystalline silicon (c-Si) appears at $\sim 510 \text{ cm}^{-1}$

133 corresponding to the transverse optical (TO) phonon for crystalline Si (Fig.3B) [23].

134 When laser energy density is lower than 800 mJ/cm^2 , depth to diameter ratio (h/D)
135 and Raman TO peak shift increase with laser energy density. Subsequent laser
136 irradiation provides more energy for the growth of the nucleus and then light-trapping
137 structures form (shown in Fig.4A and Fig.4B). When E_L is between 800 mJ/cm^2 and
138 1000 mJ/cm^2 , depth to diameter ratio and Raman TO peak shift approach maximum,
139 because the light-trapping poly-Si region extends laterally (shown in Fig.4C). When
140 E_L increases to 1200 mJ/cm^2 , the uniformity of pits have been damaged by high laser
141 energy density and produce more small pits around the boundaries simultaneously
142 (shown in Fig.4D). The melting depth of light-trapping structures remains constant
143 when E_L is higher than 1000 mJ/cm^2 , because α -Si thin film is enough to melt
144 completely. The average depth to diameter ratio in Fig.4D is lower than that in Fig.4C.
145 Therefore the optimal laser energy density ($E_L = 1000 \text{ mJ/cm}^2$) obtained from the
146 experiment results agrees fairly well with that from the simulation results.

147

148 3.3 Optical properties

149 In the light-trapping model, the reflection spectra are analyzed by FDTD
150 simulation. The reflection spectra are assumed to vary through the depth to diameter
151 ratio of pits that has a coefficient of h/D . The parameters of h/D in Tab.1, which
152 corresponds to laser energy density, are originated from characterization. It is proved
153 theoretically that the correlation between reflection spectra and h/D can be obtained
154 from FDTD simulation. Meanwhile the reflection spectra with different E_L are

155 deduced from the UV-visible spectrophotometer. The light source of UV-visible
156 spectrometer is irradiated by incident angles. The absorption spectra have been
157 displayed in Fig. 5. Absorption spectra are measured by Jasco V-570
158 spectrophotometer with integration sphere. It is found that average absorption is
159 enhanced when laser energy density increases from 600 mJ/cm^2 to 1000 mJ/cm^2 . So
160 the light-trapping structure is beneficial to enhance average absorption of thin films
161 irradiated by laser. We also obtained reflection spectra by UV-visible spectral
162 characterization as illustrated in Fig. 6A and FDTD simulation as shown in Fig. 6B.
163 The laser energy densities correspond to 600 mJ/cm^2 , 800 mJ/cm^2 and 1000 mJ/cm^2
164 respectively shown in Fig. 5 and Fig. 6.

165 In the experiment of light-trapping structures by laser irradiation, It is found that
166 the TO peaks in Raman spectra and value of h/D occur the maximum value, reflection
167 spectra arrive the minimum value at wavelength of 575 nm when the laser energy
168 density reaches to about 1000 mJ/cm^2 . From the Fig. 6, the reflection spectra of the
169 FDTD simulation results accords well to the value of reflection spectra obtained from
170 the UV-visible spectral results.

171

172 4. CONCLUSIONS

173 In this paper, the laser induced light-trapping structures of a-Si thin films are
174 numerically and experimentally investigated. The FDTD simulation model is used to
175 predict the optimal reflection spectra corresponding to depth to diameter ratio of
176 light-trapping structure. The optimized reflection spectra are achieved by laser energy

177 density of about 1000 mJ/cm² in the experiment. The surface characterization of thin
178 films with different laser energy densities accords very well to the light-trapping
179 modeling in the simulation.

180

181 ACKNOWLEDGMENTS

182 The authors gratefully acknowledge the financial support of the project funded
183 by National Science Foundation of China (Grant no. 61404080 and 51202139).

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218

219 **Table Caption:**

220

221 Table 1 Experimental and simulative parameters of α -Si thin film samples by laser irradiation
222 with different laser energy densities

223

224 **Figure Caption:**

225 Fig. 1 (A) Basic planar light-trapping structure of α -Si thin film on substrate (B) The cross section
226 of light-trapping structure after laser irradiation

227

228 Fig. 2 (A) Surface morphology of planar light-trapping structure characterized by optical
229 microscope (B) The cross section of light-trapping structure irradiated by $E_L=1000 \text{ mJ/cm}^2$
230 characterized by SEM

231

232 Fig. 3 The Raman spectra characterization of samples by laser irradiation with different laser
233 energy density. (A) Original (untreated) and $E_L = 600 \text{ mJ/cm}^2$, (B) $E_L = 800 - 1200 \text{ mJ/cm}^2$

234

235 Fig. 4 Surface morphology of light-trapping structures characterized by SEM at laser energy
236 densities of (A) $E_L = 600 \text{ mJ/cm}^2$, (B) $E_L = 800 \text{ mJ/cm}^2$, (C) $E_L=1000 \text{ mJ/cm}^2$, (D) $E_L=1200$
237 mJ/cm^2

238

239 **Fig. 5** Absorption spectra at laser energy densities of 600, 800 and 1000 mJ/cm^2 respectively

240

241 Fig. 6 (A) UV-visible reflection spectra and (B) FDTD simulative reflection spectra at laser energy
242 densities of 600 – 1000 mJ/cm^2

Figure 1
[Click here to download high resolution image](#)

(A)

(B)

Figure 2
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(A)

(B)

Figure 3
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Figure 4
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Figure 5
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Figure 6

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Table 1

Sample No.	Laser power (W)	Laser energy density (mJ/cm ²)	Depth to diameter ratio (h / D)
a	0.12	600	0.35
b	0.16	800	0.42
c	0.2	1000	0.55
d	0.24	1200	0.48
e (untreated)	0	0	0

(A)

(B)