Determination of Optical Band Gap and Heat Dissipation of Ga$_{1-x}$Mn$_x$As with Light in UV-VIS-IR Region using OSA SPECTRO 320

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Abstract

Heat generated by silicon-based transistors due to high energy photo irradiation interferes with the electronic conductivity of transistors in the ICs. There is need to search for an alternative semiconductor material for making diodes and transistors with little or no heat dissipation. Dilute magnetic semiconductor such as Gallium Arsenide (GaAs) has demonstrated to be a better candidate to substitute silicon in electronic technology. UV-VIS-IR light was illuminated on the Ga$_{1-x}$Mn$_x$As samples of thickness 500nm–1000nm of varied doping levels during the study. Reflectance and transmittance spectra were determined using OSA SPECTRO 320 with light obtained from sodium lamp (240V, 100 W) with irradiance of 33.4807 W/m$^2$. The maximum absorbance within the UV-VIS-IR range was, A$\leq$ 83.82% at $\lambda$ $\approx$ 200nm and minimum absorbance was, A$\geq$0.96% at $\lambda$ $\approx$ 300nm with Ga$_{1-x}$Mn$_x$As, x=20% having the highest absorbance value and Ga$_{1-x}$Mn$_x$As, x=1%, the least absorbance. For Ga$_{1-x}$Mn$_x$As; x=0, x=10%, x=1% and x=20%; maximum absorbance occurred at UV region while for x=50%, maximum absorbance was observed at $\lambda$ $\approx$ 707nm. The results show that GaAs generate most heat due to its wide optical energy gap of 1.43eV while for x=1% dissipates little heat because of its small optical energy gap of 0.36eV.

Keywords: Optical absorbance, photo irradiation, Gallium Arsenide, Gallium manganese arsenide, doping, heat dissipation, ultraviolet light

1. Introduction

Electromagnetic (EM) radiations interact with matter and depending on its energy it can be transmitted, reflected or absorbed by the matter of an incident material. The energy of the incident EM radiation is quantized and given by, $E = hC/\lambda$ (1) where $C$ is the speed of light, $\lambda$ is the wavelength of incident radiation and $h$ is the plank’s constant. According to eqn (1), higher energy is obtained from UV region and other short wavelengths region such as VIS region. The transmission, reflection and absorption of light depend on the thickness of the incident material. The SPECTRO 320 with IS-Spec Win software produces transmittance and
reflectance spectra for the whole EM spectrum. The absorbance is determined from the relation,
\[ A = 1 - (T + R) \]  \hspace{1cm} (2)
where T is transmission in % and R is reflection in %. The absorbed part of incident radiation is used to pump electrons from ground state to an excited state. Electrons at the higher energy levels fall back as they seek stability and emit energy in form of heat sometimes through a process of fluorescence. With regard to eqn (1), it is apparent that the short wavelength EM radiations are likely to dissipate much heat as they have a lot of energy to excite the electrons to the highest energy levels. From the latter, materials with high absorbance values with respect to the EM radiation, dissipate most heat and vice versa for materials with low absorbance values.

1.1 Photons absorbed by semiconductors

If the energy of the individual photons is greater than the semiconductor band gap, the photons can be absorbed, transferring their energy to an electron (Dholakia et al., 2003). This process pumps up the electron from the valence band to the conduction band. The absorption process thus creates an electron-hole pair as it results in an electron in the conduction band and a hole in the valence band. A substantial representation of the electron-hole pair generation is to view the valence band electron as part of a covalent bond. When the covalent bond is broken, the electron is set free to move in the crystal lattice of the semiconductor. The energy required to break the covalent bond is the energy band gap that provides the size of band gap. If the photon energy is less than band gap energy, it doesn’t carry enough energy to break the covalent bond and free an electron for conduction. Since the electrons can’t occupy the forbidden states between the valence and conduction bands, a photon with energy less than the band gap energy, cannot be absorbed and will pass through the study sample. In order to study the band gap of a semiconductor, light with variable photon energy near the band gap energy can be used. The photon energy at which transition between absorbing and non-absorbing behaviour takes place will correspond to the band gap energy.

For higher energies there is no transmission because all the light is absorbed. Destructive interference can be observed at those higher energies. This is observed from the absorption tail of the photon absorption-photon energy curve. For energies above the absorption edge, \( R + T \) gets very low because in the spectral range most photons are absorbed by the sample. In a rough approximation, we can calculate the absorption coefficient \( \alpha \) according to the equation,
\[ R + T = e^{-\alpha d} \] where \( d \) is the sample thickness.

\[ T \approx (1 - R)^2 e^{-\alpha d} \Rightarrow \alpha = -\frac{1}{d} \ln \left[ \frac{T / (1 - R)^2}{1} \right] \]  \hspace{1cm} (3)
(1 − R)² is approximately unity as the reflectivity is negligible and insignificant near the absorption edge (Dholakia et al., 2003 and Ishu et al., 2006). (3) can be reduced to

\[ \alpha = -\frac{1}{d} \ln[T] \iff \alpha = \frac{1}{d} \ln\left[\frac{1}{A}\right] \]

(4)

1.2 Energy band gap determination

Band gap is the uppermost property of semiconductors which is differed from metals and insulators that determines their special electronic and optical properties and wide device applications (Tan et al., 2005). The optical band gap of the semiconducting film is determined by applying the Tauc model,

\[ \alpha h\nu = D(h\nu - E_{g}^{\text{opt}})^{n} \]

(5)

where \( h\nu \) is the photon energy, \( E_{g}^{\text{opt}} \) is the optical band gap, \( D \) is the band tailing parameter and \( n=1/2 \) for direct band gap semiconductors e.g., GaAs (Ishu et al., 2006 and Yastruback, 2012). The dependence of the absorption coefficient \( \alpha \) in terms of the direct and indirect transitions is most often performed with the help of the formulae derived for 3-D crystals shown by Tauc model (Dholakia et al., 2003). Optical transmission is a very complex function and is strongly dependent on the absorption coefficient. The oscillating nature of the spectrum shows that the films are having uniform thickness. From a graph of \((\alpha h\nu)^{2}\) with \( h\nu \), optical band gap, \( E_{g}^{\text{opt}} \) can be determined by extrapolation of best line of fit between \((\alpha h\nu)^{2}\) and \( h\nu \) axis (Ishu et al., 2006 and Lee et al., 2009).

2. Methods

The spectrometer was used to start the experiment that calculates and analyses the data obtained and represent it in form of a spectrum (reflection spectrum). The samples were fixed at the aperture in the SPECTRO 320 to let in light. Portion of light that penetrates the sample was collimated and directed to the OSA 320 using a fibre optic cable inside it for analysis. A similar process was followed to obtain the transmission spectrum at transmission window. Transmission and reflection spectra for each sample were obtained over the same UV-VIS-IR wavelength range. From such spectra, absorption data for each sample was determined with reference to eqn (2) at particular wavelengths in percentages. The optical wavelengths were converted into optical energies using eqn (1) and recorded in Table 1. The information so far obtained was used to generate an absorption (%) spectra spanning over the entire UV-VIS-IR wavelength range. Using eqn (5) and values in Table 1, optical absorption coefficients were determined then graphs of absorption coefficient versus photon energies were drawn. Straight lines of best fit were drawn in all graphs and by extrapolation, the optical band gaps were determined.
3. Results and discussions

At wavelength $\lambda \leq 700$ nm or $E \geq 1.76$eV, $Ga_{1-x}Mn_xAs$ become porous and transparent to incident light. The maximum transmittance was observed to vary with respect to the doping levels that also dictate the maximum absorbed photon wavelength. Otherwise, it becomes opaque whereby the transmittance determines to the lowest value of 7.62% for $x=0$ at $\lambda \sim 1300$nm; 29.17% for $x=50\%$ at $\lambda \sim 1300$nm; 28.33% for $x=10\%$ at $\lambda \sim 1000$nm; 18.00% for $x=1\%$ at $\lambda \sim 1500$nm and 27.27% for $x=20\%$ at $\lambda \sim 1100$nm. In this spectral region, some photons are reflected and the amount of reflectance slightly surpasses that of transmittance such that by applying eqn (2), the absorbance is approximately zero for all samples under study. At wavelength $\lambda > 700$nm or $E < 1.76$eV, the samples become more opaque that the transmission and reflection of photons are $T \leq 50\%$ and $R \leq 48\%$ respectively for all the samples. By application of eqn (2), the absorbance is determined to be $A \neq 0$. As indicated earlier, absorbance is zero at $E \geq 1.4$eV but at $E \leq 1.4$eV, $Ga_{1-x}Mn_xAs$ for $x=50\%$, absorbs 47% of the illuminated photons as shown in Fig. 1.

The region of photon absorption defines the energy band gap of the ferromagnetic dilute magnetic semiconductor. At this region, absorbed photons with higher energies can generate electron hole pairs by excitation or stimulation. Any excess energy will be lost perhaps through fluorescence and the generated pairs are sufficient to produce electric current. The energy band gap behaves as schottky barrier or ‘uphill’. Thus, it becomes difficult for the pairs to be transported through it and energy more than $E_g$ (energy gap) is required to enhance the possibility of pair transportation. As a result of the generated current and the load (barrier) heat is generated that is due to joule heating in the energy gap. Thus, large absorbance suggests large amount of pair generation and in all samples under investigation it occurs at low $E_g$ or narrow gap DMS depending on the doping levels. Heat dissipated is dependent on the photon absorption percentage and the hall resistance of the Ferro-DMS. In view of doping level variation in reference to the absorption spectra, it is apparent that doping levels vary proportionately with the photon absorption percentages, the hall resistances and the amount of electron-hole pairs generated. It shows that the incorporation of manganese atoms into the GaAs film alters its’ crystal structure and narrows its energy band gap. For pure GaAs ($x=0$), the photon absorption energy range is $E_g \leq 1.4$eV with maximum photon absorbance peak of 66% as shown in Fig. 2.

Comparing with the case of $x=50\%$, pure GaAs is likely to generate more electron-hole pairs than the former when illuminated with UV-VIS-IR light without filters, indeed at the IR region, $\lambda \geq 1300$nm or $E \leq 1.0$eV. At 20% manganese doping level, optical transmittance and reflectance
draws towards each other seemingly to overlap such that the optical absorbance decreases. Indeed, it has the smallest higher absorbance value. This shows that it can generate little heat as compared to other doping levels under study. The optical destructive interference is observed at the beginning of the optical tailing parameter that defines the optical absorption edge at $E \geq 1.6 \text{eV}$ as in Fig. 3 according to Pereira and Dias da Silva, 2008.

From Table 1, and using eqn (4) Table 2 was generated which is a table of absorption coefficient as a function of optical energy gap and the incident photon energy. A plot of $(ah\theta)^2$ versus $h\theta$ provides a wavy-linear graph which can be used to determine the optical energy band gap for each doping levels as shown in Figs. 6, 7, 8, 9 and 10. For $x=0$, $x=1\%$, $x=10\%$, $x=20\%$ and $x=50\%$ energy band gap were 1.43eV, 0.36eV, 0.61eV, 0.69eV and 0.67eV respectively as in Table 1. A plot of $E_g^{\text{opt}}(\text{eV})$ versus doping levels $X (%)$ as shown if Fig. 4 shows a drastic drop in $E_g^{\text{opt}}$ when manganese atoms (1%) is incorporated into GaAs host. This is the case at energy gap of approximately 0.36eV beyond which it increases until 0.61eV for X=20\%. Beyond this point it becomes almost constant (an increase in X does not cause a significant change in the optical band gap). The initial drop in optical energy band gap correspond to a reduction in carrier concentration and this is attributed to the establishment of manganese interstitials according to Yastruback as shown in Fig. 5. This is a strange observation and is due to the presence of holes in the impurity band instead of the valence band. Here, an initial addition of manganese impurities create an impurity band which lies between conduction band and valence band. Photons of light incident on the band generates a hole-electron pair and the holes are excited into the conduction band with ease since the gap has been reduced by the initial impurities. This is why the optical band gap reduces to 0.36eV when impurity of 1\% is added into the GaAs lattice structure. A further increase of the impurities appears to compress the impurity band close to the valence band. Thus increasing the energy gap as the impurity band seem to overlap with the valence band. Generated holes upon impingement by the incident photons expeririences difficulty in jumping to the conduction band since the gap has so far been increased. This is observed by an increase in the energy gap to 0.61eV in Table 1 and in Fig. 4. Any further increase in the impurity density increases the stress between the impurity band and the valence band. This continues until the bands almost overlap and cannot reduce anymore. This is observed by an optimum curve between $20\% \leq x \leq 50\%$ in Fig. 4. Wavy-linear graphs, Figs. 6, 7, 8, 9 and 10, shows that the absorption coefficient increase with the incident photon energy. The wavy-like behavior shows that the thin films are uniform. The wavy line in the graphs show the experimental results and the straight lines show the theoretical ones. An increase in
doping levels implies higher dopant density. The increasing density exerts some stress on the valence band and the impurity band seems to overlap with the valence band. Due to a near band overlap, the gap between the conduction band and near overlap increases. If the photons are directed into the bands, the hole-electron pair is generated on the near band overlap but on the impurity band side. The holes are excited into the conduction band over a wider energy space. This suggests an increased energy band gap.

The overlapping increases until an optimum limit or yield point where the applied stress due to impurity density cannot be exceeded. At this point, any increase in the incident photon energy does not cause any positive effect on the optical energy gap of the semiconductors. This is the case with the direct band gap semiconductors. In indirect band gap semiconductors like pentavalent doped silicon, the holes are not in the impurity band but in the valence band. In this case, an increase in impurity density doesn’t affect impurity-valence interband gap as charge carriers are always in the valence band. If such semiconductors are illuminated by an incident photons of varied energies, as impurity densities are increased, their gaps reduces linearly until the conduction band and valence band nearly overlap. In view of this, manganese impurity at 1% absorbs photons over a wide range of optical energies of $E \leq 2.2\ eV$ For pure GaAs absorption optical energy range occurs at $E \leq 2.0\ eV$ as in Figs. 11 and 12 respectively. Taking the case when $X=0$ as the control set up, it can be observed that manganese impurity (1%) increases optical absorption range by 0.2eV.

For manganese doping at 10% as in Fig. 12 the optical absorption range reduces to $E \leq 1.6eV$ showing that the absorption optical energy range reduces by 0.4eV. For 20% and 50%, optical absorption ranges reduce by 0.2eV and 0.1eV respectively. These observations show that little impurities of manganese atoms have large photon absorption surface area and the electron-hole pair generation become the highest. This is observed from a small optical energy gap of 0.36eV. Otherwise, the photon absorption surface area reduces as shown in Figs. 1, 3 and 12. In this case beyond manganese impurity doping levels of approximately 6%, according to Yastruback, the optical energy band gap increases to 0.61eV for $x=10\%$, 0.69eV for $x=20\%$ and 0.67eV for $x=50\%$. At 50% manganese impurity concentration, the situation is degenerate and the reduction in optical absorption range reduces to 0.1eV which corresponds to optical energy gap of 0.67eV with a reduction of 0.02eV from that at $x=20\%$. 
5. Conclusion

The optical band gap of GaAs and manganese doped GaAs provides vast information on the trend of the nanotechnology advancement as to conform to the Moore’s law. The optical device advancement in optoelectronics is of great importance especially in designing optical transistors and optical diodes for making sensors. Compound semiconductors with direct band gap such as GaAs are best for this advancement. Here optical band gap of GaAs and its manganese doped counterparts have been determined. The optical band gap of GaAs is 1.43eV. Optical band gap for doped GaAs dropped significantly to 0.36eV for 1% manganese doping level. The reduction in the optical energy gap shows that the electron-hole photo generated pair can jump to the conduction band easily. The heat dissipated during such excitations is minimal for narrow band gaps as compared to GaAs with optical band gap of 1.43eV. This is in accordance with Ishu who ascertained that the addition of impurity into a semiconducting crystal lattice reduces its energy gap and dissipates little heat. Manganese doping levels in the range 1%≤x≤10% is most appropriate. It is presumed to dissipate little heat during electric current conduction as compared to undoped and highly doped GaAs. It is also observed that at X≥20% the optical band gap becomes almost constant despite of an increment in the impurity doping density.

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![Fig. 1: Absorbance (%) spectrum of Ga1-xMnxAs; x=50%](image1)

![Fig. 2: Optical absorbance with the optical energy band gap for pure GaAs](image2)
**Fig. 3:** Absorbance (%) spectrum of Ga$_{1-x}$Mn$_x$As; x=20%

**Fig. 4:** Optical energy gap with impurity doping variations of GaMnAs

**Fig. 5:** Charge carrier concentration versus impurity levels obtained from Van der Pauw experiment
Fig. 6: Absorption coefficient versus incident photon energy for GaAs

Fig. 7: Absorption coefficient versus incident photon energy for X=1%

Fig. 8: Absorption coefficient versus incident photon energy for X=10%
Fig. 9: Absorption coefficient versus incident photon energy for X=20%

Fig. 10: Absorption coefficient versus incident photon energy for X=50%

Fig. 11: Absorbance (%) spectrum of Ga_{1-x}Mn_{x}As; x=1%

Fig. 12: Absorbance (%) spectrum of Ga_{1-x}Mn_{x}As; x=10%
Table 1: Photon energy (eV) and absorbance (%) for Ga_{1-x}Mn_xAs

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<tr>
<td></td>
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Table 2: Absorption coefficient and incident optical energy

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