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Characterization for the Onset of Crystallization of Amorphous to Microcrystalline Silicon by Optical Spectroscopies

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ABSTRACT

We study the a- to μ c-Si films made at three laboratories by using Raman, photoluminescence- and optical-absorption spectroscopies. Raman spectra show no signature of the c-Si peak in most samples. Whereas, low energy PL enhancement was observed in films containing small density μ c-Si.

1. Introduction

To improve stability of a-Si:H, the edge material, i.e. amorphous (a) near the onset of microcrystalline (μ c) has attracted attention.[1-3] Both PECVD with H-diluted gas and HWCVD have been used in the production of a-Si:H solar cell and thin-film transistors. Furthermore, evidence of μ c-Si was found in films deposited with a high growth rate without H-dilution by PECVD.[4] To understand the correlation between deposition conditions, the film microstructure and its electronic properties, we studied numbers of the edge-films made by using Raman, photoluminescence- (PL) and optical-absorption spectra.

2. Samples and Results

Table I HWCVD samples deposited on glass

Sample ID	H ₂ /SiH ₄ (R)	XRD	Thickness(mm)	Dep. rate(Å/s)
1	1:1	a-Si	4.1	17.2
2	2:1	a-Si	3.0	12.5
3	3:1	a+ μ c	1.7	7.1

Table II PECVD samples with H-dilution on ss

Sample ID	Substrate surface conditions	Thickness (μ m)
10306	ss/i	0.5
10307	ss/n/i	0.5
10311	ss/n/i	1.5
10857	ss/textured Ag/ZnO/i	0.5
10859	ss/textured Ag/ZnO/n/i	0.5
10858	ss/textured Ag/ZnO/n/i	1.5
9883	ss/i	1.4

Table III PECVD samples deposited on c-Si and quartz

Sample ID	Substrate	H(sccm)	rf power (W)	d (μ m)	Rate(Å/s)
12465	c-Si	none	100	2.33	16.2
12467	c-Si	none	60	1.60	10.3
12469	c-Si	none	10	1.69	2.8
12451	quartz	none	20	2.13	14.9
12464	quartz	120	100	2.10	15.22
12466	c-Si	120	60	1.90	10.55
12468	c-Si	120	20	1.64	2.5

Table I lists films deposited by HWCVD with H-dilution ratio $1 \leq R \leq 3$. Films in Table II contain three structures which are identical to those edge materials studied by X-ray

diffraction (XRD) and the transient photocapacitance (TPC) technique[1]. Table III lists films grown at high rates; μ c- in the a-Si:H matrix was found by TPC measurements in most films[4]. Figs. 1(a) and (b) demonstrate the optical absorption and PL spectra for the a- to μ c-Si transition materials listed in Table I. When the H-dilution ratio R= 1 and 2, no c-Si peak can be seen in both XRD and Raman. Meanwhile both the a(E) and PL spectra show a-Si:H-like features, whereas, an extra band at ~ 1.2 eV is clearly seen in the a(E) spectra as shown in Fig. 1(a). At R=3, XRD shown a c-Si component, the 520 cm^{-1} c-Si Raman peak appeared.[5] Meanwhile, a low energy PL band peaked at ~ 1.0 eV appears and the a(E) spectrum became poly-Si-like. The typical features of μ c- are: a low energy PL band at ~ 1.0 eV which is corresponding to the optical absorption band peaked at ~ 1.2 eV.

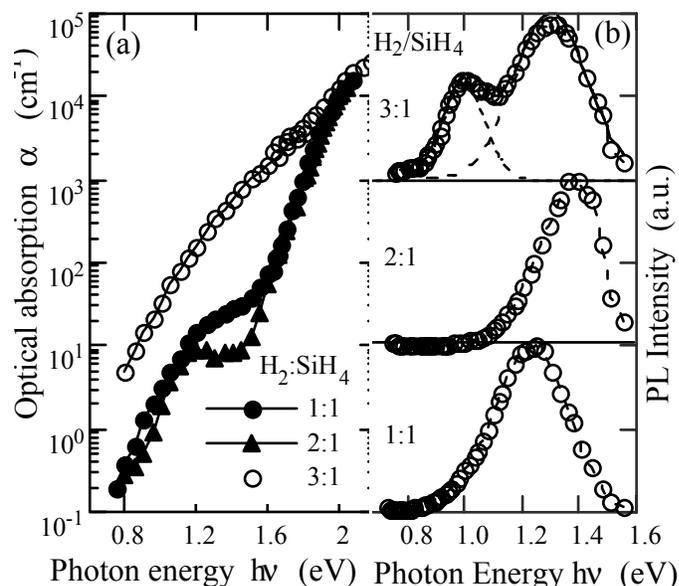


Fig. 1 (a) Optical absorption spectra and (b) PL for a-to μ c-Si

For the edge materials listed in Tables II and III, we expected to see most of them contain the 520 cm^{-1} peak in Raman; the results in Fig. 2(a) showed only the a-Si:H peak centered at 480 cm^{-1} except for sample #9883 as shown in Fig. 2(b). We double checked the films listed in Table II by XRD.[6] In consistence with the Raman results, there was no c-Si peak in all six films but only film #9883 was.

However, we found μ c-features in PL lineshape in above films. Fig. 3(a) shows the substrate effects, i.e. the low energy PL enhancement in the film grown on ss substrate. Fig. 3(b) shows thickness effects studied by varied PL excitation wavelengths on film #9883 which shows c-Si peak in Raman. The absorption depth is about 140, 600, 800 Å and

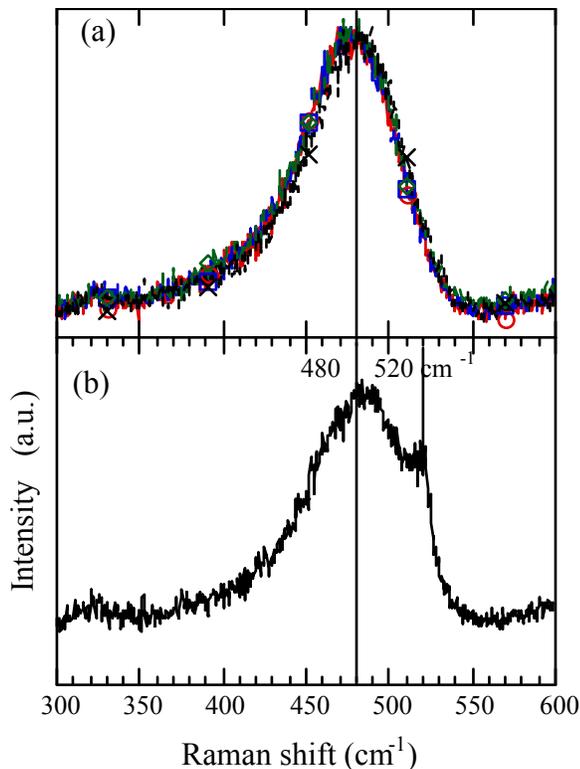


Fig. 2 Raman spectra (a) for all films listed in Tables II and III except (b) for #9883 listed in Table II

1 μm for the 325, 488, 514, and 632 nm laser in a-Si:H. As the examined layer moved to the top surface, the low energy PL was enhanced. The results imply that the structure tends to μc as the film grows thicker. Fig. 3(c) shows the PL spectra for the films deposited with the same H-dilution but varied deposition rate. The PL intensity decreases as the growth rate decreases due to μc . Meanwhile, the PL peak energy decreases from ~ 1.3 to 1.18 eV in sample #12468, that is the film with highest μc in the TPC measurement[4].

3. Summary

For a number of a/ μc films, Raman spectra showed no c-Si peak. Because that (a) growing near the a- μc transition, the resulting film properties are very sensitive to the film thickness and substrate material, so the results may not be the same unless one studies the same piece of sample; and (b) if the c-Si-grain volume fraction is only a few percentage or the grain size is ≤ 3 nm, it is below the technical limitation of Raman[7]. Whereas, low energy PL enhancement was observed in films containing small density μc -. The electronic density of states measured by PL and a(E) is more sensitive to the characterization of onset μc . Furthermore, the excitation wavelength dependence of PL can be used to study the non-uniformity along the growth direction.

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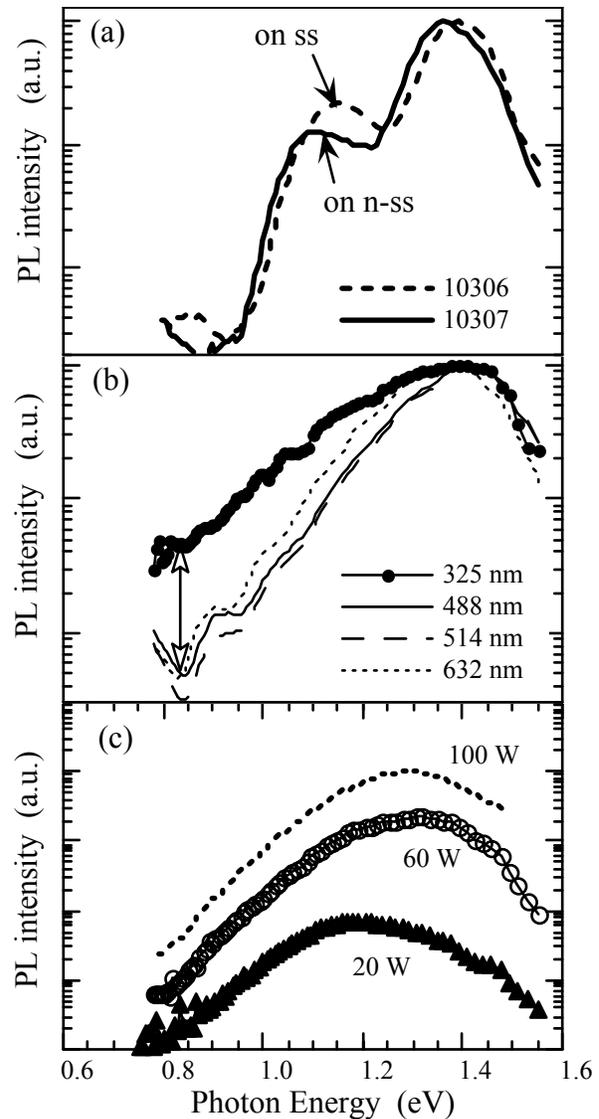


Fig. 3 PL spectra (a) for the 0.5- μm i-layer with and without an n-layer on ss substrate, (b) dependence on the excitation wavelength in a 1.4- μm thick a-/ μc -Si film, and (c) as function of rf power for H-diluted films 12464, 12466, and 12468 listed in table III.

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