Chapter III

Experimental and Calculation Technique

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3.1 . Introduction

The experimental techniques used in the present work are introduced in this chapter. The basic principles, the means and the merits of the various techniques are emphasised. Both crystalline and amorphous semiconductors are characterised by various techniques. In these characterisations, electrical, optical and structural investigations are carried out for both types of semiconductor materials. Section 3.2.1 describes the electrical characterisation of crystalline Germanium by using the four - point probe equipment (DEP02) and the Hall effect set-up (DHE-21). The section 3.2.2 briefly describes the instrumentation used for both the a.c. and the d.c. conductivity measurements of crystalline silicon. These measurements are carried out by using Hioki 3520 LCR Bridge (a.c.conductivity) and Kiethly 236 Source Measurement Units(SMU) in a Janis Research Coefficient.Inc. model CCS 100 cryostat (d.c. conductivity) respectively. This section also presents the formulae used to calculate energy gap, conductivity and other physical properties of the crystalline semiconductor. The section 3.2.3 deals with the investigations of the optical properties of crystalline silicon. The formulae used to calculate the refractive index, absorption constant and coefficient of absorption are also presented in this section. The preparation of hydrogenated amorphous silicon (a-Si:H) is described in section 3.3. The section 3.3.1 mainly focusses on the technique used to characterise the hydrogenated amorphous silicon. In section 3.3.2 the optical characterisation techniques used for a-Si:H are presented. This section also describes the formulae used to calculate the various physical parameters such as refractive index, optical thickness, absorption coefficient and hydrogen content in the material. The section

3.4.3 illustrates how the aluminium electrode coating is deposited for both the amorphous and crystalline semiconductors by using the vacuum deposition technique so that the electrical measurements on these two materials can be carried out. The section 3.3.4, describes how the electrical properties such as electrical conductivity, activation energy and the density of states at the fermi level are obtained by a.c. and d.c. conductivity measurements. The a.c. conductivity measurement is carried out by using Hioki 3520 and the d.c. current conductivity has been measured using Kiethly 236 Source Measurement Unit (SMU) in a Janis Research Co . Inc. model CCS 100 cryostat. The section 3.4 presents the detail of characterising the structures of crystalline and amorphous semiconductors. The section 3.5 focuses on the infrared spectroscopic studies on the a-Si:H to ascertain the bonding configurations present in the sample and hence to determine the purity of the sample. In the section 3.6, a brief explanation is given on the process of annealing in ambient nitrogen for crystalline and hydrogenated amorphous silicon (a-Si:H).

3.2. Characterisation of Crystalline Semiconductor

3.2.1 Electrical Characterisation of Crystalline Germanium

(I) Four Point Probe Technique [49-54]

Many conventional methods for measuring resistivity are not suitable for semiconductors because a metal-semiconductor contact is usually rectifying in nature. Also, there is a minority carrier injection by one of the current carrying contacts. An excess concentration of minority carriers in the vicinity of the electrodes will affect the potential of the contacts and change the measured resistance of the material.

The method described here overcomes the above difficulties and offer several advantages. It permits measurements of resistivity of samples having a wide variety of shapes, including the resistivity of smaller volumes within bigger pieces of the semiconductor sample. In this manner the resistivity of both sides of p-n junction can be determined. This method of measurement is not only applicable to Germanium but to other semiconductor materials as well. The basic method of the measurement is indicated in fig. 3.1. Four sharp probes are placed on a flat surface of the material to be measured, a current is passed through the two outer electrodes and the resulting floating potential is measured across the inner pair. If the flat surface on which the probes rest is adequately large and the crystal is big enough, the semiconductor may be considered to be semi- infinite in volume. To prevent minority carrier injection and to make good contacts, the surface on which the probes rest, must be mechanically lapped. The experimental circuit used for the measurement is illustrated schematically in fig. 3.2. A nominal value of the probe spacing which has been found satisfactory is an equal distance of 1.0mm between the adjacent probes. This permits the measurement with a reasonable current through the n and p-type semiconductors whose resistivity varies from 0.001 to 50 ohm cm. In order to apply the four probe method to semiconductor crystals it is necessary to assume that:

1. The resistivity of the material is uniform in the area of measurement.
2. If there is minority carrier injection in to the semiconductor by the current - carrying electrodes, most of the carriers recombine near the electrodes so that their effect on the conductivity is negligible.(This means that the measurements should be made on the surface which have a high recombination rate, such as mechanically lapped surfaces)
3. The diameter of the contacts between the metallic probes and the semiconductor should be small compared to the distance between the probes.

4. The four probes which are used for resistivity measurement must touch the surface at points that lie on straight line.
5. The surface on which the probes rest is flat with no surface leakage is possible.
6. The boundary between the current - carrying electrodes and the bulk material is hemispherical and small in diameter.

The semiconductor crystal material may either be placed upon a conducting or a non-conducting base.

a) a conducting base is one which has a much lower resistivity than the semiconductor.

b) a non-conducting base is produced when the surface of the crystals is in the contact with an insulator.

Case A : Resistivity Measurement on a Large and a Thick Sample.

One added boundary condition is required to treat this case normally , that the probes are placed far away from the boundary of the sample and the sample can then be considered of a semi - infinite volume of uniform resistivity. Fig. 3.1 shows the geometry of this case. Four probes are spaced s_1 , s_2 and s_3 apart. Current (I) is passed through the outer pair of probes (1 and 4) and the floating potential V is measured across the inner pair of probe 2 and 3. The floating potential V_f at a distance r from the current injecting electrode is given by ,

$$V_f = \frac{\rho_0 I}{2\pi r} \qquad (3.1)$$

where ρ_0 measures the material resistivity.

In the method shown in the fig. 3.1, there are two current carrying electrodes , numbered 1 and 4, and the floating potential V_f, is the difference of potentials between 2 and 3. Since, 1 and 4 carry currents of equal magnitudes in opposite directions, one finds,

$$V_f = \frac{\rho_0 I}{2\pi}\left[\frac{1}{r_1} - \frac{1}{r_4}\right] \qquad (3.2)$$

where r_1 = distance of the point from the probe number 1, r_4 = distance of the same point from probe number 4. The floating potential at probe 2, V_{f2} and at probe 3, V_{f3} can be calculated from equation (3.2) by substituting the proper distances as follows;

$$V_{f2} = \frac{\rho_0 I}{2\pi}\left[\frac{1}{s_1} - \frac{1}{(s_2+s_3)}\right] \qquad (3.3)$$

$$V_{f3} = \frac{\rho_0 I}{2\pi}\left[\frac{1}{(s_1+s_2)} - \frac{1}{s_3}\right] \qquad (3.4)$$

The potential difference V between probes 2 and 3 is then,

$$V = V_{f3} - V_{f3} = \frac{\rho_0 I}{2\pi}\left[\frac{1}{s_1} + \frac{1}{s_3} - \frac{1}{(s_1+s_2)} - \frac{1}{(s_2+s_3)}\right] \qquad (3.5)$$

and the resistivity ρ_0 is computable as,

$$\rho_0 = \frac{2\pi V}{I\left[\frac{1}{s_1} + \frac{1}{s_3} - \frac{1}{(s_1+s_2)} - \frac{1}{(s_2+s_3)}\right]} \qquad (3.6)$$

when the point spacings are equal, that is, $s_1 = s_2 = s_3 = s$, the above equation simplifies to,

$$\rho_0 = \frac{2\pi V s}{I} \qquad (3.7)$$

Case B : Resistivity Measurement on a Thin Slice(Conducting Bottom Surface)

Two boundary conditions must be met in this case , the top surface of the slice must be a reflecting (non-conducting) surface and the bottom surface must be an absorbing (conducting) surface. Since the two boundaries are parallel , a solution by the method of images is required for each current source. An infinite series of images along a line normal to the places and passing through the current source is formed. The model for this case is shown in fig. 3.3. The side surface of the slice are assumed to be far away from the area of measurement and therefore only the effect of the bottom surface needs to be considered. In this analysis the equal probe spacing (s) shall be assumed. The width of the slice is W. The array of images needed is indicated in fig. 3.3. Here the polarity and the spacing of the first few images are as shown. The floating potential V_{f2} at electrode 2 is ,

$$V_{f2} = \frac{\rho_0 I}{2\pi}\left[\frac{\sum(-1)^n 1}{\left(\sqrt{s^2}\right)+(2\pi W)^2} - \frac{\sum(-1)^n 1}{\left(\sqrt{(2s)^2}\right)+(2\pi W)^2}\right] \qquad (3.8)$$

and the resistivity becomes ;

$$\rho = \frac{\rho_0}{G_6\left(\frac{W}{s}\right)} \qquad (3.9)$$

where ρ_0 is computable from the equation (3.7). (3.6) can be used if the point spacings are different , but approximately equal. The correction G_6 (W/s) is computed from the following relationship:

$$G_6\ (W/s) = 1+4\left(\frac{s}{W}\right)\sum(-1)^n\left[\frac{1}{\left(\left\{\sqrt{\frac{s}{W}}\right\}^2+(2n)^2\right)}-\frac{1}{\left(\left\{\sqrt{\frac{2s}{W}}\right\}^2+(2n)^2\right)}\right] \quad (3.10)$$

which has been tabulated in table 3.0 and plotted in fig. 3.4.

Case C : Resistivity Measurement On A Thin Slice Non - Conducting Bottom Surface.

The model for the measurement is the similar to case B , except that the bottom surface is non-conducting. This means that all the images of fig. 3.3 have the same charge as the current source. In that case ;

$$\rho = \frac{\rho_0}{G_7\left(\frac{W}{s}\right)} \quad (3.11)$$

where ,

$$G_7\ (W/s) = 1+4\left(\frac{s}{W}\right)\sum\left[\frac{1}{\left(\left\{\sqrt{\frac{s}{W}}\right\}^2+(n)^2\right)}-\frac{1}{\left(\left\{\sqrt{\frac{2s}{W}}\right\}^2+(2n)^2\right)}\right] \quad (3.12)$$

This correction factor G₇(W/s) is tabulated in table 3.0 and plotted in fig. 3.5. For smaller values of (W/s) the function G₇(W/s) approaches the case for an infinitely thin slice or ,

$$G_7\ (W/s) = \frac{2s\ln(2)}{W} \quad (3.13)$$

Earlier it was presumed that probes are situated far away from the semiconductor boundary. In case the probes are not situated far away from the boundary , appropriate finite corrections have to be applied. The finite corrections factor 'C' has been tabulated in table 3.1.

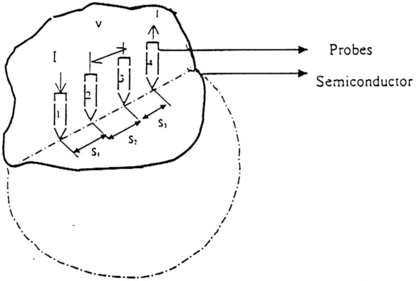


Figure 3.1 : Model for the Four - Probe Resistivity Measurement

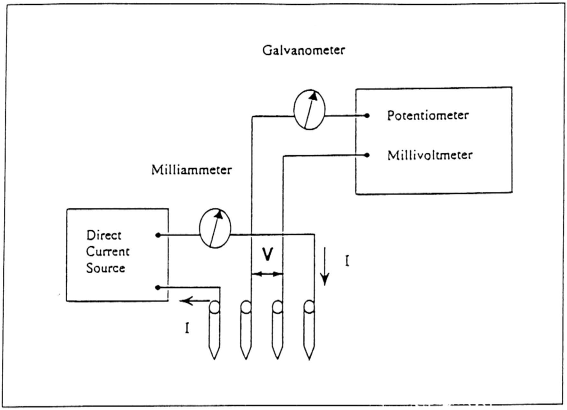


Figure 3.2 : Circuit used for Resistivity Measurement

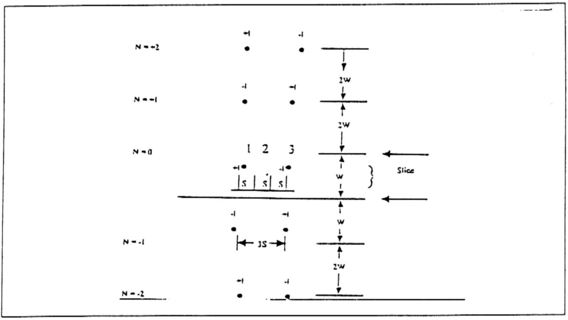


Figure 3.3 : Images for the case of the Resistivity Probes on a thin slice with a conducting bottom surface.

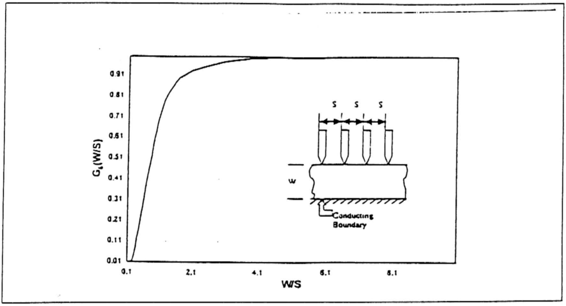


Figure 3.4 : Correction Divisor for the probes on a slice with a conducting bottom surface

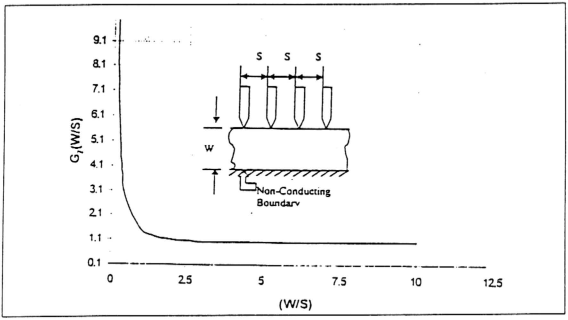


Figure 3.5 : Correction Divisor for probes on a thin slice with a non-conducting bottom surface.

S. No	W/s	$G_6(W/s)$	$G_7(W/s)$
1	0.100	0.0000019	13.863
2	0.141	0.00018	9.704
3	0.2000	0.00342	6.931
4	0.330	0.0604	4.159
5	0.500	0.228	2.780
6	1.000	0.683	1.504
7	1.414	0.848	1.223
8	2.000	0.933	1.094
9	3.333	0.9838	1.0228
10	5.000	0.9948	1.0070
11	10.000	0.9993	1.00045

Table 3.0 : Correction Divisor for thin slice

- **Brief Description of the Apparatus**

Probes Arrangement

It has four spring loaded probes , coated with Zn at the tips. The probes are collinear and are equally spaced. The Zn coating and springs ensure good electrical contacts with the sample. The probes are mounted in a Teflon bush which ensures a good electrical insulation between the probes. A Teflon spacer near the tips is also provided to keep the probes at equal distances. The whole arrangement is mounted on a suitable stand and leads are provided for current and voltage measurements. The sample which was used in this experiment is crystalline Germanium in the form of a chip/slice.

d/s	Circle diameter(d/s)	Square a/d = 1	Rectangle		
			a/d = 2	a/d = 3	a/d ≥ 4
1.00				0.9988	0.9994
1.25				1.2467	1.2248
1.50			1.4788	1.4893	1.4893
1.75			1.7196	1.7238	1.7238
2.00			1.9475	1.9475	1.9475
2.50			2.3532	2.3451	2.3541
3.00	2.2662	2.4575	2.7000	2.7005	2.7005
4.00	2.9289	3.1137	3.2246	3.2248	3.2248
5.00	3.3625	3.5098	3.5749	3.5750	3.5750
7.50	3.9273	4.0095	4.0361	4.0362	4.0362
1.00	4.1716	4.2209	4.2357	4.2357	4.2357
15.00	4.3646	4.3882	4.3947	4.3947	4.3947
20.00	4.4364	4.4516	4.4553	4.4553	4.4553
40.00	4.5076	4.5120	4.5129	4.5129	4.5129
∞	4.5324	4.5024	4.5325	4.5325	4.5325

Table 3.1 : Correction Factor (for finite sample size) for the measurement of Sheet resistance with Four-Point-Probe.

Oven

It is a small oven for the variation of temperature of the crystal from room temperature to about 200^{0}C.

Four Probe set - up

It has three subunits all enclosed in one cabinet, shown in fig. 3.6. It consists of,

i) Multirange Digital Voltmeter- In this unit intersil 3½ digit single chip A/D converter ICL7107 has been used. It has a high accuracy , auto zero to less than 10μV , zero drift less than 1μV/^{0}C , input bias current of 10pA and roll over error of less than one count.

ii) Constant Current Generator - It is a IC regulated generator to provide a constant current to the outer probes irrespective of the changing resistance of the sample due to the changes in temperatures.

iii) Oven Power Supply - Suitable voltage for the oven is obtained through a step down transformer with a low and high heating rates.

- **Experimental Procedures**

Let the sample be placed on the base plate of the four probe arrangement. Let the four probe rest in the middle of the sample. Applying a very gentle pressure, the probes are set in this position. The continuity between the probes for proper electrical contacts must be checked. *Caution : The Germanium is very brittle, therefore only a minimum pressure is required for proper electrical contacts.* The outer pair of the probes (green/black leads) must be connected to the constant current power supply and the inner pair (red leads) are to be connected to the voltage measuring instrument. The probes are placed in the oven and a thermometer in the oven is used to measure the temperature. The power is turned on to the unit. The current through the probes is next adjusted to a desired value (say 5mA). Next the voltage between the inner pair of probes is measured. The oven is turned on. The heating rate may be selected with the help of a switch - low or high, as desired. The variation of the voltage with increasing temperature from the room temperature onwards was noted, by keeping the current constant.

- **Formulae Used**

From equation 3.7 ,

$$\rho_0 = \frac{2\pi Vs}{I}$$

Since the thickness of the crystal sample is small compared to the probe distance , a correction factor for it has to be applied. Further the bottom surface is non-conducting in the present case , so equation 3.11 has to be applied as ;

$$\rho = \frac{\rho_0}{G_7\left(\frac{W}{s}\right)}$$

The function G_7 (W/s) may be obtained from table 3.0 or fig. 3.5 for the appropriate values of (W/s). Thus ρ may be calculated at various temperatures. Plot a graph for $\log_{10}\rho$ versus $T^{-1}X10^3$. Using equation 3.14

$$\log_{10}\rho = \left(\frac{E_g}{2kT}\right) - \log_{10} k \qquad (3.14)$$

$$\text{the slope is given by } \log_{10} / (1/T) = (E_g / 2k) \qquad (3.15)$$

Thus E_g may be obtained from slope of the graph.

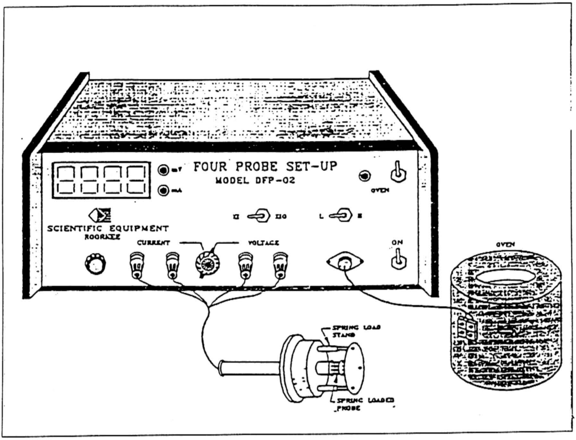


Figure 3.6 : A Four - Probe Set-up.

II) Hall Effect Measurement

A) Experimental Considerations

1. In a single crystal material the resistivity may vary smoothly from point to point. In fact, this is generally the case. The question is the amount of this variation. Often, however, it is conventionally stated that it is a constant within some limits and when this variation does in fact lie within this tolerance, it is ignored.
2. High resistance or rectification appears fairly often in electrical contacts to semiconductors and in fact it is one of the major problem in measurements.
3. Soldered probe contacts, though very much desirable, may disturb the current flow (shorting out part of the sample). Soldering directly to the body of the sample can affect

the sample properties due to the heat and contamination, unless care is taken. These problems can be avoided by using pressure contacts as in the present set-up.

4. The current through the sample should not be large enough to cause heating. By keeping the voltage drop at the contacts low enough we can prevent this phenomena from occurring. This is done to prevent "injection" during the measurement.

B) Experimental Consideration with the Measurement of Hall Coefficient.

1. The voltage appearing between the Hall probes is not generally , the Hall voltage alone. There are other galvanomagnetic and thermomagnetic effects (e.g. Nernst effect , Rhighi-Leduc effect, and Ettinghausen effect) which can also produce voltages between the Hall probes. IR drops due to probe misalignment and thermoelectric voltages due to transverse thermal gradient may also be present. When the voltage between the Hall probes is measured for both directions of the current , only the Hall voltage and IR drop reverse. Therefore , the average of these readings eliminates the influence of the other effects. When Hall voltage is measured for both the directions of the magnetic field , the IR drops does not reverse and may therefore be eliminated.
2. The Hall probes must be rotated in the field until the position of the maximum voltage is reached. This is the position when direction of the current in the probe and the magnetic field would be perpendicular to each other.
3. The resistance of the sample changes when the magnetic field is turned on. This phenomena is known as the magnetoresistance effect and it occurs due to the fact that the drift velocity of all carriers is not the same, when the magnetic field is on. The Hall voltage compensates exactly the Lorentz force for carriers with the average velocity. By

using a constant current power supply, this problem can be eliminated and this would keep the current constant irrespective of the resistance of the sample.

4. In general, the resistance of the sample is very high and the Hall voltages are very low. This means that practically there is hardly any current-not more than few micro amperes. Therefore , the Hall voltage should be measured with a high input impedance ($\cong 1M\Omega$) devices such as an electrometer, electronic millivoltmeters or good potentiometers.
5. Although the dimensions of the crystals do not appear in the formula except the thickness, but the theory assumes that all carriers are moving only length-wise. Practically it has been found that a closer to ideal situations may be obtained if the length may be taken three times the width of the crystals.

C . Brief Description of The Apparatus

The Hall effect measurement set-up has five sub units and all are shown in fig. 3.7, fig. 3.8 and fig. 3.9. The sub units are , Hall probe (Ge crystal and InAs) , Hall effect set - up (digital) DHE-21 , Electromagnet Newport series N38 , Constant Current Power supply, DPS-175 or DPS-50 and Digital Gaussmeter, DGM-102.

D . Experimental Procedure

The width wise contacts of the Hall Probes are connected to the terminals marked "Voltage" and lengthwise contacts to terminals marked 'Current'. The power to the Hall effect set - up is turned on and a current of a few mA is passed through the sample. There may be some voltage reading even when the sample is outside the magnetic field. This is due to the imperfect alignment of the four contacts and is generally known as the 'zero field potential'. In case its value is comparable to the Hall voltage , it should be adjusted to a minimum possible (for Hall probe Ge only). In all cases, this error should be subtracted from the Hall voltage reading. Next, the sample is placed in the magnetic field as shown in fig. 3.10 and the electromagnetic power supply is turned on. The current is next adjusted to a desired value. The sample is rotated till it becomes perpendicular to the magnetic field. Hall voltage will be maximum in this adjustment.

The Hall voltages are measured for both the directions of the current and magnetic field (i.e. four observation for a particular value of current and magnetic field). The Hall voltage is measured as a function of the current keeping a suitable value of the magnetic field as constant. Next, graphs are plotted for V_H against I and V_H against H. The magnetic field is measured by the Gaussmeter.

E) Formulae Used :

From graph of Hall voltage versus the magnetic field, the Hall coefficient is calculated by using the following equation:

$$R = \frac{V_H Z}{IH} \qquad (3.16)$$

where V_H = Hall voltage, I= current, H= magnetic field and Z= thickness of the sample. The charge carrier density can be calculated as follows ;

$$R = \frac{1}{nq} \qquad (3.17)$$

$$n = \frac{1}{Rq}$$

The carrier mobility can be also calculated by using the following equation 3.18:

$$\mu_n \text{ (or } \mu_p) = R\sigma \qquad (3.18)$$

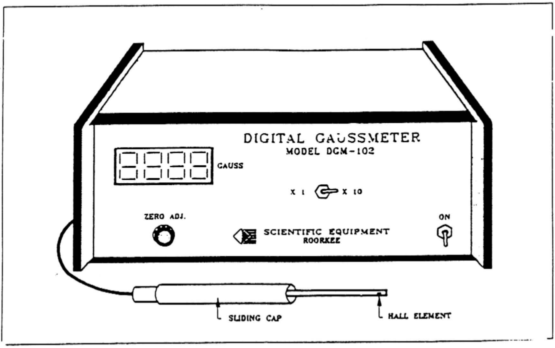


Figure 3.7 : Digital Gaussmeter , model DGM - 102

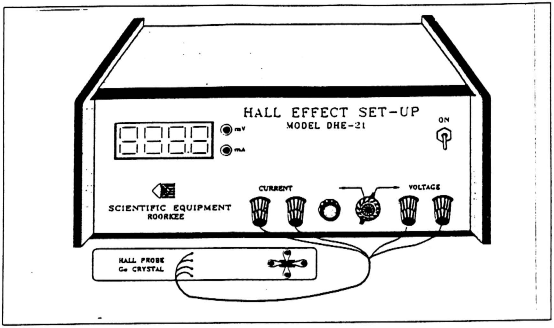


Figure 3.8 : Hall Effect Set-Up, Model DHE-21

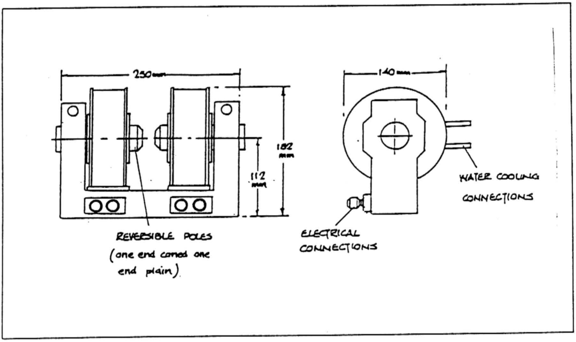


Figure 3.9 : Electromagnet Newport Series, N 38

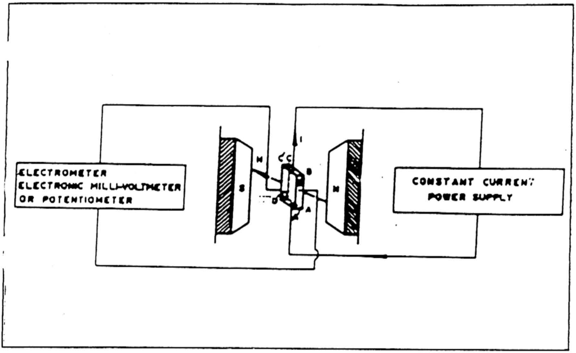


Figure 3.10 : Placement of probe in Magnetic Field

3.2.2. Electrical Characterisation of Crystalline Silicon

(A) D.C.Conductivity Measurement

i) Measurement Technique

Since the conductivity measurement for the crystalline silicon could not be measured by the Four Point Probe technique because of its very low conductivity, aluminium electrodes were deposited on top and bottom surface of the sample to measure its conductivity directly. The technique of the deposition of the aluminium electrode by using vacuum deposition system is well elaborated in section 3.3.3. The d.c. conductivity of the crystalline-Si was measured using the VPF 100 Cryostat and 236 Keithley Source Measurement Unit (SMU) and the current - voltage measurement was carried out between 297 ^{0}K - 338 ^{0}K. The Lake Shore 320 autotunning temperature controller was used throughout the measurement. The configuration used in the SMU during current voltage measurement for crystalline - Si is given in table 3.2 and the table 3.3 gives the configuration measurement for crystalline - Si is given in table 3.2 and the table 3.3 gives the configuration in SMU during the empty trap for crystalline - Si. Before starting all measurements , the pump should be turned off and one should make sure that the gas inlet is closed to avoid up surging of oil in to the cryostat. It is necessary to turn on the power supply to the temperature controller, SMU and computer at least for half - an hour before making any measurement in order to warm up the system. Before all measurements, a constant voltage of 100 volts has to be applied for about half an hour to elevate the electrons trapped in the mobility gap.

Mode	Sweep
Type	Linear
Measurement	Voltage and Current
Start	0 V
Stop	100 V
Number of points	2.1
Interval	0.5 V
Time delay	0 sec
Integration	50 Hz
Filter	4 Readings

Table 3.2 : Configuration used in SMU during current voltage measurement in crystalline-Si

Mode	Constant
Type	Linear
Stimulus Measure	Voltage and Current
Value	100 V
Delay	0 sec
Intergration	50 Hz
Filter	4 Reading

Table 3.3 : Configuration used in SMU during empty trapping for crystalline - Si.

The brief description of SMU system and the VPF 100 Cryostat will be discussed more in detail in section 3.3.4.

ii)Formulae Used:

When the current voltage reading is obtained from the SMU system, a graph of current (I) versus voltage (V) for the different temperature has to be plotted and it must be a linear graph. Then the slope of the graph in the ohmic region has to be calculated which is expressed as,

$$\text{slope (m)} = \frac{\Delta I}{\Delta V} \qquad (3.19)$$

The expression for the conductivity σ (= $1/\rho$) may now be written as,

$$\frac{1}{\rho} = \left(\frac{1}{R}\right)\left(\frac{t}{A}\right) \qquad (3.20)$$

$$\sigma = \left(\frac{I}{V}\right)\left(\frac{t}{A}\right) \qquad (3.21)$$

$$\sigma = \left(\frac{mt}{A}\right) \qquad (3.22)$$

where m is the slope of the I-V graph in the ohmic region , t is the thickness of the sample and A is the area of the aluminium electrodes which was deposited on top of the crystalline - Si. The energy gap (E_g) of the crystalline - Si can then be obtained from the slope of the graph $\log_{10}\rho$ versus (1 / T), as presented in the following equation:

$$\ln \sigma = \left(\frac{E_g}{2kT}\right) - \ln K \qquad (3.23)$$

$$m = \left(\frac{\ln \sigma}{T^{-1}}\right) = \left(\frac{E_g}{2k}\right) \qquad (3.24)$$

where m is the slope of graph $\ln\sigma$ versus T^{-1} .

b) A.C. Conductivity Measurement

A.C. method represents the most popular approach to the determination of the electrical conductivity of materials. This is because, simple cells using inert blocking electrodes are used to determine the bulk electronic properties, even though the theory to interpret the measurements is very complex. Impedance spectroscopy refers to the measurement of real and imaginary parts of the impedance over a wide range of frequencies. This helps in separating out the true bulk conductivity from the conduction due to the grain boundaries and interfacial impedance[58]. In impedance spectroscopy, a sinusoidal signal of low voltage amplitude is applied across the cell containing the sample. The output signal which is also a sinusoidal wave is compared with the input signal to determine the impedance modulus and the phase shift. It is because the impedance is frequency dependent, we can extract the information about the different electrical properties of the sample [59].

The result of an a.c. experiment can also be presented in the form of Y(admittance), C_s (serial capacitance), C_p (parallel capacitance), D (loss coefficient), G (conductance), θ (phase angle) and Z (impedance) [60]. The complex impedance plot of RC circuit in series and parallel connections are shown in fig . 3.11.

The measurement unit which was used in the experiment is a HIOKI 3520 LCR HI TESTER BRIDGE where it can run the measurement for all the parameters mentioned earlier in the frequency range 42 Hz - 5.0 MHz. The layout of the a.c. measurement set - up will be described in section 3.3.4. The crystalline - Si which was deposited with the aluminium electrodes on both sides has to be connected with copper wires on both of its sides by using silver paste (resistivity 0.03Ω/sq). Then one end of both wires has to be connected to the Hioki Tester bridge and the crystalline-Si has to be placed in an oven so that the temperature stabilises at 302 ^{0}K(room temperature). The frequency range was from the lowest 42 Hz to the highest 5.0 MHz and the readings for all the parameters for the particular temperature are recorded by using the Hioki software. How the electrodes and the silver paste were mounted will be explained briefly in section 3.3.3. The experiments have to be repeated for crystalline-Si after the annealing process. The experimental results described in this section will be presented and analysed in the following chapter.

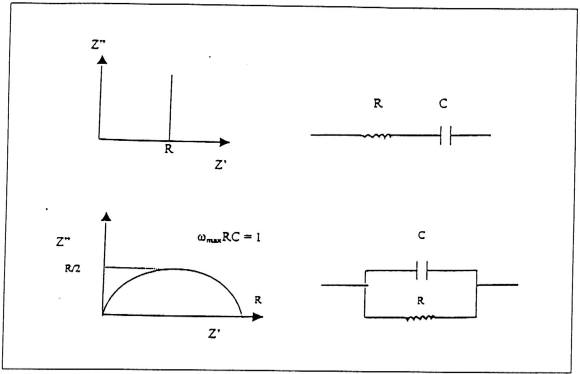


Figure 3.11 : Complex impedance plots in an RC circuit in a) series and b)parallel

3.2.3. Optical Characterisation of Crystalline - Si

i) UV - Vis Transmission Spectroscopy

The optical transmission spectrum of crystalline - Si has been taken over a range of 200 nm - 3000 nm and this has been done by using a Shimadzu UV-VIS spectrophotometer model UV - 3101PC. A schematic block diagram has been shown in fig. 3.12. The optical schematics of UV-3101PC will be discussed more in section 3.3.2. The set-up consists of a light source, a monochromator, a sample compartment (which hold the sample and the reference holder), a photomultiplier tube (detector) and a computer to automate the measurement. Primarily, the base line was obtained by using air as the reference and scanned in the range 200 nm - 3000 nm. Once the base line measurement has been completed, the sample holder was loaded with crystalline - Si and the transmission spectrum of the sample was obtained.

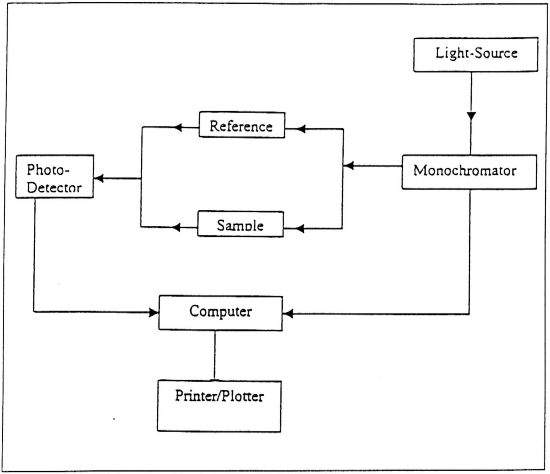


Figure 3.12: A Schematic block diagram of UV - VIS spectrophotometer

ii) Formulae used to calculate refractive index(n), absorption constant(k) and coefficient of absorption(α).

The refractive index of the sample was calculated by assuming that the absorption constant is equal zero and using the equation 2.17. The absorption constant (k) was calculated from reflectance data at each wavelength by using the equation 2.17, when the refractive index can be obtained. The coefficient of absorption (α) was next calculated by substituting the appropriate value of k for each wavelength by using equation 2.18, and finally the graph of (α) against wavelength(λ) was plotted.

3.3. Preparation of Hydrogenated Amorphous Silicon (a-Si:H)

3.3.1 Sample Preparation

For any particular deposition run , samples have to be prepared for the various measurement techniques. The total surface area for deposition is usually the top of the base electrodes , which in our case is ≈ 182 cm^2. This will limit the number of samples which can be prepared for each measurement. Two types of substrates are usually used, such as, the glass slides and the crystalline - Si wafers. The glass substrates are usually used to study the electrical and the optical properties. The crystalline - Si wafer substrates are used to study the infra-red absorption properties. The procedure mentioned below refers to the preparation of glass slides to be used as substrates for the a-Si:H film:

1. The glass slides are to be cut to appropriate dimensions using the diamond glass cutter. The optical and electrical samples must have areas ≈ 3.90 x 2.40 cm^2.
2. To remove the gross dirt and oils , the samples are held under the tap and washed using a commercial detergent.
3. The slides are then immersed in a beaker of water, and shaken in an ultrasonic bath for five minutes. After this stage onwards, tweezers have to be used to handle the slides.
4. The slides are next removed and immersed in a beaker of isopropyl alcohol and shaken in the ultrasonic bath for at least 5 minutes.
5. Then the slides are immersed in acetone and shaken ultrasonically for 2 minutes.
6. The slides are then placed in the petri dishes and stored in the oven at 50 °C so that it is free from dust and grease.

For the crystalline - Si , a special care has to be taken when the cutting is done due to its brittleness. The preliminary cleaning is done by etching with 10% solution of hydrogen fluoride (HF). The rest of the cleaning procedure follows that of the glass slides. The aluminium deposition mask which was used to prepare the electrical characterisation and optical characterisation samples, has to be polished with sand papers prior to the normal cleaning to remove any a-Si:H deposition on them. The handling of the samples after deposition can have a critical effect on the film characteristic. Oxygen , nitrogen and water vapour are common contaminants. In addition, exposure to strong lights has to be avoided in view of the known photostructural effects. The electrical sample will require the aluminium electrodes to be deposited on them as soon as possible.

3.3.2. Preparation of a-Si:H thin film sample

The a-Si:H samples which were used in this work were deposited by using horizontal plasma glow discharge system. This system is a home built system designed and built originally by K.S.Wong [61] in the Solid State Research Laboratory, Physics Department, University Malaya. In this system, the silane gas (SiH_4) is discharged at an ionization current of 12 mA and to maintain this ionization current, the d.c. voltage was varied from 500 volt-580 volt. The deposition of silane was carried-out at room temperature and the deposition was done for 90 minutes. The silane deposition pressure was monitored by using Pirani head and the pressure was maintained at 0.8 mbar. In this work, two sets of a-Si:H films were prepared to characterise the films. The two sets of sample were obtained by producing samples using silane flow-rates of 5 sccm and 25 sccm during the deposition. A Hasting Automated Mass flow controller, model 400 was used to monitor the flow-rates of silane. The deposition parameters for 5 sccm and 25 sccm samples are presented in table 3.4. The film were deposited simultaneously on crystalline silicon and soda lime glass substrates. The films on crystalline silicon substrate were used for infra-red analysis whereas the films on glass substrate were used for optical characterisation, structural characterisation and electrical characterisation. Aluminium electrodes were deposited in a co-planar structure using an Edwards Evaporating system for electrical characterisation.

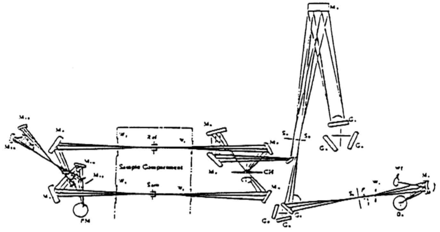
Parameters	**Flow Rate : 5 sccm**	**Flow Rate : 25 sccm**
Deposition Pressure	8 x 10^{-1} mbar	8 x 10^{-1} mbar
Ionisation Current	12 mA (maintaining voltage 80V)	12 mA (maintaining voltage 75V)
Deposition Time	90 minutes	90 minutes
Deposition Temperature	23 ^{0}C	23 ^{0}C
D.C. Voltage	500 volt - 580 volt	500 volt
Substrate	glass and crystalline - Si	glass and crystalline - Si
Sample Position	Base	Base
A.C. Voltage	90 volt	90 volt

Table 3.4 : The deposition parameters of the hydrogenated amorphous silicon (a-Si:H).

3.3.3. Optical Characterisation of a-Si:H

I) UV - Visible Spectroscopy

A Shimadzu UV - VIS / UV - VIS - NIR 3101PC scanning spectrophotometer (fig. 3.13) was used to obtain the optical transmission spectrum for the hydrogenated amorphous silicon (a-Si:H) sample. The spectrophotometer system consists of a light source, a sample compartment, a monochromator and a detector system. The light sources used to produce light in the ultra-violet to near infra-red wavelength region in this system consists of a halogen lamp and a deuterium lamp. The monochromator unit consists of entrance and exit slits, a mirror system and a prism. The detector system consists of a PbS photocell.



D_2:	Deuterium lamp	$W_1 - W_3$:	Window plates (W_1, W_2, 30mm dia.; W_3, 40mm dia.)
WI	Halogen lamp		
F:	Filter	CH:	Chopper mirror
$G_1 - G_3$:	Gratings of first monochromator	$M_1 - M_{13}$:	Mirrors (M_{11} is detector switching mirror)
$G_4 - G_6$:	Gratings of second monochromator	Ref:	Reference cell
S_1:	Entrance slit	Sam:	Sample cell
S_2:	Intermediate slit	PM:	Photomutiplier
S_3:	Exit slit	PbS:	PbS cell

Figure 3.13 : Optical Schematics of UV - 3101PC.

A typical UV and Visible transmission spectrum for a-Si:H is shown schematically in fig. 3.14.

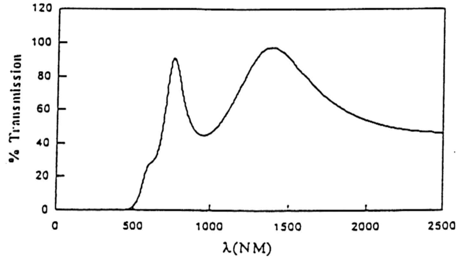


Figure 3.14: A typical transmission spectrum of the hydrogenated amorphous silicon (a-Si:H)

Visible and UV spectroscopy have a variety of applications associated with the local structure of the materials. This is because the position of the absorption and transmission bands are sensitive to co-ordination environment and bond character. For this work , the scanning range was selected is from 300 nm - 3000 nm. A diagnostic programme appears on the computer monitor when it is turned on to ensure that the system is functioning. The base line is first obtained by scanning with two glass slides which were used as substrates for the thin film in both the reference and the sample holders. One of the glass slides is used as reference and is replaced by the thin film a-Si:H sample. The transmission spectrum of the sample is then obtained. A typical transmission spectrum for a-Si:H thin film sample is shown earlier in fig. 3.14. However not all thin film samples produce transmission spectrum with interference fringes since the appearance of this fringes are strongly dependent in the refractive index and the thickness of the film.

II) Determination of refractive index , thickness and optical energy gap of a-Si:H thin films.

The of film thickness and refractive index at various wavelengths are determined using the technique which was proposed by J.G.Manifacier , J.Gasiot and J.P.Fillard [62]. The refractive index and the film thickness are determined by considering a continuous function of interference maxima T_{max} and interference minima, T_{min} to be a continuous function of wavelength. The refractive index at a particular wavelength is determined using the following equation:

$$n(\lambda) = [\, N + (N^2 - n_0 n_1)^{1/2}\,]^{1/2} \qquad (3.25)$$

where;

$$N(\lambda) = \frac{(n_0^2 + n_1^2)}{2} + 2n_0 n_1 \frac{(T_{max} - T_{min})}{T_{max} T_{min}} \qquad (3.26)$$

where n_o and n_1 are the refractive indices of air and the substrate (glass) respectively. The expression for the thickness of the thin film (d) is then determined by using the interference maxima condition for two different wavelength λ_1 and λ_2, as given below:

$$d = \frac{M\lambda_1\lambda_2}{2[\lambda_2 n(\lambda_1) - \lambda_1 n(\lambda_2)]} \qquad (3.27)$$

where M is the number of oscillations between the two extremea occurring for λ_1 and λ_2 and $n(\lambda_1)$ and $n(\lambda_2)$ are the refractive indices at λ_1 and λ_2 respectively. The dispersion curve of refractive index versus wavelength is obtained by using the Cauchy relationship,

$$n = n_o + (b/\lambda^2)$$

where n_0 is the static refractive index and b is a constant. The dispersion curve is then used to determine the hydrogen content of a-Si:H thin film. The transmission spectrum of the a-Si:H is also been used to determine the optical band gap of the film. The absorption coefficient (α) is calculated from the transmission curve by the following relationship ,

$$\alpha = \frac{1}{d}\ln(\frac{1}{x}) \qquad (3.28)$$

where d is the film thickness , x is derived from expression for transmission (T) coefficient through the air - film -substrate interference as given in Brodsky [63]:

$$T = \frac{(1-R_1)(1-R_2)(1-R_3)e^{-\alpha d}}{(1-R_1R_3)[1-(R_1R_2+R_1R_3(1-R_2)^2)e^{-2\alpha d}]} \qquad (3.29)$$

where R_1 , R_2 and R_3 are the reflectivities at the air-film , film-glass and glass-air surfaces respectively. Bahl's relation [64] is used to determine the reflectivities.

$$R_1 = \frac{(n_f-1)^2}{(n_f+1)^2} \qquad (3.30)$$

$$R_2 = \frac{(n_f-n_s)^2}{(n_f+n_s)^2} \qquad (3.31)$$

$$R_3 = \frac{(n_s-1)^2}{(n_s+1)^2} \qquad (3.32)$$

where n_s is the refractive index of the substrate (glass) and n_f is the refractive index of the film. The refractive index of air is 1.0. Using $x = e^{-\alpha d}$ and,

$$A = (1-R_1)(1-R_2)(1-R_3) \quad (3.33)$$

$$B = R_1 R_3 \quad (3.34)$$

$$C = R_1R_2 + R_1R_3(1-R_2)^2 \quad (3.35)$$

the equation (3.29) can be written in the following form :

$$T = \frac{Ax}{(1-B)(1-Cx^2)} \quad (3.36)$$

which can be rewritten in the following quadratic form:

$$(TC - TBC)\, x^2 + Ax - (T - TB) = 0 \quad (3.37)$$

Solving (3.37) for x, one obtains

$$x = \frac{-A \pm \sqrt{A^2 + 4T^2C(1-B)^2}}{2TC(1-B)} \quad (3.38)$$

The absorption coefficient is then calculated for different wavelengths using equation (3.28).The optical energy gap of the material, is determined from the Tauc's plot of $(\alpha E)^{1/2}$ versus E where E is the photon energy. The intercept of the most linear region of this plot near the absorption edge with the energy axis is the optical energy gap of the film. The Tauc's plot of $(\alpha E)^{1/2}$ versus E is only applicable when the density of states is of parabolic dependence.

II) Calculation of the Hydrogen Content

The refractive index of the material can be expressed as[33,65] ,

$$n^2 - 1 = \frac{E_d - E_0}{E_0^2 - E^2} \quad (3.39)$$

where n is the refractive index , E_0 is the energy of the effective dispersion oscillator , E is the photon energy and E_d is the dispersion energy which measures the average strength of the inter band optical transition. Equation (2.66) can be written as ,

$$\frac{1}{n^2-1}=\frac{E_0^2-E^2}{E_d E_0} \qquad (3.40)$$

Values of E_d and E_o are obtained from values of the intercept and the slope of the most linear region of the $1/n^2$-1 versus E^2 plot. The E_d and E_o values are derived from the following relationship:

$$E_d = \sqrt{\frac{1}{\mathrm{int}\,ercept x slope}} \qquad (3.41)$$

$$E_o = \sqrt{\frac{\mathrm{int}\,ercept}{slope}} \qquad (3.42)$$

The density of valence electrons, n_v,, is next obtained from the model of C.Ance.et.all[34].

$$n_v = \frac{0.0143 E_d^0 X 10^{23}}{\varepsilon_0 - 1} \qquad (3.43)$$

where ε(0) is taken as square of the standard refractive index in the long wavelength region. One can calculate the hydrogen content in the hydrogenated amorphous silicon as ;

$$C_H = \frac{1}{3}\frac{n_v}{n_s}\left[4-\sqrt{\frac{E_d}{2.8}}\right] \qquad (3.44)$$

where n_s is the density of valence electrons in the crystal silicon ($n_s \approx 2 \times 10^{23}$ electrons cm^{-3}) [35,36].

III) Calculation of the Width of the Band Tail

It is well known that potential fluctuations due to the internal electric field occurs in amorphous solids. The fluctuation results in tailing of valence and conduction bands into the forbidden band gap. This "Urbach Tail" is expected to be observed in polycrystalline thin films also. The absorption coefficient for polycrystalline material may be expressed as,[66,67].

$$\alpha \approx \exp\left(\frac{E}{E_e}\right) \qquad (3.45)$$

where E is the photon energy (eV) and E_e is the width of the band tail (eV). Therefore the gradual decrease of the absorption edge extending up to a few tenth of eV into the forbidden gap is called "Urbach Edge"[68]. The equation mentioned above can therefore be used to determine the Urbach Tail band width, which measures the extent of band tailing into the forbidden gap. The value of E_e can be obtained by plotting a graph $\ln(\alpha)$ versus photon energy (E) and the slope of graph in the linear region has to be found by using regression technique. The inverse slope of the graph gives the width of the band tail.

3.3.4 Electrical Characterisation

(A) . D.C. Conductivity Measurement

i) Measurement Technique

The sample used in the d.c. conductivity measurement was placed in a Janis VPF-100 cryostat. The reason for placing the sample in the cryostat is that a heater and a thermocouple are conveniently attached to the sample holder which is connected to a Lake Shore 321 Autotuning Temperature Controller so that measurement can be done at temperature between 297^0K-338^0K. Also the cryostat encloses and shield the sample from external electric field which can effect the current-voltage measurement since the current magnitude is very small. Current - voltage measurement was done at a fixed temperature by using Keithley 236 - Source Measurement Unit (SMU) supported by metrics computer software. The experimental set-up for the d.c. conductivity measurement is illustrated in fig.

3.15. The aluminium electrodes of co-planar structure was deposited earlier by evaporation technique. The dimension of the electrodes was measured by using a sliding microscope. The conductivities σ, of this sample at the various measurement temperature were calculated from the current-voltage plot. The activation energy for the sample is determined from the graph of $\ln(\sigma)$ versus inverse temperature. Before current - voltage measurement is carried out, the trap emptying process is done to ensure that the states within the forbidden gap is emptied. The configuration used in running the SMU for the emptying trap process is tabulated in table 3.5. During this process, the sample was subjected to a constant voltage of 100 volts for half an hour. The electric circuit for current - voltage measurement is illustrated in fig. 3.16. The configuration used when running the SMU for the conductivity measurements is tabulated in table 3.6.

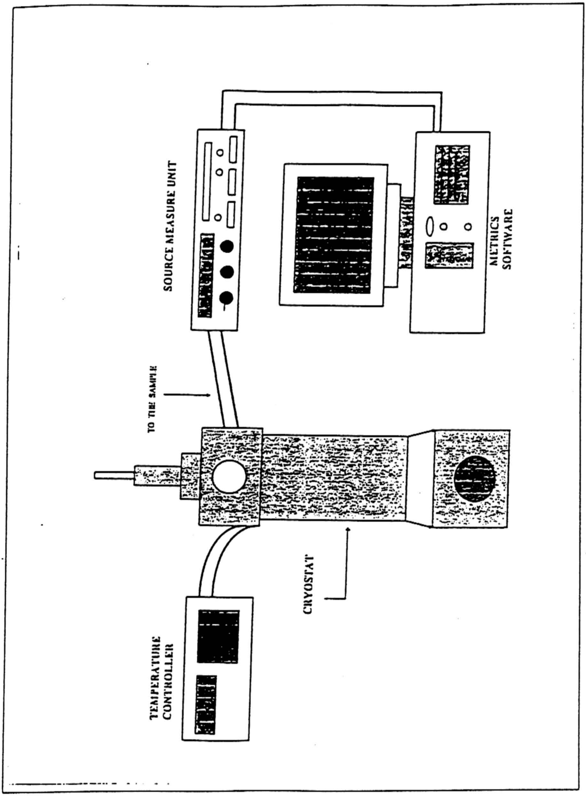


Figure 3.15 : Experimental set-up for direct current (d.c.) conductivity measurement

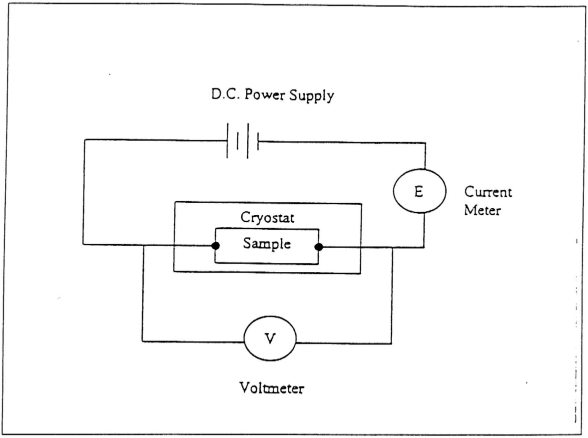


Figure 3.16: Electrical circuitry for the current - voltage measurement.

Mode	Constant
Type	Linear
Stimulus Measure	Voltage and Current
Value	100 V
Delay	0 sec
Intergration	50 Hz
Filter	4 Reading

Table 3.5 : Configuration used in SMU during empty trapping for a-Si:H.

Mode	Sweep
Type	Linear
Measurement	Voltage and Current
Start	0 V
Stop	100 V
Number of points	2.1
Interval	0.5 V
Time delay	0 sec
Integration	50 Hz
Filter	4 Readings

Table 3.6 : Configuration used in SMU during current voltage measurement in a-Si:H

ii)Formula for Calculation of D.C. Conductivity

Figure 3.17 illustrates the co-planar configuration for d.c. conductivity measurement. The conductivity of the a-Si:H sample on the glass substrate is calculated by using the following expression ;

$$\sigma = \left(\frac{I}{V}\right)\left(\frac{d}{wt}\right) \qquad (3.46)$$

where I is the current measured , d is the width of the gap, V is the voltage across the sample , w is the width of the electrode and t is the thickness of the sample between the electrodes (refer fig. 3.17).

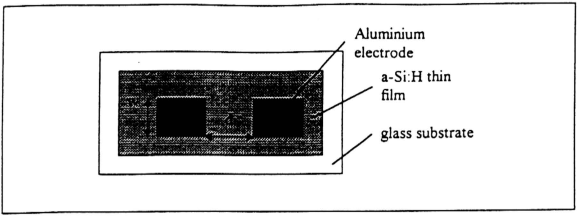


Figure 3.17: Coefficient-planar configuration for d.c. conductivity measurement

ii) Calculation to determine the activation energy (E_c - E_f)

The dependence of conductivity on measurement temperature is expressed by the equation:

$$\sigma = \sigma_0 \, e^{-\left(\frac{E_c - E_f}{kT}\right)} \qquad (3.47)$$

where σ_o is a constant, (E_c-E_f) is the activation energy, k is the Boltzmann constant and T is the measurement temperature. Thus by plotting ln(σ) versus 1/T, the activation energy can be determined. Measurement temperatures are confined to temperatures where extended state conduction is a dominant conduction mechanism. In this case, the range between 297°K to 338°K is suitable.

(B) Alternating Current (a.c.) Conductivity Measurement

i). Measurement Technique

The a.c. conductivity measurement were carried out by using Hioki 3520 LCR Hi Tester Bridge. Measurement were done in the frequency range of 42 Hz - 5.0 MHz. The a.c. measurement set-up which was used in this work is illustrated in fig. 3.18. The samples were placed in the oven so that the measurement temperature can be stabilised. Aluminium electrodes were deposited in a transverse configuration on samples deposited on crystalline silicon while co-planar electrodes were deposited on samples deposited on glass substrate. Capacitance versus frequency measurement at room temperature was done on the film deposited on crystalline silicon substrate to determine the thickness of the film. Conductance and capacitance versus frequency measurements were done on film deposited on glass substrates at temperatures between 302^{0}K to 338^{0}K. The measurement parameters were recorded using the Hioki Software interfaced to the experimental set-up.

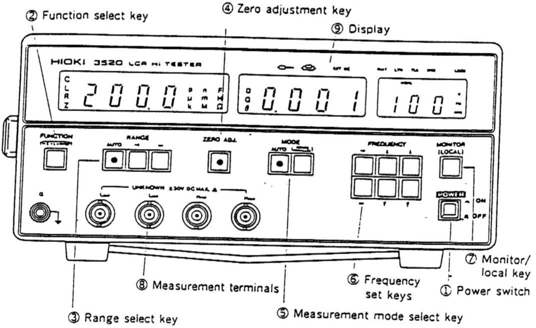


Figure 3.18 : The Hioki Tester Bridge.

ii) Calculations for Sample on Glass Substrate

The density of states at Fermi Level is evaluated from the conductance (G) versus frequency results. The frequency range for this calculation is between 42 Hz to 1 MHz. The conductivity of the sample, is calculated from expression:

$$\sigma_{(a.c.)} = G\left(\frac{l}{A}\right) \qquad (3.48)$$

where l is the gap between the electrodes, and A is the cross-section normal to the direction area of current flow. The thickness of the film has been obtained from the optical measurement. The conductivity is then calculated for all the measured temperatures and a graph of conductivity versus the temperature is plotted. The graph expected should be a linear and the slope of the graph (m) is determined by the least square method. From this slope, the density of states at the fermi level $N(E_f)$ was obtained using the following expressions:

$$\sigma(\omega) = \left(\frac{\pi}{3}\right) e^2 kT\left(N(E_f)\right)^2 \alpha^{-5}\omega\left[\ln\left(\frac{\upsilon_{ph}}{\omega}\right)\right]^4 \qquad (3.49)$$

where ν_{ph} is phonon frequency (10^{13} s^{-1}), $\omega \approx 10^6$ s^{-1}, α^{-1} is effective range of wave function ($\alpha^{-1} \approx 10$ Å), e is the electron charge, k is the Boltzmann Constant.

iii) Calculation of thickness of film on crystalline - Si substrates

The thickness of the film on the crystalline silicon substrate is determined using the plot of parallel capacitance versus frequency. From the capacitance value in the high frequency range where the capacitance saturates to a constant value. The thickness of the film was determined using the expression:

$$C_p = \frac{\varepsilon_0 \varepsilon_r A}{d} \quad (3.50)$$

$$\text{(thickness) } d = \frac{\varepsilon_0 \varepsilon_r A}{C_p} \quad (3.51)$$

where ε_r is the dielectric constant of the sample, A is the area of the aluminium dot on the a-Si:H film and C_p is the parallel capacitance value in the high frequency region and d is the film thickness. Figure 3.19 illustrates the transverse electrode configuration used in the experiment. The dielectric constant is determined from the square of the refractive index of the film.

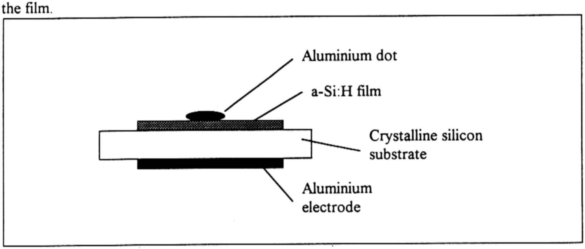


Figure 3.19: Transverse configuration of electrodes on a-Si:H deposited on crystalline silicon

3.4 Structural Investigation for Crystalline and Amorphous Semiconductors.

X-ray diffractograms for crystalline and amorphous semiconductor samples were taken using a Philips Compact X-ray Diffractometer System PW1840. The Diffractometer consists of a goniometer of a Bragg - Brento design and with an automatic divergence slit and a solid state Si - Array detector [70]. A long fine focus x-ray tube is used for optimum results for peak intensity and resolution. A copper anode material is used for the powder diffractometry , with k_α line at 0.1542 nm as in fig. 3.20. X-ray powder diffraction pattern consists of a sets of peaks , each of different intensity and position (Bragg's angle , θ or d-spacing) on a length of a chart paper. The peak position for the irradiated substances are essentially fixed and are characteristic of that substance. The intensity may vary somewhat from sample to sample. Bragg's law is used to relate the observed diffraction angle 2θ to the spacing of the lattice planes in the samples which give rise to the diffraction. Bragg's law can be written as ,

$$n\lambda = 2d \sin\theta \qquad (3.52)$$

where λ is the wavelength of the x-ray radiation , d is the interplanar spacing , θ is the angle of incedence and n is an integer. Powder X-RAY DIFFRACTION has several applications including quantitative identification between , crystalline , amorphous and polycrystalline compounds. Each sample has its own characteristic powder diffraction pattern which may be used for its identifications. The configurations which was used in the x-ray Diffractometer for crystalline and amorphous semiconductor in the experiment is described in the table 3.7.

Parameters	Crystalline Semiconductor	Amorphous Semiconductor
Source	Cu - K_{α} (λ=1.544nm)	Cu - K_{α} (λ=1.544nm)
Voltage	40 KV	40 KV
Current	30 mA	30 mA
Scan Type	Continous	Continous
Scan Step Size	0.002	0.002
Scan Step Time	20 min	20 min
Range (c.p.s)	10.00 - 70.00	10.00 - 70.00

Table 3.7 : Configuration used in X-ray Diffractometer.

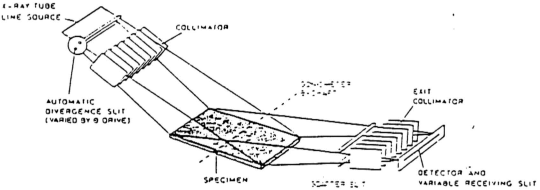


Figure 3.20 : Goniometer X - Ray Path.

3.5 Fourier Transform Infrared Spectroscopy for a-Si:H

Fourier - Transform Infrared (FTIR) spectroscopy technique is utilised to analyse the chemical bonding structure in a-Si:H films which was produced by d.c. plasma glow discharge technique. These studies, provide very useful information which identifies the spectrum signatures for sites containing one H atom , SiH , one or more than one hydrogen atoms , SiH_2 and SiH_3. The SiH environment usually contains a bond-stretching mode at 2000 cm^{-1} and a bond-bending mode at 630 cm^{-1}, whereas sites with more than one H atom exhibit additional features in bond-bending frequency regime , 800 - 900 cm^{-1} , as well as new bond-stretching modes between 2050 and 2150 cm^{-1}. In this experiment , the concentration of bonded hydrogen at wave number 2200 cm^{-1} - 1800 cm^{-1} and within 1200cm^{-1} - 500 cm^{-1} have been calculated by using the equation below. In the experiment , Perkin Elmer model 1600 FTIR spectrophotometer has been used to scan thin film a-Si:H deposited on crystalline - Si substrate. The latter was used because the Crystalline - Si substrate will not absorb the infrared photons due to its crystal symmetry. Firstly , the background was scanned over the range 4000 to 200 cm^{-1} followed by the crystal silicon substrate and then the a-Si:H film on crystal silicon is then scanned over the same range. The infra-red spectra for a-Si:H may then be derived.

ii)Determination of Integrated Intensity under peaks of IR Absorption Spectrum

The integrated intensity of the Si-H stretching mode (S_s) at ≈2000 cm^{-1} and Si-H bond wagging mode (S_w) at ≈ 600 cm^{-1} bands are determined by first converting the transmission spectra to absorption coefficient spectra using the equation:

$$\alpha(\omega) = \frac{1}{d}\ln\left(\frac{100}{\%T}\right) \qquad (3.53)$$

where $\alpha(\omega)$ is the absorption coefficient , d is the thickness of the a-Si:H thin film and %T is the transmission percentage. Then the Gaussian lineshape is used to deconvolute component peaks from the absorption spectrum. The general equation used for Gaussian lineshape is as below :

$$\alpha(\omega) = \alpha(\max) \exp\left(-\frac{\left[4\{\ln 2\}\{\omega - \omega_0\}^2\right]}{\Delta\omega} \right) \qquad (3.54)$$

where ,

$$\alpha(\max) = \frac{2(\ln 2)^{1/2} S_{band}}{\pi^{1/2}\Delta\omega} \qquad (3.55)$$

and

$$S_{band} = \int \alpha(\omega) d\omega \qquad (3.56)$$

where S_{band} is the area under the curve , $\Delta\omega$ is the full width half maximum (FWHM) of the absorption peak, $\alpha(\max)$ is the maximum absorption coefficient and ω_0 is the peak position. A typical curve-fitting graph for the a-Si:H stretch absorption band at 2000 cm^{-1} is illustrated in fig. 3.21. Equation (3.54) is rewritten in the form of ,

$$y = A \exp\left(-[Bx]\right) \qquad (3.57)$$

where,

$$A = B^{1/2} S_{band} / \pi^{1/2} \qquad (3.58)$$

$$B = \frac{4\ln(2)}{(\Delta\omega)^2} \qquad (3.59)$$

$$x = [\omega - \omega_0]^2 \qquad (3.60)$$

Equation 3.57 can be rewritten as ,

$$\ln y = \ln A - B\,[\omega - \omega_0]^2 \qquad (3.61)$$

The integrated intensity of the absorption peak representing a bonding configuration is ,

$$I = \int \frac{\alpha(\omega)}{\omega_0} d\omega \qquad (3.62)$$

From equation (3.56) the integrated intensity under peaks can be expressed as below,

$$I = \frac{S_{band}}{\omega_0} \qquad (3.63).$$

iii) Formulae for Calculation of bonded Hydrogen Concentration

The hydrogen concentration can be obtained from this equation which is expressed below,

$$N_H = \frac{\gamma(1+2\varepsilon)^2\left(\sqrt{\varepsilon}\right) N_A S_{s,w}}{9\varepsilon^2 (T/\xi)} \qquad (3.64)$$

where $\varepsilon = 12$ for Si , N_A is the Avagadro's number , γ is the 'fudge' factor to take into account the inadequacies in the local field correction which is taken to be 0.5 and (T / ξ) is the integrated strength of the corresponding bond in the gaseous hydride given in cm / mole bond is taken to be 3.5. Thus , for silicon the expression can be written as [71] ,

$$N_H = A_s \int_{w,s} \frac{\alpha(\omega)}{\omega} d\omega \qquad (3.65)$$

with $A_s = 1.4 \times 10^{20}$ cm^{-2} and $A_w = 1.6 \times 10^{19}$ cm^{-2} for the stretching and the wagging bands respectively [72]. The hydrogen content of the a-Si:H thin film samples in this work is defined as the percentage of the hydrogen concentration calculated from the total integrated intensities of the Si-H wagging absorption band at 640 cm^{-1} to the concentration of silicon atoms in crystal silicon which is taken to be 5 x 10^{22} atoms / cm^3. This introduces significant error in the magnitude of hydrogen content when microvoid concentration in the film is high. The results of the hydrogen percentage will be presented in the next chapter.

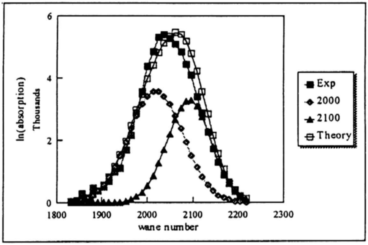


Figure 3.21 : A typical curve fitting graph which was done in the experiment to obtain the integrated intensity under the peak by using Gaussian equation.

3.6 Annealing Process

Annealing is a process by which a material is heated in a furnace for a specific time at a specific temperature. In this work, the sample is annealed in ambient nitrogen to make sure that oxygen contamination on the sample does not take place during the process. The furnace is heated by setting the temperature controller switch to the required temperature. A steady flow of the nitrogen gas is allowed to pass through the Pyrex tube. When the temperature is stable, the sample is put into the sample holder which is then inserted into the furnace together with the thermocouple sensor. In this work, the samples is annealed in ambient nitrogen at 300^0C and 500°C for half an hour each. The samples are allowed to cool down in the furnace in a continuous flow of nitrogen gas to room temperature. The furnace used in this experiment is of the carbolite model CFN 1271 and the set-up for annealing process is shown in fig. 3.22.

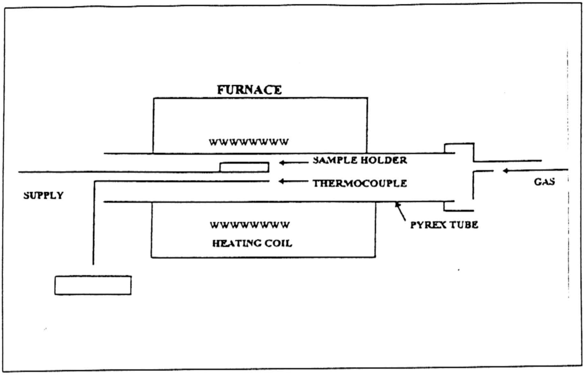


Figure 3.22 :Experimental arrangement for the annealing process