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Optical Properties of Nanocrystalline Silicon Thin Films in Wider Regions of Wavelength

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Abstract

Nanocrystalline silicon thin films were prepared on corning (7059) glass substrates by means of a 150 MHz very high frequency plasma-enhanced chemical vapour deposition. An analysis about the effect of deposition times and substrate temperatures on the optical properties of nanocrystalline silicon is reported. Analysis by UV-Vis-Nir spectrophotometer showed that nc-Si films were almost transparent throughout the visible and infrared (IR) region mainly at $\lambda > 500$ nm, while strongly absorbed incident light occurred in the ultraviolet (UV) region. A blue-shift changes at energy around 2.3 eV is observed for absoprtion coefficient if compared to those of bulk silicon crystal due to quantum confinement of nc-Si. The effect of film thickness showed a strong relation in the absorption coefficient value. Thicker films at longer deposition times and lower substrate temperatures reduced absorption coefficient of the films. However, grain size and surface roughness also plays a major role. Optical energy band gap, E_g^{opt} deduced from Tauc's plot were found to be higher than 1.1.eV within the range of 1.7 - 2.3eV. These results were consistence with those obtained using PL measurements. The existence of nc-Si was previously confirmed using EDX and Raman analysis.

Keywords: nanocrystalline silicon; optical properties; absorption coefficient; energy bandgap

1. INTRODUCTION

Silicon is the main component used in semiconductor devices. However, due to its inability to emit light efficiently, their application is limited. After a report is made on visible photoluminescence (PL) from porous silicon in 1990, it has attracted much interest on the probability of developing silicon as principal material in optoelectronic devices [8, 9]. Extensive research on this particular material has shown that the existence of small crystallites, typically around 10 nm that is embedded in an amorphous matrix (nanocrystalline silicon) has effectively create new and unique properties compared to those of bulk crystalline silicon.

Nanocrystalline silicon (nc-Si) thin films are grown through various techniques such as pulsed laser deposition (PLD), magnetron sputtering, hot wire CVD (HW-CVD) and plasma enhanced CVD (PE-CVD). Among the techniques, the latter is the most used because of its ability to grow high quality nc-Si thin films at high deposition rate [3, 9].

Over the decade, various range of plasma excitation frequencies has been developed in hope to determine an optimum condition to grow high quality nc-Si thin films by using PECVD. However, research is more focused on the usage of low and medium high frequency (MHF). There are only a few report on nc-Si thin films grown using very high frequency (VHF) PECVD. In this paper, we grow nc-Si thin films using the highest plasma excitation frequency ever reported, which is a 150MHz VHF-PECVD. The purpose of this work is to see the effect of varied growth condition on the optical properties of the films.

2. EXPERIMENTAL DETAILS

Nc-Si thin films were prepared by a 150MHz VHF-PECVD technique on 7059 corning glass substrate with SiH_4 (g) as feed gas. To enhance the nucleation of nc-Si, SiH_4 is diluted in argon (g) with 1:9 ratios. Total gas flow rate and RF power is kept fixed at 10 sccm and 24 watt. Meanwhile, deposition time, t_D and substrate temperature, T_s are varied from 5 to 20 minutes and 100°C to 400°C, respectively. The thickness of the films were about 100-300 nm. The films thicknesses were determined from ellipsometer analysis.

Transmittance spectra for the films were analysed using UVVis-Nir. Data obtained from transmittance spectra is then used to determine the absorption coefficient, α (cm^{-1}). The optical energy gap, E_g^{opt} is found out by using Tauc's plot.

3. RESULTS AND DISCUSSION

3.1 Transmission and Absorption Coefficient

As light enter a medium, the loss of its intensity, if any, is caused by absorption. Portion of light that are not absorbed is said to be transmitted. Changes in deposition time and substrate temperature are found to be insignificant in the changes of light being transmitted for nc-Si thin films. Throughout the visible (vis) and infrared (IR) region, mainly at $\lambda > 500$ nm, only a very small portion of light is being absorbed, thus films are almost transparent in these regions. However, a strong light absorption occurred in the ultraviolet (UV) region.

The absence of absorption in the visible and infrared region is because in these regions, photons do not have sufficient energy to cause electronic transition from valence band (VB) to higher energy state. The transition can only occur if the incident photon corresponds exactly to the energy gap associated with the films. Electronic transition does not occur in the condition where photons are insufficiently energetic or too energetic. However, the energy of incident photon is sufficient enough to be absorbed in the ultraviolet region thus; absorption is present in this region [11]. Figure 1 shows the transmittance spectra for films prepared at various substrate temperatures.

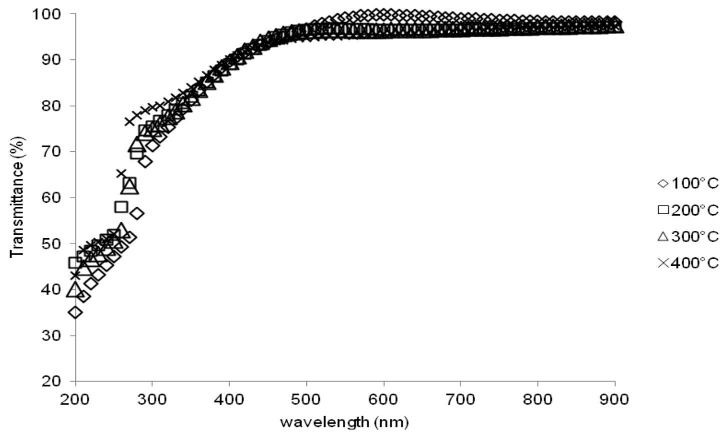

Figure 1: Transmittance spectra for samples prepared at various substrate temperature

In this study, the domination of quantum confinement effect on the optical properties of nc-Si can be observed from the blue-shift of the absorption threshold value with respect to bulk c-Si. The reduction to nanoscale size also causes a decrease in electrons state densitywhich reduces the absorption coefficient value as observed in figure 2 and 3 [6].

The shifting of absorption threshold value is strongly related to the variation in grain sizes. As grain size gets larger, the interaction between electrons in Si-Si bond grows stronger and causes a band gap widening. Therefore, enhancement in grain size is likely to shift the absorption threshold value to lower energy [10]. The observed red-shift as growth time is prolonged and substrate temperature is higher complies with larger grains as determined by Raman analysis.

It is also observed that the values of absorption coefficient are lower for sample prepared at longer deposition time. The reduction in absorption value is a result of increased film thickness. As samples are prepared at a longer deposition time, the film becomes thicker. Since absorption coefficient is inversely proportional to the thickness of film, *d* as shown by eq. (1), the obtained results correspond well with the theory [2, 7]. On the other hand, samples prepared at higher substrate temperature have lower thickness, therefore, higher absorption.

$$\alpha = -\frac{1}{d}\ln T \qquad (1)$$

With α = absorption coefficient, d = thickness of film and T = transmittance (%)

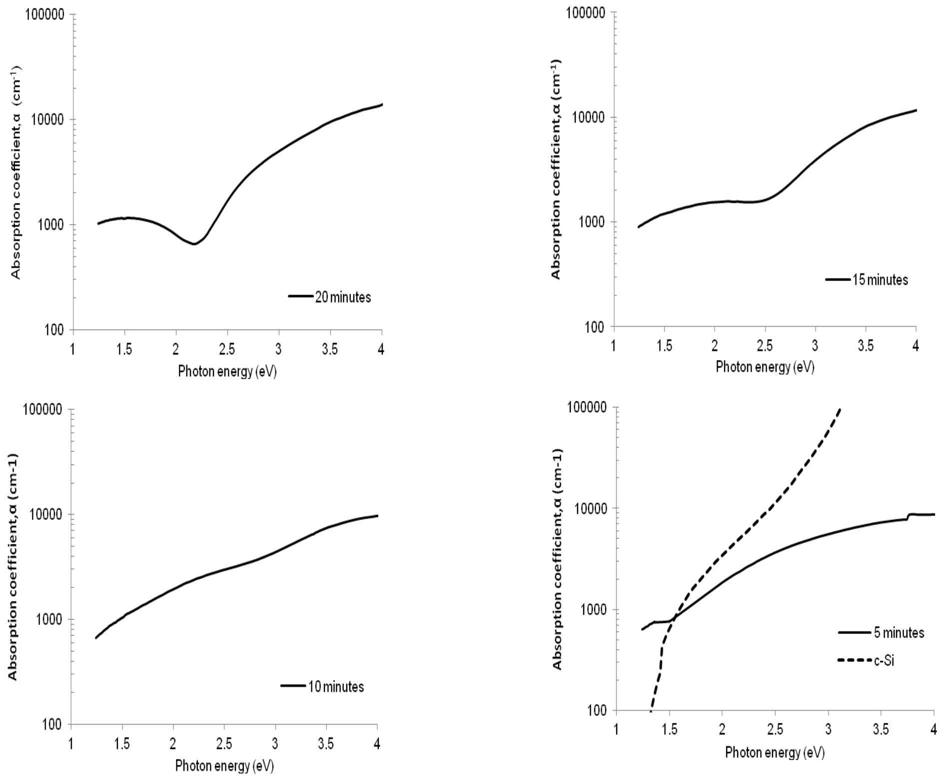

Figure 2: Absorption coefficient for nc-Si thin films prepared at deposition times of 5, 10, 15 and 20 minutes

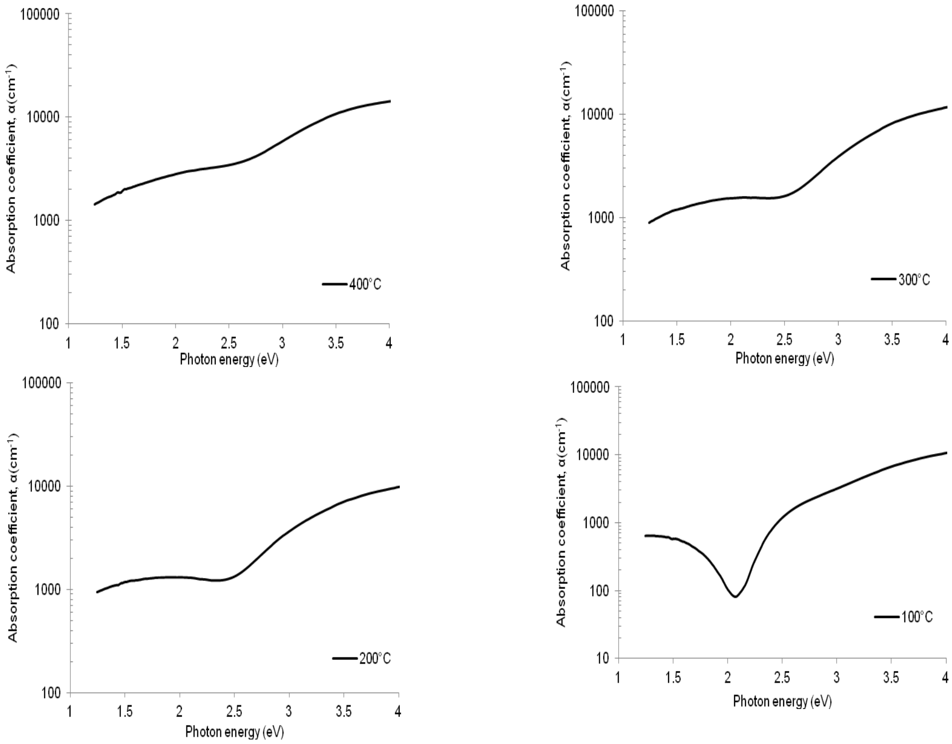

Figure 3: Absorption coefficient for nc-Si thin films prepared at substrate temperature of 100°C, 200°C, 300°C and 400°C

3.2 Optical Energy Band Gap

Optical energy band gap, E_g^{opt} is obtained by plotting $(\alpha h\nu)^{1/2}$ vs $h\nu$ and extrapolating the linear part of the graph to where $(\alpha h\nu)^{1/2} = 0$. Table 1 tabulates the E_g^{opt} obtained from the samples.

Table 1: Optical energy band gap, E_g^{opt} for samples prepared at different deposition conditions

Growth conditions		Optical band gap, E_g^{opt} (eV)
Deposition time (minutes)	5	-
	10	2.02
	15	2.00
	20	1.98
Substrate temperature, °C	100	2.18
	200	2.02
	300	2.00
	400	1.89

From table 1, E_g^{opt} obtained from analysis on the films are higher than bulk c-Si (1.12eV). The energy band-gap widening is consistent with quantum confinement effect expected with the shrinking of Si grains into nanoscale. A similar declining trend is observed in E_g^{opt} as growth process progressed. The trend is in good agreement with enlargement in grain size at longer deposition time and higher substrate temperature [10,16,5]. The decrease in E_g^{opt} was also previously reported as a result of increasing film thickness [12, 4, 2]. This is true for the films grown at increasing deposition time. However, thinner films obtained as substrate temperature is higher do not comply with the report. This contradictive result might be due to the differences in the film thickness where in previous report, the film thickness is reported as 190 nm, 405 nm and 490 nm whereas in this study, the film thickness is below 300 nm. This shows that at lower thickness, E_g^{opt} is dominated by grain size instead of thickness of the films.

4. CONCLUSIONS

We prepared nc-Si thin films by a PECVD tehnique using a SiH_4/Ar gas mixture. The optical properties were studied by increasing deposition time from 5 to 20 minutes and substrate temperature from 100°C to 400°C. It was found that due to quantum confinement effect, the absorption threshold value shifted to higher energy compared to those of bulk c-Si. Although film thickness strongly affect total absorption coefficient value, it does not play a major role in the determination of E_g^{opt}. Instead, enlargement of grain size causes red-shift in absorption threshold value and decrease E_g^{opt}.

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REFERENCES

[1] Ali, A.M. (2007). Optical properties of nanocrystalline silicon films deposited by plasma-enhanced chemical Vapor deposition. *Optical Materials.*30, 238-243.

[2] Bakry, A.M. (2008). Influence of film thickness on optical properties of hydrogenated amorphous silicon thin films. Egypt. J. Solids, Vol. (31), No. (1), 11-22.

[3] Cao, G. (2004). *Nanostructures & Nanomaterial: Synthesis, Properties,& Applications,* New Zealand: John Wiley & Sons.

[4] Demichelis, F., G.Kanidakis, E.Mezzetti, P.Mpawenayo, A.Tagliaferro, E.Tresso, P.Rava and G.Della, (1987).Influence of film thickness on optical and electrical properties of hydrogenated amorphous silicon. *Thin Solid Films*, 150, 1.

[5] Iori, F. and S.Ossicini, (2009). Effect of Simultaneous Doping with Boron and Phosphorous on the Structural, Electronic and Optical Properties of Silicon Nanostructures. *Physica E: Low-dimensional Systems and Nanostructures.* 41 (6), 939-946.

[6] Jadkar, S.R., A.M.Funde, N.A.Bakr, D.K.Kamble, R.R.Hawaldar, and D.P.Amalnerkar, (2008). Influence of hydrogen dilution on structural, electrical and optical properties of hydrogenated nanocrystalline silicon (nc-Si:H) thin films prepared by plasma enhanced chemical vapour deposition (PE-CVD). *Solar Energy Materials & Solar Cells.* 92, 1217-1223.

[7] Jenkins, F.A. and H.E. White, (1981). *Fundamentals of Optics Fourth Edition*. Singapore: McGraw-Hill, Inc.

[8] Jutzi, P and U.Schubert, (Eds.).(2003). *Silicon Chemistry – From the Atom to Extended System.* (44-57).

[9] Weinheim : Wiley-VCH Kumar, V. (2008). *Nanosilicon (1^{st} ed)*, Oxford, UK: Elsevier.

[10] Nakajima, A., Y.Sugita, K.Kawamura, H.Tomita, and N.Nokoyama, (1996). Microstructure and optical absorption properties of Si nanocrystals fabricated with low-pressure chemical-vapor deposition. *J. Appl. Phys.* 80 (7), 4006-4011.

[11] Poole Jr, C.P. and F.J. Owens, (2003). *Introduction to Nanotechnology.* New Jersey: John Wiley and Sons.

[12] Talukder, G., J.A.Cowan, D.E.Brodie and J.D.Leslie, (1984). Thickness and doping effects observed in impure vacuum deposited a-Si films. *Can.J.Phys.*, 62, 848