CHAPTER 3

EXPERIMENTAL AND CALCULATION TECHNIQUE

3.1 Introduction

Hydrogenated amorphous silicon (a-Si:H) prepared by the glow discharge decomposition of silane (SiH₄) has become very important in the field of thin film device applications. The growth conditions of a-Si:H films have been defined by a set of discharge parameters such as gas pressure, silane concentration, gas flow rate, radio frequency power and substrate temperature. Varying the discharge parameters in a wide range will lead to the optimization of the processing conditions for the growth of a-Si:H. In order to achieve further improvements in its physical properties, chemical reactions during the plasma deposition has to be clarified quantitatively, not only in regard to the compositions of excited molecules in the plasma, but also on the mutual interaction among the reactive species in the gas phase as well as on the substrate surface.

In this work, argon gas is used to interfere the deposition process of silicon. Argon gas and silane gas is allowed to flow together at different argon to silane flow rate ratio ranging from 3.00 to 0.25. A total of eight sets of samples have been prepared including two sets prepared without argon dilution. The set of samples without argon dilution was fixed at silane flow rate of 20 sccm and 5 sccm. These samples are meant to be the controlling set of high silane flow rate and low silane flow rate respectively.
<table>
<thead>
<tr>
<th>Argon to silane flow rate ratio</th>
<th>± 0.05</th>
<th>0.25</th>
<th>0.5</th>
<th>0.75</th>
<th>1.00</th>
<th>2.00</th>
<th>3.00</th>
<th>Pure silane 5 sccm</th>
<th>Pure silane 20 sccm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deposition pressure (mbar)</td>
<td>± 0.01</td>
<td>0.40</td>
<td>0.50</td>
<td>0.60</td>
<td>0.26</td>
<td>0.37</td>
<td>0.46</td>
<td>0.10</td>
<td>0.46</td>
</tr>
<tr>
<td>Ionization current (mA)</td>
<td>± 1</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Ionization voltage (V)</td>
<td>± 1</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>600</td>
</tr>
<tr>
<td>Substrate temperature (°C)</td>
<td>± 1</td>
<td>27</td>
<td>27</td>
<td>27</td>
<td>27</td>
<td>27</td>
<td>27</td>
<td>27</td>
<td>27</td>
</tr>
</tbody>
</table>

Table 3.1: Discharge parameters of the deposition process.
The gas pressure is monitored throughout the deposition process whereas other discharge parameters are fixed at the same values for every deposition. Table 3.1 shows the discharge parameters of the experiment.

3.2 Plasma Glow Discharge Technique

a-Si:H films have been prepared by plasma decomposition of silane gas since 1969. Glow discharge preparation units can be divided into two groups\(^1\), depending on the method of coupling the radio frequency excitation into the plasma. The first glow discharge deposition of amorphous silicon was carried out in an inductively coupled system designed by Sterling\(^2\) and his collaborators. The Dundee\(^3\) group then adopted the same approach in the studies of the electronic properties of material. In the latter, inductively coupled reactors are still used as a convenient method for depositing small area specimens. Of all the preparation techniques, a-Si:H deposited by silane glow discharge is found to have structural, chemical and electronic properties which are very dependent on the deposition conditions.

The system used to deposit a-Si:H films in this experiment is the horizontal plasma glow discharge system in which the discharge chamber is placed in horizontal position. The characteristics of the films produced by the plasma glow discharge technique are governed by numerous variables such as the reactor geometry, electrode configuration and separation, power level and frequency, gas composition, gas flow rate, deposition pressure and substrate temperature.
The schematic diagram of the horizontal plasma glow discharge system is presented in figure 3.1. The system consists of five major components consisting of the deposition chamber, the pumping system, the gas distribution system, the high voltage direct current power supply and the detoxification system. Details of every component will be discussed later in this chapter.

3.2.1 The Deposition Chamber

The DC horizontal plasma glow discharge deposition chamber used in this experiment was first designed by Wong King Seng\textsuperscript{4} in 1992. Some modifications have been made to the system by Faiz Abdul Rahman\textsuperscript{5} who later worked on it. The chamber is a cylindrical stainless steel vessel with dimensions of 300mm in length, 150mm in diameter and 6mm thick. A pair of stainless steel plates is screwed on to both ends of the vessel. In order to assure good vacuum, Viton O-rings are placed in between the ends of the vessel and the plates. A stainless steel rotary shaft is placed at the center of the front plate to support an aluminum block that acts as the cathode. The cathode, which also acts as a sample holder, is inclined at 45° to the horizontal. An electrical lead through on the front plate connects the cathode to the power supply. The back plate holds a gaughead which connects the chamber to the Pirani 501 pressure meter.

A quartz tube with dimensions of 96mm in diameter, 200mm in length and 5mm in thickness encloses the anode and the cathode in the discharge area. The anode, which is a stainless steel plate of 65mm diameter and 5mm thick holds a stainless steel wire mesh, is connected to the power supply through an
electrical lead through at the back plate. Figure 3.2 illustrate a schematic diagram of the deposition chamber.

3.2.2 The pumping system

The pumping systems for the plasma deposition system used in this experiment consists of an EM 28 Edwards Rotary Vacuum Pump and a Pirani 11 pressure meter. The pumping unit is fixed directly to the deposition chamber through an inlet catchpot. The detoxification system is attached to the exhaust of the pump. The pressure in the chamber is measured by a Pirani 11 pressure meter which is connected via a PRE-10K gauge head fixed at the back plate of the deposition chamber. The pressure meter has a range of $10^{-2}$ to 1.0 mbar.

3.2.3 The Gas Distribution System

The gas distribution lines are made of 0.25-inch stainless steel tubing. It connects the deposition chamber to the various gas cylinders namely silane (SiH$_4$), argon (Ar), and nitrogen (N$_2$). The silane gas, being a heavily toxic gas is placed in a gas safety cabinet to ensure safety in case of leakage. Silane gas is first flown through a special gas regulator (Soxal 450-BS4-100) with special purging system. This purging system is connected to a nitrogen gas cylinder.

Gases from the cylinders are separately directed through these tubing to a gas distribution panel that distributes the gases to various systems in the laboratory. Before reaching the deposition chamber, the gases have to go through separate metering valves, which then direct the gases to separate Hastings mass flow meter controller. Hastings mass flow meter controller,
DC: Deposition Chamber
DT: Detoxification Tank
PS: DC Power Supply
gh: gauge head
gi: gas inlet
gv: gas valve
mfm: mass flow meter
cv: check valve
vv: vacuum valve
bv: bypass valve
aa: air admittance

Figure 3.1: A schematic diagram of the DC horizontal plasma glow-discharge system.
Figure 3.2: A schematic diagram of the reaction chamber.
which is connected to the system, monitors the gas flow rates. On exiting the flow meters, the gases pass through one way valves to prevent back flows. For safety purposes, a bypass line is made after the metering valve of the silane line to allow silane gas to be pumped out even if a blockage occurs at the mass flow controller. The silane gas and argon gases are joined at a single gas line, which direct the mixed gases into the deposition chamber.

3.2.4 The Detoxification System

Various kinds of gases are released during the deposition process and some of them are dangerously toxic. The detoxification system, which is meant to dilute the toxic gases, removes excess silane. It consists of a nitrogen gas line, which is bled into the oil bath of the rotary pump and a plastic container containing a solution of potassium permanganate (KMnO₄). The exhaust from the pump unit is directed to the KMnO₄ container. In this container, the silane is transformed into harmless products as the following chemical reaction occurs.

\[ 2\text{KMnO}_4 + \text{SiH}_4 \rightarrow 2\text{KMnO}_2 + \text{K}_2\text{SiO}_4 + 2\text{H}_2 \]

The chemical process totally eliminates the excess silane gas.

3.2.5 The Electrical System

The electrical system consists of two major components that are the DC power supply and the electrical control panel. The DC power supply is connected to the system through a full wave diode rectifier bridge which consists of 32 diodes. A step-up transformer with an input of 240V and output of 3kV is used to step-up the main power supply which is then rectified.
The transformer is immersed in an oil filled container for cooling purposes. A series resistors is used to control the current magnitude during the glow discharge process as well as to protect the transformer from any current overload. The DC potential across the electrodes in the deposition chamber is measured by an Iwatsu high voltage probe model HV-P30 and an Iwatsu Oscilloscope model SS-5710. The ionization current is measured by an analog milliammeter with a range of 0 to 100mA.

3.3 Deposition of a-Si:H by DC Glow Discharge.

In this work, amorphous silicon is deposited by the horizontal DC glow discharge technique. Two kinds of substrate is used that is glass and crystal silicon. The substrates are cut to a size of 2 cm times 1.5 cm rectangle. It is then cleaned and placed on the inclined cathode that also acts as a sample holder.

Before starting the deposition process, it is very important to make sure that the system is free from any leakage because the silane gas used in the deposition process is a highly toxic gas. Therefore, pre deposition and post deposition procedures had been observed strictly.

3.3.1 Pre deposition Procedure

The pre deposition procedure starts with pumping the deposition chamber using the rotary pump unit until the pressure is about 0.05 mbar. Then the gas lines are pumped stage by stage starting with opening the valves leading to the mass flow controller. Then the flowmeters are fully opened followed by the metering valves. Finally, the valves leading to the gas cylinders are opened.
The lines are pumped until the pressure of the entire system is less than 0.1 mbar. The next step is purging the silane gas line with oxygen-free nitrogen gas in order to remove any excess of silane from the previous deposition. After purging, the silane line is filled with nitrogen. A liquid called Snoop is used to check any leakage in the system where it will be indicated by bubbles that appear at leakage points. Once the system is detected to be free from leakage, it is pumped down again before it is set into operation.

### 3.3.2 Deposition Procedure

In this work, deposition process is done at room temperature using different gas flow rates. The desired argon and silane flowrates are set on the mass flow controller. Then the cleaned glass and crystal silicon substrates are placed on the sample holder. The system is then pumped down to a base pressure of about 0.05 mbar. The pre deposition procedure is carried on until it is save to operate using silane gas. Then nitrogen is introduced slowly into the oil bath of the rotary pump to dilute away excess silane.

Now the pump is ready for operation. With the silane valves closed, argon gas is first flown into the deposition chamber and the chamber pressure is measured. When the pressure has come to a stable state, silane gas is then allowed to flow into the chamber. Again, the new chamber pressure is measured. After the chamber pressure stabiles, the glow discharge is started by applying a required voltage across the electrodes. As the deposition takes place, parameters such as pressure, flow rate, ionization current and the DC voltage are monitored every 10 minutes and maintained at the desired settings. At the
end of the deposition, the DC power supply is turned off thus stopping the discharge process.

3.3.3 Post deposition procedure

Turning off the DC power supply ends up the glow discharge process. The silane gas tank regulator is then closed and so is the argon gas. The gas line is pumped until the flowmeter indicate zero flow rate readings and the chamber pressure is about 0.05 mbar. Finally, the silane gas line is purged again with nitrogen in order to flush out any excess silane in the line. The nitrogen gas line which leads to the oil bath of the rotary pump is closed after there is no more silane flowing in the line.

3.4 Substrate Cleaning Procedure

The most important requirement before starting any deposition is to clean the substrate from any dust, organic and inorganic matter that is trapped on the surface of the substrate which can significantly influence the properties of the film prepared. The substrate cleaning procedure underlined for glass substrate and crystal silicon substrate have to be followed very strictly. Once the substrate is considered clean, it is placed immediately in the reaction chamber to avoid recontamination. Different procedures are done for silicon substrate and glass substrate.
3.4.1 Silicon Substrate

The crystal silicon wafer is first cut into small pieces and rinsed with deionized water. Then they are boiled for about 10 minutes in a solution of $H_2O : H_2O_2 : HCl$ with a ratio of $86 : 11 : 3$ respectively. Then the small pieces of silicon are rinsed with deionized water in order to wash out any inorganic excess on the substrate surface. The silicon are then immersed in a solution of $H_2O : H_2O_2 : NH_4OH$ with a ratio of $7 : 3 : 3$ respectively to remove any organic contamination. Then again it is rinsed in deionized water. After that the silicon pieces are immersed in a solution of $H_2O : HF$ with a ratio of $10 : 1$ respectively. Finally the silicon pieces are rinsed again in deionized water.

3.4.2 Glass Substrate

Similar to the crystal silicon substrate, the glass substrate is first cut into small pieces. Then it is immersed in a beaker containing soap water. The whole beaker is then put into the ultrasonic bath for about 15 minutes. Then the substrates are rinsed in distilled water followed by aceton and ethanol. Finally they are rinsed again in distilled water.

3.5 Optical Transmission Spectroscopy Measurement

In this work, the ultra violet-visible spectrum (UV-VIS) is used to characterize the optical properties of the films prepared. Parameters obtained from this technique are the refractive index (n), the film thickness (d), and the optical energy gap ($E_g$). The optical transmission spectrum is obtained using the Jasco UV-VIS-NIR 3102-PC double beam spectrophotometer in the range of
200 to 2500 nm. A block diagram of the optical transmission set-up is shown in figure 3.3. The instrument consists of a light source, a monocromator, a sample compartment which holds a reference and a sample, a photo detector and a computer to control the measurement. In starting the measuring process, the spectral baseline is first obtained. In order to obtain the spectral baseline, two slides of glass are placed one in each reference and sample holder. Once the spectral baseline is obtained, the glass in the sample holder is removed and replaced by the sample deposited on glass. Then the measurement begins and the optical transmission spectrum is observed.

3.5.1 Calculations of the Refractive Index, Film Thickness and Optical Energy Gap.

The refractive index and the thickness of the film are deduced from the optical transmission spectrum of the film using the interference fringes in the low absorption region. In calculating the values, combination of Manifacier technique and Davies technique is used. The configuration of film on a transparent substrate is shown in figure 3.4. A typical transmission spectrum of the samples is shown in figure 3.5.

The values of the refractive index, \( n \), and the thickness, \( d \), of the film are deduced from the interference pattern in the long wavelength region. The transmission can be expressed as

\[
T = \frac{AX}{(1 - B)(1 - CX^2)} \tag{3.0}
\]

where \( A = (1 - R_1)(1 - R_2)(1 - R_3) \)
Figure 3.3: Block diagram of the optical transmission set-up.
Figure 3.4: A thin film on a transparent substrate.
\[ B = R_2 R_3 \]
\[ C = R_1 R_2 + R_1 R_3 (1 - R_2)^2 \]
\[ X = \exp(-\alpha d) \quad \text{(3.1)} \]

And \( R_1 \) = reflectance at air-film
\( R_2 \) = reflectance at film-substance
\( R_3 \) = reflectance at substance-air
\( \alpha \) = absorption coefficient
\( d \) = film thickness

Using the Manifacier technique which is accurate when transmission is almost 100\%, the refractive index of film is
\[ n = \left[ N + (N_2 - n_0^2 n_1^2)^{1/2} \right]^{1/2} \quad \text{(3.2)} \]
where \( N = (n_0^2 + n_1^2)/2 + 2n_0 n_1 (T_{\text{max}} - T_{\text{min}})/(T_{\text{max}} T_{\text{min}}) \quad \text{(3.3)} \)

The film thickness, \( d \), can be calculated from the following equation.
\[ d = M (\lambda_1 \lambda_2)/2 [\lambda_1 n_2(\lambda_2) - \lambda_2 n_1(\lambda_1)] \quad \text{(3.4)} \]

where \( M \) = number of complete oscillations between two extremes, and \( n_2(\lambda_2) \) and \( n_1(\lambda_1) \) are refractive indices at \( \lambda_2 \) and \( \lambda_1 \) where the two extremes are observed. In manipulating Manifacier technique, greater accuracy is gained if \( n \) is determined at the longest wavelength.

In the Davies\(^8\) technique, equation 2nd \( \sin \theta = m\lambda \) is used. Since in the system, \( \theta \) is 90\(^\circ\), the equation becomes 2nd = \( m\lambda \) where \( m = 1/2, 1, 3/2, \ldots \). From the transmission spectrum, wavelengths where maximum and minimum occurs are determined from the longest wavelength downwards. Then the values of \( m\lambda/2 \) is plotted versus wavelength and the value of \( m \) is changed.
until a curve similar to figure 3.6 is obtained. The particular value of \( m \) is assumed to be the correct \( m \) value for the spectrum.

The \( n \) value at the longest wavelength corresponds to the correct \( m \) is then used to determine the film thickness, \( d \) where \( d = m\lambda/n \). Then, this \( d \) is used to determine the values of \( n \) at the rest of the wavelengths. Plotting these values of \( n \) versus \( 1/\lambda^2 \) and fitting it to Cauchy equation

\[
 n = a + b/\lambda^2 \tag{3.5}
\]

will allow us to determine the values of \( a \) and \( b \). \( a \) is called the static refractive index of the film or also known as \( n_0 \). If \( n \) for the whole spectrum is determined, dispersion of the refractive index can be obtained (Figure 3.7).

From equation 3.1, absorption coefficient, \( \alpha \), can be written as

\[
 \alpha = (1/d) \ln (1/X) \tag{3.6}
\]

where

\[
 X = -A + \left[A^2 + 4CT^2 (1 - B)^2 \right]^{1/2} \over 2CT (1 - B) \n\]

In determining the optical energy gap, photon energy for the whole spectrum is calculated through equation 3.7. \( \alpha \) is then calculated for the whole spectrum. Then the values of \( (\alpha E)^{1/2} \) is plotted versus \( E \). From its linear portion, energy gap, \( E_g \) can be determined by dividing \( c \) over \( m \) where \( c \) is its intercept and \( m \) is its slope, \( E_g = c/m \).
Figure 3.5: A typical transmission spectra.
Figure 3.6: The curve for the correct $m$ value.

Figure 3.7: Dispersion of the refractive index.
\[ E = \frac{hc}{\lambda e} \]  

Where \( h \) = Planck constant  
\( c \) = velocity of light  
\( e \) = electronic charge

3.5.2 Calculations of the Refractive Index and Film Thickness for Films with Very Weak Absorption

The calculation method of film thickness for films that gives very little interference fringes was utilized from the method proposed by Khedr M. Hassan\(^{11}\) which he developed to estimate the thickness of transparent thin film deposited onto transparent substrate. The condition for the application of the proposed method is the existence of a region in the transmission spectrum in which the assumption \( n \gg k \) is valid and \( n \) is almost independent of the incident photon wavelength. \( n \) is the real part of the refractive index, \( k \) is the extinction coefficient.

The calculation method was based on the existence of two interference fringes which frequently appear in the transparent region of the transmission spectrum. Considering a very weak absorption, Khedr\(^{11}\) utilised the Fresnel coefficients and approximated the transmittance and the reflectance for normal incidence as follow.

\[
T = \frac{16 n_1 n_3 n^2 A}{C_1^2 + C_2^2 A^2 + 2C_1C_2 A \cos(4\pi nt/\lambda)} \quad \text{------(3.8)}
\]

\[
R = \frac{B_1^2 + B_2^2 A^2 + 2C_1C_2 A \cos(4\pi nt/\lambda)}{C_1^2 + C_2^2 A^2 + 2C_1C_2 A \cos(4\pi nt/\lambda)} \quad \text{------(3.9)}
\]
Where \( C_1 = (n + n_1)(n + n_3) \)
\( C_2 = (n - n_1)(n_3 - n) \)
\( B_1 = (n - n_1)(n + n_3) \)
\( B_2 = (n + n_1)(n_3 - n) \)
\( A = \exp(-4\pi kt/\lambda) = \exp(-\alpha t) \)
\( \alpha = \) absorption coefficient of the film
\( n = \) real part of the refractive index
\( k = \) extinction coefficient

The indices 1, 2 and 3 correspond to air, film and substrate respectively. Generally, the transmission \( T \) is a function of \( n, k \) and \( \lambda \) thus the derivative of \( T \) takes the form below.

\[
\frac{dT}{d\lambda} = \frac{\partial T}{\partial \lambda} + (\frac{\partial T}{\partial n})(\frac{dn}{d\lambda}) + (\frac{\partial T}{\partial k})(\frac{dk}{d\lambda})
\]

\( \text{-------(3.10)} \)

In the region of the spectrum below the absorption edge \( k = 0 \), the term \( \frac{dk}{d\lambda} \) can be ignored. In this region, \( n \) is a slowly varying function of \( \lambda \), hence the variation of \( n \) with respect to \( \lambda \) can be neglected. Thus the slope of the interference edge is due mostly to the term \( \frac{\partial T}{\partial \lambda} \) i.e. \( \frac{dT}{d\lambda} \equiv \frac{\partial T}{\partial \lambda} \). From the expression of \( T \) in equation 3.8 and its derivative with respect to \( \lambda \), two equations for thickness in terms of \( T, n, \lambda \) and \( \frac{dT}{d\lambda} \) can be deduced as follow.

\[
t = \frac{\lambda}{4\pi n} \cos^{-1} \left[ \frac{16 n_1 n_3 n^2 - T(C_1^2 + C_2^2)}{2TC_1 C_2} \right] - \frac{m\lambda}{2n}
\]

\( \text{-------(3.11)} \)

\[
t = -\frac{2\lambda^2 n_1 n_3 n}{T^2 \pi C_1 C_2} \left[ 1 - \left( \frac{16 n_1 n_3 n^2 - T(C_1^2 + C_2^2)}{2TC_1 C_2} \right)^2 \right]^{-1/2}
\]

\( \text{-------(3.12)} \)

Where \( m \) is an integer.
Equation 3.11 and 3.12 can be solved to determine $n$ and $t$ for any point at any interference edge. The slope $dT/d\lambda$ can be deduced for a particular wavelength with known corresponding value of $T$. Solving these two equations for that particular wavelength will lead to a pair of solutions of $n$ and $t$ for each value of $m$. These pair of solutions can be matched with other pairs of solutions calculated for another wavelength within another interference edge with the same value of $T$. The correct pair of solution which give the closest values of $n$ and $t$ for the two wavelengths can be chosen bearing in mind that the difference between the values of $m$ for two wavelengths having some values of $T$ onto two consecutive edges is unity and $m$ is larger for the longer wavelength.

3.6 Fourier Transform Infrared Spectroscopy Measurement

Infrared transmission measurement technique is used to study the nature of bonding of silicon in a-Si:H network. The void concentration is also calculated from this technique using the microstructure parameter $R$. The infrared transmission spectrum of amorphous silicon is obtained by scanning a sample of amorphous silicon deposited on a crystal silicon substrate. Crystal silicon is the favoured substrate as symmetry considerations prevent it from absorbing infrared photons.

In this work, Fourier Transform Infrared (FTIR) spectrum is obtained with a Perkin Elmer system 2000 FTIR spectrophotometer within the scanning range of 300 to 3000 $\text{cm}^{-1}$. The basic outline of the instrument is shown in figure 3.8 which illustrates the optical components in the interferometer unit.
Figure 3.8: Schematic representation of the FTIR instrument configuration.
Figure 3.9: A typical IR spectrum of an a-Si:H thin film.
The crystal silicon substrate without any deposition is first scanned as a background. After the background spectrum is obtained, the empty substrate is replaced by the sample deposited on a crystal silicon substrate. The FTIR spectrum for the film is the resultant of the sample spectrum minus the background spectrum. The spectrum is averaged over 20 scans. A typical infrared spectrum of an a-Si:H thin film in the range of 200 to 2500 cm\(^{-1}\) is shown in figure 3.9.

3.6.1 Determination of Integrated Intensity and Hydrogen Content.

In this work, the SiH environment is characterized by a bond-stretching mode at 2000 cm\(^{-1}\) and a bending-mode at 630 cm\(^{-1}\). The transmission spectra is first converted to absorption coefficient spectra using equation 3.13. Then the Gaussian\(^{10}\) or Doppler lineshape is used to deconvolute component peaks from the absorption spectrum. The equation used for the Gaussian lineshape is given is equation 3.14.

\[
\alpha(\omega) = (1/d) \ln (100/ T\%)
\]

\[
\alpha(\omega) = \alpha(\text{max}) \exp \left[-\frac{4 \ln 2}{\omega - \omega_0} \right] / \Delta \omega
\]

\[
\alpha(\text{max}) = 2 (\ln 2)^{1/2} S_{\text{band}} / (\pi^{1/2} \Delta \omega)
\]

where \( S_{\text{band}} = \int \alpha(\omega) \, d\omega \)

\[
\text{and } S_{\text{band}} = \int \alpha(\omega) \, d\omega
\]

\( S_{\text{band}} \) is the area under the curve, \( \Delta \omega \) is the full width half maximum of the absorption peak, \( \alpha(\text{max}) \) is the maximum absorption coefficient and \( \omega_0 \) is the peak position.

In the form of

\[
y = A \exp (-Bx)
\]
equation 3.14 can be rewritten with $A = B^{1/2} S_{\text{band}} / \pi^{1/2}$, $B = (4 \ln 2) / (\Delta \omega)^2$ and $x = (\omega - \omega_o)^2$. Rewriting equation 3.16, $\ln y = \ln A - B(\omega - \omega_o)^2$. The integrated intensity of the absorption peak which represents a bonding configuration is therefore

$$I = \int_0^\infty \frac{\alpha(\omega)}{\omega_o} \ d\omega$$

The integrated intensity can also be derived from equation 3.15 thus be written as

$$I = S_{\text{band}} / \omega_o$$

Calculating the hydrogen content is the continuation from integrated intensity. Assuming the hydrogen concentration in the film as $N$, thus $N = A_1$ with $A_1 = 1.6 \times 10^{19} \ cm^{-1}$ for the SiH wagging mode at 640 cm$^{-1}$. The microstructure parameter, $R$ is then determined by the following equation.

$$R = \frac{I_{\text{2100}}}{(I_{\text{2100}} + I_{\text{2000}})} \quad ------(3.17)$$

The total hydrogen content is

$$H\% = \frac{N}{N_{\text{Si}}} \quad ------(3.18)$$

with $N_{\text{Si}} = 5 \times 10^{22}$ is the silicon atom concentration in crystal silicon samples. The microstructure parameter is utilized to determine the hydrogen content at the internal surface of microvoids and at isolated SiH bonds.

Hydrogen content at the internal surface of the microvoids is

$$H(v) = R \times H\% \quad ------(3.19)$$

Hydrogen content at isolated SiH bonds

$$H(\text{SiH}) = (1 - R) H\% \quad ------(3.20)$$

The values of $H(v)$ and $H(\text{SiH})$ indicates the structure of the film. If the value of $H(\text{SiH})$ is bigger than $H(v)$, the film has an amorphous structure.
whereas if $H(v)$ dominates the film with its value bigger than $H(\text{SiH})$, the film has a columnar structure.

### 3.7 References