

## Band gap Measurement of *P* – type Monocrystalline Silicon Wafer

G. Hashmi<sup>1\*</sup>, M. K. Basher<sup>2</sup>, M. Hoq<sup>2</sup> and M. H. Rahman<sup>1</sup>

<sup>1</sup>*Department of Electrical and Electronic Engineering, University of Dhaka, Dhaka-1000*

<sup>2</sup>*Institute of Electronics, AERE, Bangladesh Atomic Energy Commission, Savar, Dhaka*

### Abstract

Band gap of P-type monocrystalline silicon wafer has been measured using spectral response measurement system. To see the spectral response a SR510 lock in amplifier, SR540 optical chopper, monochromator (400nm-1200nm), optical detector and lab view software has been used. From spectral response of polished P-type monocrystalline silicon wafer absorption, reflection and transmission has been respectively seen from 400nm-550nm, 550nm-1050nm and 1050-1200nm. Assuming band gap of silicon is (1.12eV), this result has been theoretically verified using Planck–Einstein relation. Moreover, theoretical band gap of silicon has been calculated (1.127362 eV). The band gap measurement process uses partial concept of Tauc’s downhill negative slop and Planck–Einstein relation. Experimental result shows that, the band gap of silicon is 1.127907 eV.

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### Introduction

One of the most important properties of a semiconductor which distinguish it from metals and insulators is band gap. Band gap is defined as the energy difference (in eV) between the top of upper band (valence band) and the bottom of the lower band (conduction band) in insulators and semiconductors (Streetman, 1993). Furthermore, band Gap measurement has a significant role in semiconductor, nanomaterial and solar cell fabrication industries (Dharma and Pisal, 2009). As band gap measuring equipment’s are very pricy sometimes resource management is necessary. For this purpose, the main goal of this research work has been to utilize an equipment rather than its primary purpose. Although, the primary purpose of spectral response measurement system is to measure the spectral response of a material, this system has been used to measure the band gap of P-type monocrystalline silicon wafer. The measurement shows that, the band gap of polished P-type monocrystalline silicon wafer is 1.127907 eV. Furthermore, the band gap of silicon has been

theoretically calculated which is 1.127362 eV. There are various techniques like UV-VIS spectroscopy, Tauc’s plot and equation, reflection, and absorption coefficient or spectra, four point probe etc. are used to determine the band gap of semiconductor. But here only partial concepts of Tauc’s method has been used. Additionally, spectral response of polished P-type monocrystalline silicon wafer has been investigated. Then this result was theoretically verified after calculating the photon energy with Planck–Einstein relation and relating the photon energy with band gap of silicon (1.12eV).

### *Description of spectral response measurement system*

The spectral response measurement system, as shown in Figure 1, is composed of a SR510 lock in amplifier, SR540 optical chopper, monochromator (400nm-1200nm), optical detector and lab view software. This system emits and directs lights upon a material and form the reflected lights it determines the spectral response of a material (Darmont, 2009).

\*Corresponding author e-mail: [galib\\_90@yahoo.com](mailto:galib_90@yahoo.com)

Here, light emits from a tungsten-halogen lamp which is then focused onto the entrance slit of the monochromator using a condenser lens. Furthermore, a stepper motor is attached to the monochromator which rotates and varies the monochromator output wavelength between 400 nm to 1200 nm. Also a SR540 optical chopper is placed at the exit slit of the monochromator to provide reference signal to the SR510 lock-in amplifier to ensure all the stray light is rejected by the system and enhance system sensitivity from nV to mV range. The output from the monochromator is directed to the material (silicon wafer) with a simple rotatable mirror. After that, the reflected

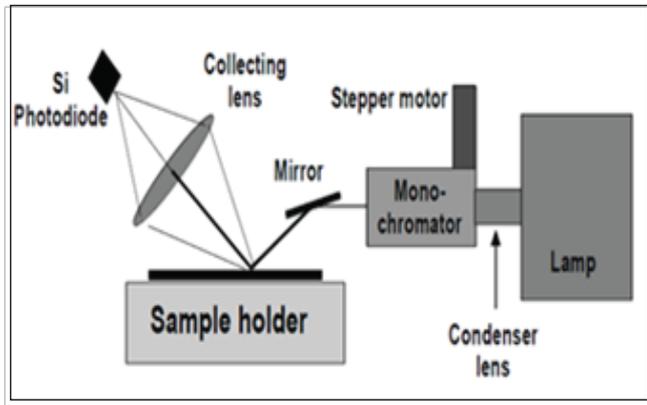


Fig. 1. Schematic diagram of spectral response measurement system

light falls upon a large convex lens close to the surface of the material thus collecting the reflected and scattered light which is then focused onto an optical detector. The optical detector (which converts optical signal to electrical signal) is connected to SR510 lock-in amplifier for measurement through the LabVIEW interface. Here, LabVIEW interface is used for system control, data acquisition and to view the spectral response of the material. The primary purpose of the spectral response measurement system is to plot the spectral response of a material and then from the plotted graph relative reflectivity (in respect to mirror) can be obtained.

*Spectral response of polished P - type monocrystalline silicon wafer*

Figure 2 shows the spectral response of polished P-type monocrystalline silicon wafer. To interpret the spectral response one has to understand about the relationship between photon energy and band gap. It is seen that, if the (photon energy)  $hf > E_g$  (Band gap) then absorption will happen (Rogers *et al.*, 2015). How much absorption will

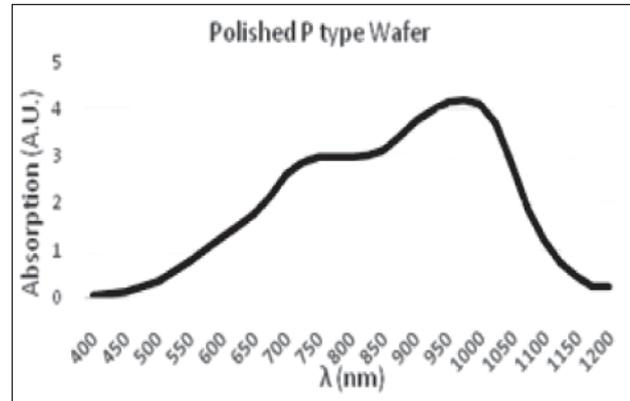


Fig. 2. Spectral response of polished p - type monocrystalline silicon wafer

happen it will depend upon refractive index, absorption coefficient, thickness, surface roughness etc. of the semiconductor material. Moreover, if  $hf = E_g$  then electron hole pair is created and light is efficiently absorbed. Whereas, if  $hf < E_g$  then light interact weakly and pass through the semiconductor as if it was a transparent material. So to see, these relationship, the Planck-Einstein equation has been used to determine the photon energy of different wavelength by the following equation.

$$E = hf \dots (1)$$

Where h is the Planck constant, E is the photon energy and f is the associated wave frequency.

$$\text{Or, } E = \frac{hc}{\lambda} \text{ (Neamen, 2003)}$$

$$= \frac{(4.135667516 \times 10^{-15} \text{ eVs})(299792458 \text{ ms}^{-1})}{\lambda}$$

This equation can be reduces to

$$E \text{ (eV)} = \frac{1239.84193}{\lambda \text{ (nm)}} \dots (2)$$

From equation (2) photon energy of different wavelength along with its corresponding frequency and color are calculated and tabulated in Table I.

Now, the band gap of silicon is 1.12 eV (Sze *et al.*, 2007; NSM Archive, Website). So, photon energy more than 1.12 eV will get highly absorbed. Therefore when 400-550nm (violet to green, photon energy 2.75-2.50 eV) wavelength falls on the P-type wafer, these wavelength is highly absorbed. As the wavelength increases (from red to infrared wavelength (550-1050nm)) the photon energy eV becomes lower and as photon energy become close to silicon band gap

**Table I. Photon energy of different wavelength along with its corresponding frequency and color**

Color	Wavelength	Frequency	Photon energy
violet	380–450 nm	668–789 THz	2.75–3.26 eV
blue	450–495 nm	606–668 THz	2.50–2.75 eV
green	495–570 nm	526–606 THz	2.17–2.50 eV
yellow	570–590 nm	508–526 THz	2.10–2.17 eV
orange	590–620 nm	484–508 THz	2.00–2.10 eV
red	620–750 nm	400–484 THz	1.65–2.00 eV
infrared	700 -1050 nm	430 THz -300 GHz	1.24 mili eV - 1.7eV

1.12 eV, absorption decreases and reflection increases. At 975 nm, peak is observed, where reflection is highest. After infrared region photon energy is lower than band gap of silicon (1.12eV) so transmittance happen, so roll off of spectral response is seen.

#### *Literature review and theoretical calculation of band gap of silicon*

Although most of the books and journals specified band gap of silicon as 1.12 eV, literature review of band gap of silicon suggested that the band gap of silicon varies from 1.11 eV to 1.13 eV. This is due to the fact that, as temperature varies, the intrinsic carrier concentration ( $n_i$ ), effective density of states of the conduction band ( $N_c$ ) and effective density of states of the valance band ( $N_v$ ) also varies. The theoretical and experimental of these values are considered different in books and journals and that's why the band gap of silicon varies from 1.11 eV to 1.13eV. However, it is suffice to say that the band gap of silicon will always lie between 1.11 eV to 1.13eV.

$$V_T = \frac{KT}{q} = \frac{1.380 \times 10^{-23} \times 300}{1.602 \times 10^{-19}} = 0.2584 \text{ v}$$

Where K is the Boltzmann constant, T is the temperature in Kelvin and q is the electron charge in coulomb.

Now, the conduction band energy at intrinsic level is determined by the following equation

$$E_c = V_T \times \ln \left( \frac{N_c}{n_i} \right)$$

Where,  $N_c$  is the conduction band state concentration (at intrinsic) =  $2.86 \times 10^{19} \text{ (cm}^{-3}\text{)}$  (McEvoy *et al.*, 2012)

And  $n_i$  is the intrinsic carrier concentration of silicon =  $1 \times 10^{10} \text{ cm}^{-3}$  (Vivien and Pavesi, 2013; NSM Archive Website)

Therefore, conduction band voltage  $E_c = 0.02584 \ln$

$$\frac{2.86 \times 10^{19}}{1 \times 10^{10}} = 0.562642 \text{ eV}$$

Now, the valance band energy at intrinsic level is determined by the following equation

$$E_v = -V_T \times \ln \left( \frac{N_v}{n_i} \right)$$

Where,  $N_v$  is the valance band state concentration (at intrinsic) =  $3.10 \times 10^{19} \text{ cm}^{-3}$  (McEvoy *et al.*, 2007)

Therefore, valance band voltage  $E_v = -0.02584 \ln$

$$\frac{3.10 \times 10^{19}}{1 \times 10^{10}} = -0.56472 \text{ eV}$$

Now, the band gap ( $E_g$ ) of silicon is

$$E_g = E_c - E_v = 1.127362 \text{ eV}$$

#### *Band gap measurement*

From the spectral response measurement system, the data of P-type monocrystalline silicon wafer has been successfully obtained and tabulated in Table II. Moreover, with that data the spectral response curve has been proficiently drawn in Microsoft Excel. However, the experimentally obtained data directly does not provide the band gap of silicon.

There are various techniques like UV-VIS spectroscopy, Tauc's plot and equation, reflection, and absorption coefficient or spectra, four point probe etc. are used to determine the band gap of semiconductor. Nevertheless, in all the band gap measurement cases the technique and the data used to find the band gap of semiconductor are different as the data are not collected form spectral response measurement system.

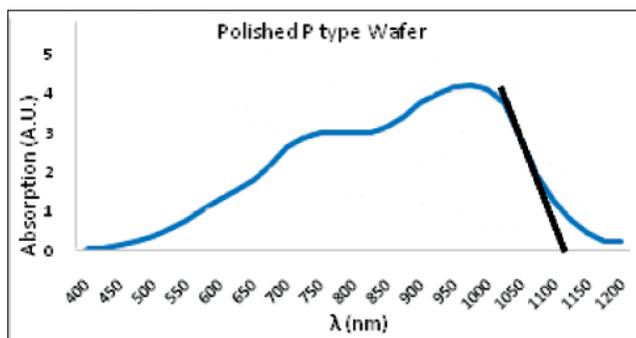
So, a new approach has been applied to measure the band gap of P-type monocrystalline silicon using spectral response measurement system. Apart from spectral response measurement system's data, partial concept of Tauc's band gap measurement process is used in this band gap measurement process. Major difference between Tauc's band gap measurement process (Tauc, 1968) and this work is that, Tauc's band gap measurement process uses the photon energy (eV) vs. absorption coefficient plot of the material whereas here, arbitrary unit (A.U.) and wavelength ( $\lambda$ ) of the material has been used to determine the band gap of semiconductor.

**Table II. Spectral response data of P-type monocrystalline polished silicon wafer**

$\lambda$ (nm)	A.U.	$\lambda$ (nm)	A.U.	$\lambda$ (nm)	A.U.	$\lambda$ (nm)	A.U.
400	0.05	625	1.53	850	3.12	1075	1.89
425	0.07	650	1.78	875	3.40	1100	1.23
450	0.12	675	2.13	900	3.74	1125	0.76
475	0.23	700	2.63	925	3.98	1150	0.45
500	0.36	725	2.85	950	4.14	1175	0.25
525	0.55	750	2.98	975	4.19	1200	0.23
550	0.76	775	2.99	1000	4.10	1075	1.89
575	1.024	800	2.99	1025	3.72	1100	1.23
600	1.28	825	3.00	1050	2.84	1125	0.76

*Procedure of Band gap measurement*

To determine the band gap of P-type monocrystalline polished silicon wafer, the spectral response of P-type monocrystalline silicon wafer needs to be drawn first. From the Table II data the spectral response curve has been drawn in Microsoft Excel. Next, drawing of a negative slope along the downhill part of the spectral response of P-type monocrystalline polished silicon wafer is necessary, as shown in Fig. 3.

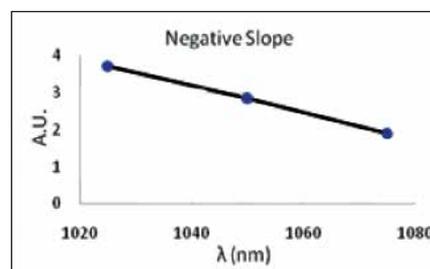
**Fig. 3. Negative slope drawn along downhill part of spectral response of polished p - type monocrystalline silicon wafer**

Now, to draw the negative slop along the downhill spectral response, downhill part spectral data are selected from Table II (Highlighted by yellow color).

From the highlighted color at least 3 wavelengths along with A.U (Arbitrary Unit) are needed to form a straight line. Here it can easily be done using Microsoft Excel software. Just selecting and then removing the unnecessary points (wavelengths) will easily form a straight line, which is actually the negative slop (shown in Fig. 4). The negative slop formation wavelengths and associated A.U. are tabulated in Table III. Now, extension of the negative slop will intersect the horizontal axis and will give away the required wavelength. Lastly, by putting the value of the wavelength in Planck-Einstein equation the band gap of P-type monocrystalline silicon wafer can be determined.

**Table III. The three wavelengths and associated A.U. which form the negative slope**

Wavelength (nm)	Arbitrary unit (A.U.)
1025	3.724194
1050	2.840405
1075	1.890594

**Fig. 4. Negative slope****Results and discussion**

By extending the negative slope, it intersects a point in the horizontal axis. This intersection point in the horizontal axis is the required wavelength. To find out the intersection point of horizontal axis, it is considered that  $P_1$  (1050, 2.840405);  $P_2$  (1075, 1.890594);  $P_3$  ( $\lambda$ , 0) these three points are in the same line. It is only possible if and only if the slope for both the lines are same. As  $\lambda$  is the intersection point of

horizontal axis all these points will be in the same line and slope will be the same.

$$\begin{aligned} \text{So, } m (\text{slope}) &= \frac{y_1 - y_2 = y_1 - y_3}{x_1 - x_2 = x_1 - x_3} \\ \frac{3.84045 - 1.890594}{1050 - 1075} &= \frac{3.840405 - 0}{1050 - x_3} \\ \frac{1.949811}{-25} &= \frac{3.840405}{1050 - x_3} \\ 1.949811(1050 - x_3) &= -96.010125 \\ 2047.30155 - 1.949811x_3 &= -96.010125 \\ -1.949811x_3 &= -2143.311675 \\ \text{Therefore, } x_3 \text{ or } \lambda &= 1099.240734 \text{ nm} \end{aligned}$$

Now putting the wavelength value in equation 2 (Planck-Einstein equation) we get,

$$\text{Band Gap} = \frac{1239.84193}{1099.240734} = 1.127907 \text{ eV ; which is the band gap of P-type monocrystalline silicon wafer.}$$

However, the theoretical calculation shows the band gap of silicon is 1.127362 eV. So the error is

$$\frac{1.127907 - 1.127362}{1.127362} \times 100 = 0.04834\%, \text{ which can be}$$

considered negligible. So from spectral response measurement system band gap of P-type monocrystalline silicon can be successfully measured.

## Conclusion

Although the relative reflectivity is normally measured by spectral response measurement system, it is seen that band gap of polished P-type monocrystalline silicon wafer can also be measured by this system. Experimental measurement shows band gap of silicon is 1.127907 eV. Whereas, theoretical calculated value is 1.127362 eV. As error is 0.04834%, it can be considered as negligible. With this spectral response measurement system the absorption coefficient cannot be determined, so direct and indirect band gap semiconductor identification is not possible. But, it can be concluded that spectral response measurement equipment can be used as a band gap measurement equipment if the semiconductor material spectral response lies between 400 nm to 1200 nm. The main purpose of this work has been to

use an equipment rather than its primary purpose. As spectral response measurement system can measure the band gap of silicon the primary purpose of this work has been fulfilled. Furthermore, from spectral response of polished P-type monocrystalline silicon wafer absorption, reflection and transmission has been observed and the result has been theoretically verified using Planck-Einstein relation.

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