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Structural, Optical and Electronic Properties of Hydrogenated Amorphous Silicon Thin Films

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Abstract

In the present research paper of hydrogenated amorphous silicon thin films have been deposited by plasma enhanced chemical vapour deposition (PECVD) technique. Normally device quality Hydrogenated amorphous silicon (a-Si:H) films are deposited at very low power but our aim is to deposit this thin films at high growth rate by applying high power density to cathode. The influence of the nature of the high growth rate on the structural, optical and electronic properties of the Hydrogenated amorphous silicon (a-Si:H) films has been studied. Structural properties were investigated by using x-ray diffraction and atomic force microscope, optical ones by using a UV–visible spectrophotometer and electronic properties by means of dc four-probe resistivity measurements. The refractive index, extension coefficient, energy band gap with various thickness of thin film is investigated using Manificier et.al method.

Keywords: Amorphous Material, PECVD technique, surface morphology, refractive index, extinction coefficient, energy band gap, Resistivity measurements.

Introduction

Hydrogenated amorphous silicon (a-Si:H) has evolved into an ubiquitous materials system in large-area electronics for many commercial applications ranging from liquid-crystal displays to medical imaging[1-4]. Its play a prominent role in microelectronics industry and silicon IC industry for device fabrication. Since a notable fraction of the device processing cost lies in photolithographic techniques, last few years hydrogenated amorphous silicon (a-Si:H) has received a great demand in the field of Thin Film Transistor (TFT), Solar cells and Opto-electronics device technology[5-8]. Structural and Optical properties of a-Si: H is varying due to deposition method and its structural flexibilities in the Plasma Enhance Chemical Vapour Deposition (PECVD) technique. While we apply glow discharge to SiH_4, the plasma will generate in the chamber and deposit on the glass substrate[9]. The properties of a-Si: H is influenced by the amount of hydrogen bond to silicon, which is controlled by substrate temperature and the hydrogen-silicon surface chemistry.

In this research paper structural and optical property of a-Si: H films have been studied by Plasma Enhance chemical Vapour deposition technique at high growth rate by applying high power (3-14 w) density to cathode [10]. Optical properties, such as absorption coefficient, energy band gap and refraction index have been investigated by UV-VIS double beam spectrometer (Shimadzu, Japan, Model UV 2401 PC SHIMADZU) and structural and morphological properties of the films analyzed by X-Ray diffraction and atomic force microscopy (AFM). While electronic properties investigated by means of dc four-probe resistivity measurement technique.

Methodology

Experimental Technique: Plasma Enhance Chemical Vapour Deposition (PECVD) technique is the most commonly used technique for deposition of a-Si:H thin films. In Plasma Enhance Chemical Vapour Deposition (PECVD) technique processing glow discharge plasma sustain within chamber where simultaneous CVD reaction occur. Deposition of a-Si: H is done using RF-PECVD technique in capacitive coupling mode. In this we use a vacuum chamber, the body of chamber is taken as anode and inside the chamber a cathode plate is used for feeding recently saline SiH4 and Ar with flow rate 24-25 sccn. The deposition of a-Si:H films based on the generation of an Ar plasma using high rf power density of 3.18 w/cm^2. The films thickness was different at different pressure 6×10^{-6} Torr to 7×10^{-6} Torr. The temperature during deposition was fixed at 300^0 C without turning on the bias rf power. We kept Si vapors inside the chamber at the desired vacuum for the thin film deposition. As the Si plasma generated in the chamber then it will be deposited on the glass substrate. Our all films were grown in the similar ways. The thickness of a-Si:H films was measured by UV Spectrometer. The surface Morphology of each sample was scanned by atomic force microscopy (AFM) on a 1×1 μm area at a scan rate of 1Khz and structure of a-Si:H is investigated by x-ray diffraction (XRD) at scan angle (0.5^0 – 1^0) with slow motion.

Optical properties: Transmission spectra of a-Si:H films were recorded at room temperature with the help of UV-VIS double beam spectrometer Shimadzu JAPAN (model UV 2401 PC Shimadzu) in the wavelength range 300-900 nm. The optical constants such as refractive index, extinction coefficient and thickness of a-Si: H thin films have been investigated from transmission spectra by using Manifacir's envelope method which shows the interference pattern[11]. The transmission spectra of a-Si: H films have been recorded in the range from 300-900 nm. The refractive index (n), extinction coefficient (k), thickness (t) and optical bend gap has been determined from transmission spectra Figure-1 a and b. The value of n, k and t are shown in Table-1 a and b and determined by the following formulas [12, 13].

$$n = \sqrt{[N + (N^2 + n_0^2 n_1^2)^{1/2}]} \quad (1)$$

Where n is refractive index of given substrate thin film, n_0 and n_1 are the refractive index of air and substrate respectively

The number N is given by the following equation

$$N = \left[\left(n_0^2 + n_1^2\right)^2 / 2\right] + 2 n_0 n\left[\left(T_{\max} - T_{\min}\right) / T_{\max} T_{\min}\right] \quad (2)$$

Where $T_{\max}$ and $T_{\min}$ are the upper extreme point and lower extreme point at a particular wavelength respectively

The excitation coefficient

$$k = \left(-\lambda / 4\pi t\right) \log P \quad (3)$$

Where t is the thickness of the film and P is given by the following equation

$$P = C_1 / C_2 \left[\frac{1 - \left(T_{\max} / T_{\min}\right)}{1 + \left(T_{\max} / T_{\min}\right)}\right] \quad (4)$$

with $C_1 = (n + n_0)(n + n_1)$ and $C_2 = (n - n_0)(n_1 - n)$

The optical band gap is determined from UV Transmittance by Tauc relation

$$(\alpha h\upsilon)^{1/2} = B\left(h\upsilon - E_{opt}\right) \quad (5)$$

The graph between $(\alpha h\upsilon)^{1/2}$ and $h\upsilon$ as shown in Figure-2 a and b, which gives the values of optical band gap.

Structural properties: The X-Ray diffraction pattern of a-Si:H films is also reported with the help of a X-Ray diffractometer by using CuKα radiation (λ = 1.54045Å)[14]. The d values are obtained from the spectra were compared with standard ASTM data and confirm the structure of a-Si: H film.

The morphological properties of deposited thin films have been investigated by AFM and related to optical properties[15, 16]. AFM measurement was made in air by a nano Rth AFM system (HTMDT, NTEGRA) Institute Instrumentation Center, IIT Roorkee 247667, operating in close contact mode. Silicon canonical tips of 10 nm radiuses mounted on silicon cantilever of 125 μm length 42 n/m force constant and 320 KHz reasonable frequency wave used. Physical topography, roughness and dimension of the surface features were evaluated.

Resistivity measurements: Electrical resistivity of the a-Si:H thin films was determined by the dc four-probe resistivity method in the temperature range 15–300 K. The resistivity curve Figure-5 of the a-Si:H films deposited on glass substrate show a negligible change in the resistivity in going from 40 to 300 K. a-Si: H thin films show its behavior similar to heavily doped semiconductors[17].

Result and Discussion

Figure-1 a and b shows the transmission spectra of a-Si: H thin film. The values of T_{max} and T_{min} were determined at different wavelengths and values of N and n were calculated by substituting T_{max} and T_{min} in a standard equation. The obtained data is reported in Table-1 a and b. It is observed that as the wavelength (λ) increases, refractive index (n) decreases and there it again increases above the wavelength 787.67nm and the extinction coefficient is also decreases. The transmission spectrum varies from 80% to 60% which is nearest to the Manifacir's transmission spectra (85%). So we can say that our sample is good fabricated. The thicknesses of these films are also estimated by this method. Which were found to be in the range of all three samples 0.6 μm to1.5μm.

The optical band gap of film found from UV Transmittance and plotting a Tauc graph between $(\alpha h\upsilon)^{1/2}$ and hυ.

From Tauc graph the values of optical band gap varies from 1.93 to 1.72 ev. Which is suitable for optoelectronic devices and the structural properties are reported by X-Ray diffraction and AFM technique.

The x-ray diffraction studies were done on all the samples without exception as grown and heated, were amorphous in nature Figure-3 a and b illustration the nature of diffractograms obtained. The small hump seen in the diffractogram is characteristic of the short range ordering present a-Si:H films. However no peaks indicating the non crystalline nature of a-Si:H were seen. This can be expected since the amount of material (a-Si: H) for scattering x-ray may not be sufficient. This shows that the material is amorphous in nature.

The structural properties of a-Si:H is also reported by AFM. Figure 4 a and b shows that the AFM 2×2μm^2 images of the surface of the films deposition respectively at (3 -14 w) as it can be seen Average roughness Sa 5.47517, RMS Sq 7.5549, surface skewness (Ssk) 1.47316 and entropy 8.38606. When rf plasma power increases from 3 W to 14W the particle size varies from 92 nm to 20 nm. These films are very flat and rms roughness rises from 15 nm to 5 nm.

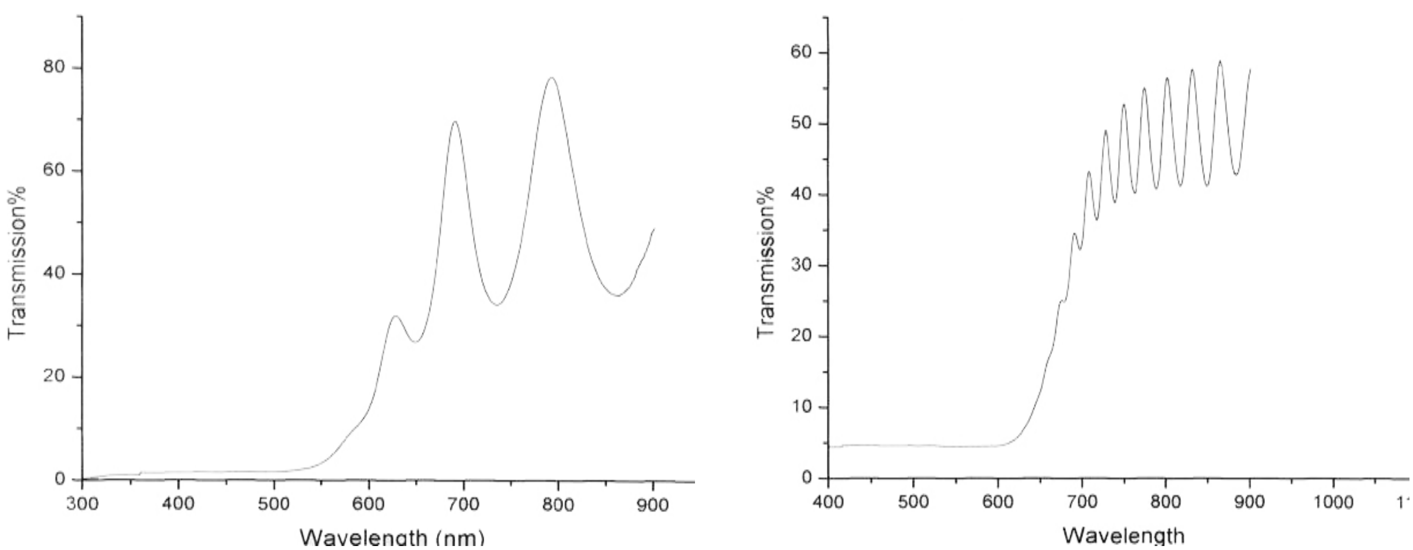
Table-1
Variation of refractive index (*n*) and extinction coefficient (*k*) for a-Si: H thin films with wavelength. Where λ is wavelength in nm, T_{max} and T_{mi}n upper extreme point and lower extreme point, k extinction coefficient, t thickness in μm and n refractive index

(1-A)

S.No.	λ (nm)	T_{max}(%)	T_{min} (%)	N	t (μm)	k
1.	649	69.17	27.4	2.123029	0.6	-7275166
2.	733.83	77.627	34.141	2.100369	0.6	-7963804

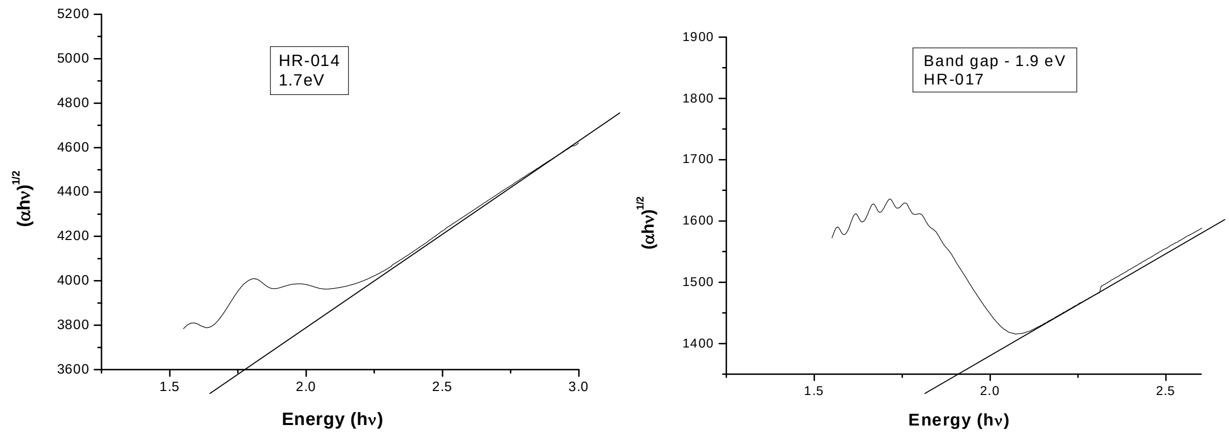
(1-B)

S.No.	λ (nm)	T_{max} (%)	T_{min} (%)	N	t (μm)	k
1.	696.91	43.04	32.29	2.065748	1.5	-152717.3
2.	717.64	48.77	36.51	2.062374	1.5	-159655.2
3.	739.21	52.73	38.78	2.062122	1.5	-174535
4.	761.9	54.738	40.4	2.06078	1.5	-178380.8
5.	787.67	56.21	41.19	2.060795	1.5	-188579.6
6.	817.36	57.266	41.45	2.061492	1.5	-202610.6
7.	847.89	58.47	41.3	2.063267	1.5	-223424.9



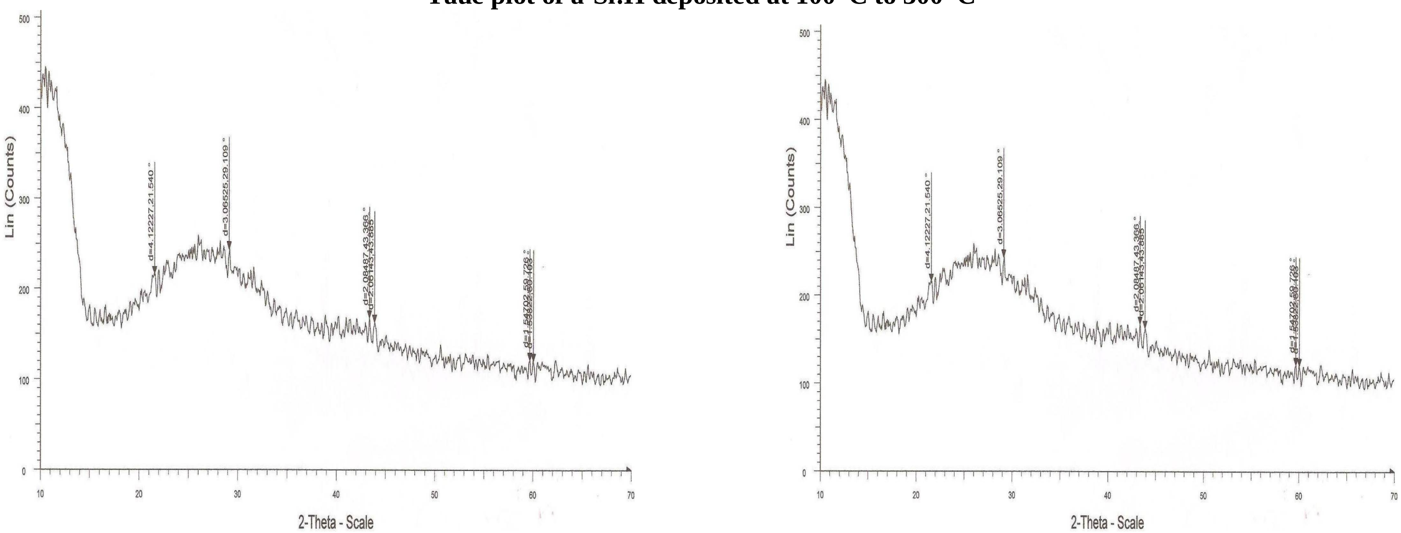
(a) **(b)**

Figure-1
Optical transmission spectra of a-Si: H thin film



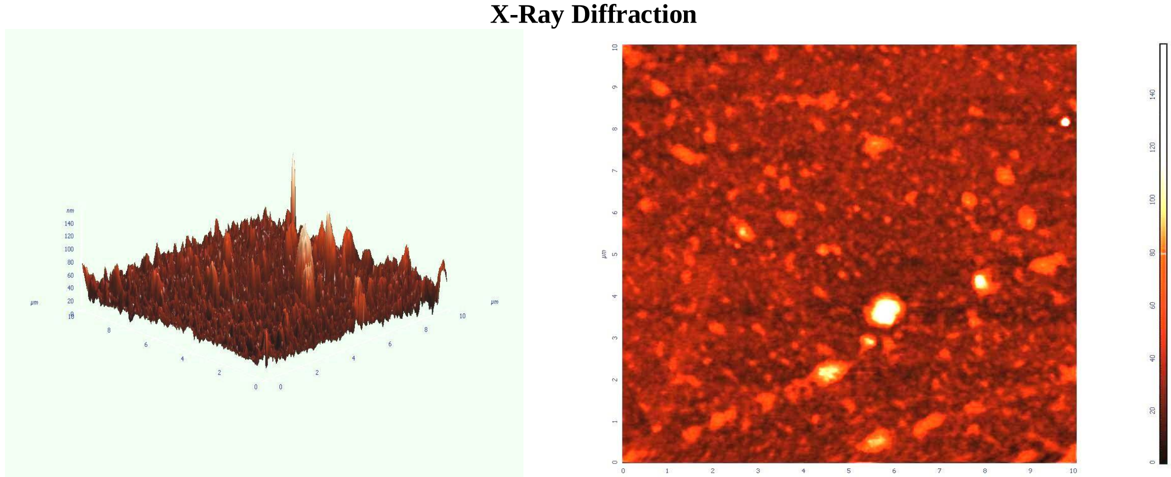
(a) **(b)**

Figure-2
Tauc plot of a-Si:H deposited at 100^0 C to 300^0 C



(a) **(b)**

Figure-3
X-Ray Diffraction



(a) **(b)**

Figure-4
Atomic Force Microscope

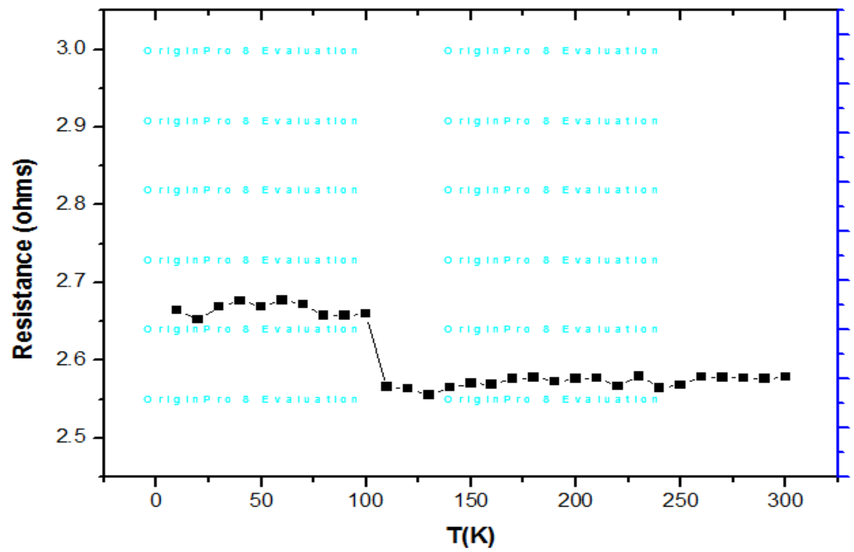


Figure-5
Resistivity measurements of a-Si:H thin film.

Conclusion

Our work to deposit thin film of a-Si:H by high rate PECVD technique, which play a prominent role in thin film technology. As conclusion from our study is Si crystalline vapor converted into plasma and it is deposited on the substrate due to disorder in the crystallization. Si becomes in the amorphous structure and increase the density of state near the conduction and valance band. The narrowing of energy band gap and increasing of the absorption tail with rf plasma both confirm the defects which is better explained by concentration of dangling bonds and due to dangling bonds the localized states will be increased in the sample. The resistivity data showed that deposited film a-Si:H have heavily doped semiconductors nature. This work is useful and powerful in PECVD technique for solar cell and device fabrication (TFT) technology.

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