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Optical Transmission Measurements on Glow-Discharge Amorphous Silicon Nitride Films

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Abstract

Hydrogenated amorphous silicon nitride films have been prepared by the glow-discharge decomposition of ammonia/silane gas mixture. From optical transmission measurements in the wavelength range from 400 nm to 1100 nm refractive indices absorption coefficients and optical Tauc gaps of the films have been obtained. A systematic investigation of optical parameters has been carried out as a function of the nitrogen content of samples.

Key Words: A. Optical transmission; B. Refractive index; C. Swanepoel method D. Hydrogenated amorphous silicon nitride

1. Introduction

Hydrogenated amorphous silicon ($a\text{-}Si{:}H$) and its alloys ($a\text{-}Si_{1-x}C_x{:}H$, $a\text{-}SiN_x{:}H$ etc.) are important materials for photovoltaic and microelectronic devices. In this study we report the effect of nitrogen on the optical properties of hydrogenated amorphous silicon nitride films ($a\text{-}SiN_x{:}H$). Optical transmission measurements were carried out to determine the film thickness, the wavelength dependence of the refractive index and optical absorption coefficient. The optical constants were determined from the optical transmission measurements using the method described by Swanepoel [1].

1.1. Swanepoel method:

A thin film on a transparent substrate is shown in Figure 1. In the figure d, n, α and T denote the film thickness, the refractive index, the absorption coefficient and the transmission, respectively. The transparent substrate has a thickness several orders of magnitude larger than d and has index of refraction s and absorption coefficient $\alpha_s = 0$.

The index of refraction for air is taken to be $n_0 = 1$. The transmission spectrum can roughly be divided into four regions. In the transparent region (α=0) the transmission is determined by n and s through multiple reflections. In the region of weak absorption α is small and the transmission begins to decrease. In the medium absorption region α is large and the transmission decreases mainly due to the effect of α. In the region of strong absorption the transmission decreases drastically due almost exclusively to the influence of α.

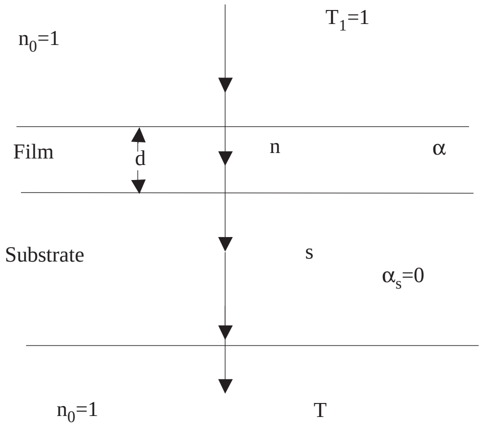

Figure 1. System of an absorbing thin film on a thick finite transparent substrate.

If the thickness d is uniform, interference effects give rise to the spectrum, shown by the full curve in Figure 2. These interference fringes can be used to calculate the optical constants of the film. The basic equation for interference fringes is

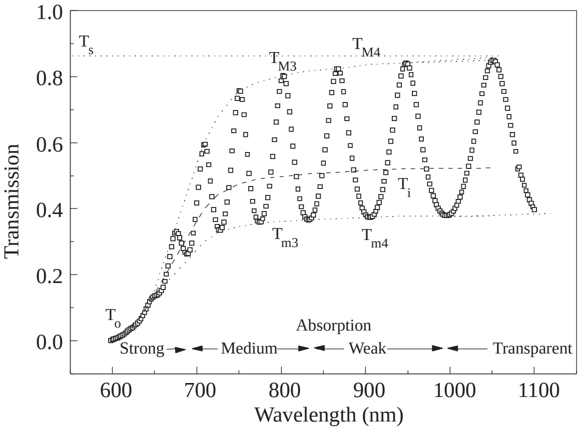

Figure 2. Measured transmission spectra of *a-Si:H* thin film on glass substrate.

$$2nd = m\lambda, \tag{1}$$

where m is an integer for maxima and half integer for minima.

The transmission T, for the case of Figure 2, is given as

$$T = T\left(n, x\right) = \frac{Ax}{B - Cx\cos\phi + Dx^2}, \tag{2}$$

where

$$A = 16n^2 s \tag{3a}$$

$$B = \left(n+1\right)^3\left(n+s^2\right) \tag{3b}$$

$$C = 2\left(n^2-1\right)\left(n^2-s^2\right) \tag{3c}$$

$$D = \left(n-1\right)^3\left(n-s^2\right) \tag{3d}$$

$$\phi = 4\pi nd/\lambda \tag{3e}$$

$$x = \exp\left(-\alpha d\right). \tag{3f}$$

If T_M and T_m are maximum and minimum values of the transmission and T_s is the maximum value of the transmission in the absence of the film, then substrate refractive index s, T_M and T_m are given by the following equations:

$$s = \frac{1}{T_s} + \left(\frac{1}{T_s^2} - 1\right)^{1/2} \tag{4}$$

$$T_M = \frac{Ax}{B - Cx + Dx^2} \tag{5}$$

$$T_m = \frac{Ax}{B + Cx + Dx^2}. \tag{6}$$

The absorption coefficient α for the regions of weak and medium absorption will be non-zero. From the equations (5) and (6) we obtain an equation that is independent of x:

$$\frac{1}{T_M} - \frac{1}{T_m} = \frac{2C}{A}. \tag{7}$$

1.2. Determination of $n(\lambda)$, $\alpha(\lambda)$ and the thickness d:

The method to determine the optical constants is based on the parabolic fitting procedure of adjacent maximum (T_M) and minimum (T_m). Substituting equation (3) into (7) and solving for n yields

$$n = \left[N + \left(N^2 - s^2\right)^{1/2}\right]^{1/2}, \tag{8}$$

where

$$N = 2s\frac{T_M - T_m}{T_M T_m} + \frac{s^2+1}{2}. \tag{9}$$

If n_1 and n_2 are the refractive index at two adjacent maxima (or minima) at λ_1 and λ_2, then the film thickness is given by

$$d = \frac{\lambda_1 \lambda_2}{2\left(\lambda_1 n_2 - \lambda_2 n_1\right)}. \tag{10}$$

Once $n(\lambda)$ is known, all the constants in equation (3) are known and x can be calculated. Addition of the reciprocals of equations (5) and (6) gives

$$\frac{2T_M T_m}{T_M + T_m} = \frac{Ax}{B + Dx^2}. \tag{11}$$

Solving for x yields

$$x = \frac{F - \left[F^2 - \left(n^2-1\right)^3\left(n^2 - s^4\right)\right]^{1/2}}{\left(n-1\right)^3\left(n - s^2\right)}, \tag{12}$$

where

$$F = \frac{8n^2 s}{T_i} \tag{13}$$

and

$$T_i = \frac{2T_M T_m}{T_M + T_m}. \tag{14}$$

$\alpha(\lambda)$ can be calculated from x and d using Equation (3f).

1.3. Determination of optic band gap, B parameter and E_{04} energy:

The relation between absorption coefficient and optic band gap are given by Tauc equation [2,3]:

$$\sqrt{\alpha h\nu} = B(h\nu - E_g^{opt}), \tag{15}$$

From the graph of $(\alpha h\nu)^{1/2}$ versus $h\nu$ one obtains E_g and B parameter. B is also a useful diagnostic of the material since it is inversely proportional to the extent of the tail state (ΔE) at conduction and valance band edges. B is given by

$$B \approx \pi^2 \sigma_0 (nc\Delta E)^{-1}, \tag{16}$$

where σ_0 is the minimum metallic conductivity, n is the refractive index and c is the velocity of light. E_{04} is the photon energy at which the absorption coefficient reaches α=10^4 cm^{-1}.

2. Experimental Details

The samples were prepared in an rf glow-discharge apparatus, using $SiH_4 + NH_3$ gas mixtures. Corning 7059 glass were used as substrates. The substrate temperature was kept constant at 300 ^{o}C, the rf power was held at 5 W, and the total gas pressure was fixed at 200 mTorr. Nitrogen content in the samples has been obtained from the relative partial pressure of NH_3 and SiH_4 gases in the glow-discharge system, defined by the following ratio;

$$r = \frac{[P_{NH_3}]}{[P_{NH_3}] + [P_{SiH_4}]} \quad . \tag{17}$$

Transmission spectra in range from 400 nm to 1100 nm were recorded using a CVI DK-240 monocromator. The film thickness, refractive index, absorption coefficient with dependence of wavelength were determined using the Swanepoel method. In addition, dependence of these parameters upon nitrogen content was also investigated.

3. Experimental Results

The refractive index $n(\lambda)$ and optical absorption coefficients $\alpha(\lambda)$ as functions of wavelength were determined from the optical transmission measurements. As a result of absorption coefficient data we calculated E_{04} energy, E_g optical band gap and the B parameter from the Tauc equation. The film thicknesses d were determined by refractive index data. For all samples, E_g, B, E_{04}, $n(\lambda$=700 nm) and film thickness values are given in Table 1.

The wavelength dependence of the refractive index has been calculated in the range between 400 nm to 1100 nm on the a-SiN_x:H films. As shown in Figure 3 , the refractive index becomes constant in the long wavelength region and increases slowly in the short wavelength range.

A plot of the refractive index n at λ=700 nm versus nitrogen content r is presented in Figure 4. The refractive index remains constant for the small amount nitrogen content (r=0.1) and then decreases very rapidly with further increases in r. Similar behaviour in refractive index has been observed by Sotiropoulus et al. [4] and Güngör et al. [5] for the samples prepared in rf glow- discharge system mixing $N_2 + SiH_4$ gasses.

Table 1. For all samplesE_g, B, E_{04}, $n(\lambda$=700nm) and film thickness values which determined from the optical transmission measurements.

Sample	***r***	***E_g^{opt} (eV)***	***B ($cm^{-1}eV^{-1}$)***	***E_{04} (eV)***	***n(λ=700nm)***	***d(μm)***
S112	0.00	1.70	632.7	1.92	3.57	1.44
NH111	0.05	1.82	1011.2	1.91	3.62	1.17
NH122	0.10	1.83	991.8	1.95	3.53	1.23
NH151	0.15	1.83	930.1	1.98	3.23	1.42
NH131	0.25	1.90	686.3	2.06	3.02	1.31
NH141	0.50	1.96	499.7	2.27	2.53	1.33
NH83	0.90	3.30	790.4	3.56	1.73	0.43

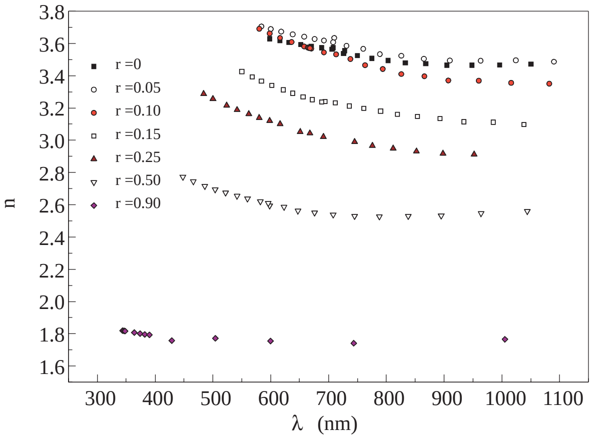

Figure 3. The refractive index as a function of the wavelength for various nitrogen content r.

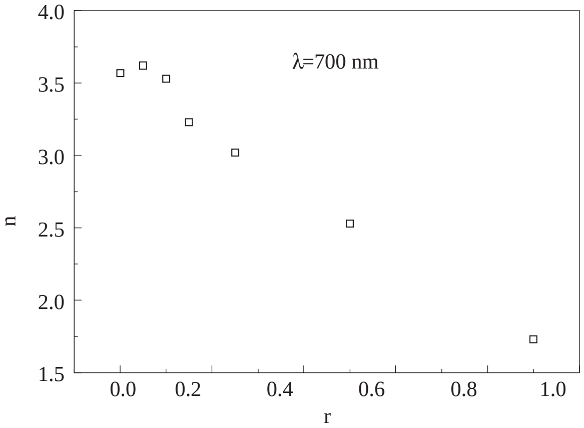

Figure 4. The refractive index as a function of nitrogen content at λ=700 nm.

The optical gap E_g was determined for each sample. The resulting values are shown as a function of nitrogen content in Figure 5. E_g is nearly independent of nitrogen content below a threshold concentration of r=0.5 and increases rapidly above this concentration. This observation is consistent with the band edge energies calculated by Robertson [6] and the optical gap measured by Herak et al. [2] and Hasegawa et al. [7]. We have also plotted E_{04} versus r in Figure 6. It seems clear that E_{04} increases with increasing nitrogen content. It means that absorption edge goes to a high energy level with increasing r and films become transparent at the highest nitrogen content (r = 0.90).

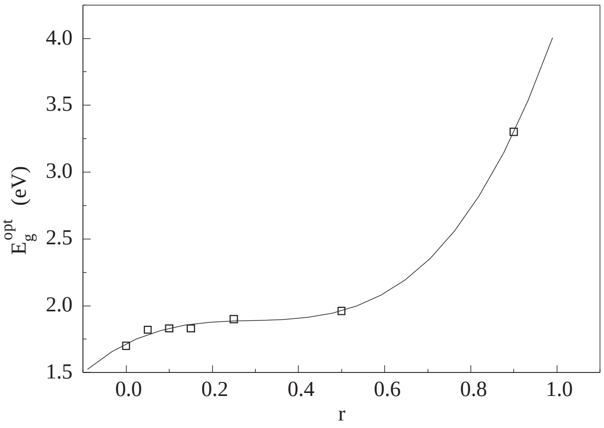

Figure 5. The optical band gap E_g deduced from Tauc plots as a function of nitrogen content r.

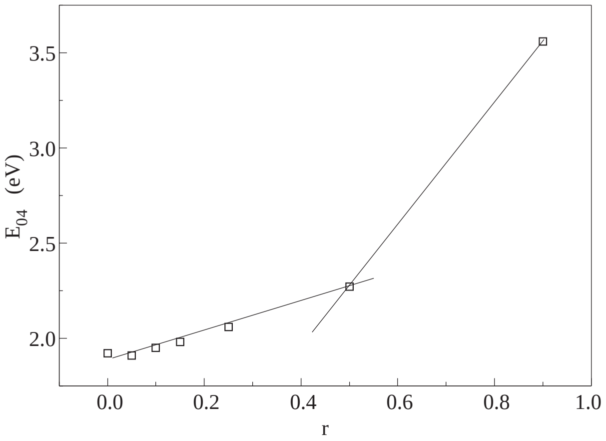

Figure 6. The E_{04} energy as a function of nitrogen content r.

The parameter B decreases when the nitrogen rate increases as shown in Table 1.

Since B is inversely proportional to the extent of the tail states as given in (16), ΔE must increase with increasing nitrogen content.

4. Conclusions

The experimental results obtained in this study are summarized as follows:

1) Refractive index is constant in the long wavelength range and increases in the short wavelength range.

2) Refractive index is nearly unchanged for a very small nitrogen concentration region ($0 < r \leq 0.10$) but decreases rapidly with further increase in r.

3) The optical gap is approximately independent of nitrogen content for $r \leq 0.5$.

4) Absorption edge goes into the high energy range with increasing nitrogen content.

5) The films become transparent for the highest nitrogen content (r=0.90).

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