Bulk Germanium Optical Properties: The Effects of Extinction/Absorption Coefficients and Crystal Momentum in the Infrared Region

BULK GERMANIUM OPTICAL PROPERTIES: THE EFFECTS OF EXTINCTION/ABSORPTION COEFFICIENTS AND CRYSTAL MOMENTUM IN THE INFRARED REGION

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ABSTRACT

Study on the optical behaviours of bulk germanium (Ge) transmitting in infrared (IR) region with respect to parameters such as wavelength and frequency has been an area of interest. Influence of absorption and extinction coefficients and crystal momentum on the optical properties of Ge semiconductor in the IR region were investigated. Developed models and data from existing works on Ge semiconductor were analyzed using a theoretical approach. Optical properties such as absorption and extinction coefficients were found to greatly influence the behavior of Ge semiconducting material, which determines the amount of light absorbed by the materials, most especially in the Infrared region of spectrum. The data and the models used were able to predict the effects on the properties of Ge semiconductor in the IR region.

Keywords: Bulk germanium; infrared region; semiconductor; solid state; quantum confinement

Introduction

The two outstanding single semiconductor materials of germanium (Ge) and silicon (Si) are proven to be the most considered materials in the field of solid-state device technologies and also nanotechnology in recent years (Frey et al., 2006). In the area of infrared (IR) lens design, these materials are essentials. For window or lens applications in the 1.6-1.8µm spectrum region, Ge semiconductor substrate is mostly used (Koester et al., 2006). Due to its high refractive index, Ge plays part in optical interconnect devise if incorporated in Si waveguide for improved silicon photonics devices (Cho et al., 2014). Chromatic aberration in several applications can be avoided if high refractive index and low dispersion bulk materials across different range of temperature are used (Koester et al., 2006). Performance of Si and Ge optical devices transmitting in the infrared region can harness effectively when these materials are cooled to cryogenic temperatures, thereby

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improving the signal from the device background radiation (Frey *et al.*, 2006). Nowadays, Ge is used as a component of glass in telecommunications fiber optics; as a polymerization catalyst for polyethylene terephthalate (PET), an IR night vision device and also as a semiconductor substrate in electronic circuitry (Adams, 1990, Koester *et al.*, 2006). Recently, Nanocrystals Si and Ge have been used in photonic devices that emit light in the visible region of the spectrum(Isiyaku & Ghoshal, 2016). This is due to quantum confinement, surface state effects and exciton binding energy (Abdu *et al.*, 2016, Wu & Yang, 2000).

Ge semiconductor material is a lustrous, brittle, hard and greyish white metalloid that is essential in many new-solid state electronic and optical devices with an indirect band gap of 0.66eV and hence does not emit light in the visible range (Isiyaku & Ghoshal, 2016, Aliyu *et al.*, 2016). This semiconductor is obtained in

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the form of a single crystal or apolycrystalline material. It is softer than silicon and very much softer than the diamond form of carbon. Polycrystalline Ge is less expensive and is available in larger sizes than mono-crystalline material. Ge crystallizes in the covalently bonded cubic diamond structure from which it melts at 937.4 °C (Audzijonis *et al.*, 2010, Dasgupata and Amitava, 2014). It has an infrared refractive index of 4.00, a room temperature density 5.32 grams per cubic centimeterandradiative recombination coefficient 6.4 x 10⁻¹⁴ cm³/s for which is stable in air up to 400°C, above which it begins to oxidize (Pearson & Brattain, 1955).

Extinction coefficient (k) which is proportional to both absorption coefficient a and wavelength λ is an important parameter for examining the trend of optical and electronic properties of a semiconductor (Harris, 2010). It is an optical property of the semiconductor material that determines how much light is absorbed by the material and is related to the index of refraction n (Audzijonis et al., 2010). The excitation range performance at a given wavelength is also estimated by the absorption coefficient α which also links to k, the imaginary part of the index of refraction. This property gives the amount of intensity absorbed per unit length by the material. Optical properties are also related with the increase in crystal momentum for which the wave number decreases. In this work, the effect of the optical absorption coefficient, extinction coefficient and crystal momentum on the optical properties of bulk Ge material with respect to certain varying wavelengths and frequencies are investigated.

Theory and Methods

The behaviour of electromagnetic radiation depends on its wavelength or energy (i.e. frequency). Higher frequencies indicate shorter wavelengths and vice versa. This interactive electromagnetic radiation exhibit both wave-like and particle-like properties. Here, a theoretical method has been used in determining the effects of optical absorption, extinction coefficients and crystal momentum of an optical germanium. It provides an important part in examining the optical properties of germanium, especially in the far infrared region of the electromagnetic spectrum.

For a complete one full cycle (one period of a wave), we could say that the wave has moved by one wavelength. Since speed is distance traveled with respect to time spent, and a wave moves a distance of one wavelength in a time of one period, the speed *v* is given as,

$$v = \frac{\lambda}{t}$$
(1)

If the frequency is given to be;

$$f = \frac{1}{t}$$
(2)
Thus,

$$f = \frac{v}{\lambda \eta}$$
(3)

The speed of light in a medium is related to the speed in vacuum by the index of the refraction

$$\mathbf{v} = \frac{c}{\eta} \tag{4}$$

Therefore, Eqn. (2) becomes;

$$f = \frac{c}{\lambda \eta}$$
(5)

Similarly, looking at the Beer Lambert law, $I_x = I_{(0)}e^{-ax}$ (6)

where $I_{(x)}$ indicates the intensity at point *x* in the material, $I_{(0)}$ represents the intensity of light entering the material while *x* is number of molecules per centimeter cube.

Optical absorption coefficient (α) of a semiconductor material depends mostly on the wavelength of light, causing some wavelength to be absorbed in a medium, while the same medium is transparent to another wavelength. Since the intensity is proportional to the square of the magnitude of the electric field and taking only the first term for the sake of simplicity, we assumed that if the electric field is decreasing with $e^{k\beta x}$, then the intensity of the wave is

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decreasing proportionally to $(e^{k\beta x})^2 = e^{-2k\beta x}$. Comparing the expression with Beer Lambert law, we obtain the relationship between the absorption coefficient (α) and the extinction coefficient(k) as:

$$\alpha = 2k\beta = \frac{2kw}{c} = \frac{4\pi k}{\lambda}$$
(7)
Therefore,

$$k = \frac{\alpha \lambda}{4\pi}$$
 (8)

where k and α are the extinction and absorption coefficients while β is given as;

$$\beta = \frac{W}{c} \tag{9}$$

Similarly, the wave number k as a function of crystal momentum P of the material is taken as the relation in Equation (10) as reported previously (Harris, 2010).

$$k = \frac{2\pi p}{h}$$
(11)

Equation (3) is used to calculate the frequency of the optical germanium at different wavelengths range 2.5-12µm for index of refraction values n_i from the work of Adams (1990). The calculated values of extinction coefficient (k) at different absorption coefficient (α) andwavelength (λ) are obtained using Equation (7). Furthermore, wave number k_i dependent momentum P were calculated with the aid of Equation (10) (Harris, 2010).

Results and Discussion

Calculated frequencies (Hz) of the bulk germanium in the infra-red region are presented in Table 1. The corresponding frequencies were obtained using equation (3) after careful consideration of the work of Adams (1990).

Table 1: Infrared wavelength ranges and their corresponding frequencies for decreasing refractive index.

λ (μm)	<i>n</i> (refractive index)	$f(s^{-1})$
2.5	4.0653	2.95×10^{13}
3.0	4.0446	$2.47 \mathrm{x} 10^{13}$
4.0	4.0225	$1.86 \mathrm{x} 10^{13}$
5.0	4.0170	$1.49 \mathrm{x} 10^{13}$
6.0	4.0122	$1.25 \mathrm{x} 10^{13}$
7.0	4.0092	$1.07 x 10^{13}$
8.0	4.0074	$0.94 x 10^{13}$
9.0	4.0061	0.83×10^{13}
10.0	4.0052	$0.75 x 10^{13}$
11.0	4.0042	0.63×10^{13}
12.0	4.0039	$0.62 \mathrm{x} 10^{13}$



It is observed that even in infrared region the increase in the wavelength which corresponds to decrease in refractive index lead to decrease in the corresponding frequencies of the optical germanium as shown in Fig. 1. At extreme IR region, the frequencies increases sharply as the wavelength decreases up to long wave IR region, revealing higher energy at range close to visible region. Similarly, the frequencies Bulk Germanium Optical Properties: The Effects of Extinction/Absorption Coefficients and Crystal Momentum in the Infrared Region Aliyu Kabiru Isiyaku et al

decrease as the wavelengths increases toward the microwave IR region indicating a decrease in energy.

Equation (7) is used to calculate the values of extinction coefficient (*k*) at different values of absorption coefficient (α) and wavelength (λ) extracted from the work of Adams (1990) as shown in Table 2.

 Table 2: Calculated extinction coefficient for different absorption coefficient

α (cm ⁻¹)	$\lambda (\mu m)$	K (c)
0.0047	2.0	0.09x10 ⁻⁸
0.0047	2.5	0.11x10 ⁻⁸
0.0047	3.0	0.15x10 ⁻⁸
0.0051	4.0	0.20×10^{-8}
0.0068	5.0	0.32×10^{-8}
0.0107	6.0	0.59x10 ⁻⁸
0.0150	7.0	0.83x10 ⁻⁸
0.0178	8.0	1.30×10^{-8}
0.0215	9.0	1.70×10^{-8}
0.029	10.0	2.58x10 ⁻⁸

The excitation of electrons in the valence band depends on the absorption coefficient of the material, this extinction coefficient (k) parameter provides the framework for testing the number of electrons absorb by the material. This is evidenced in Equation (7), where k>0means absorption, while k = 0 means the light travels straight through the material. A plot of absorption coefficient (α) against extinction coefficient (k) is presented in Fig. 2 using a tabulated data in Table 2. This indicates that the increase in extinction coefficient leads to increase in the corresponding absorption coefficient of an optical germanium in infrared region. This resulted into the optimum emission of IR light region in germanium material. The result shows that even for those photons which have energy above the band gap the absorption coefficient is not constant, but still depends strongly on wavelength.





Table 3 gives the calculated values of crystal momentum P, for a range of wave number from the work of (Harris, 2010), calculated using equation (10). The calculated results were graphically presented in Fig. 3

 Table 3: Calculated crystal momentum for some established values of wave number

Wavenumber (<i>k</i>)	Momentum (P)
2.208X10 ⁻²⁸	$2.0 ext{ x10}^{5}$
1.656 X10 ⁻²⁸	1.5×10^5
1.326 X10 ⁻²⁸	1.2×10^5
1.104 X10 ⁻²⁸	$1.0 \ \mathrm{x10^{5}}$
$0.946 \ \mathrm{X10^{-28}}$	$0.9 ext{ x10}^{5}$
$0.828 \ \mathrm{X10^{-28}}$	$0.8 ext{ x10}^{5}$
$0.736 \mathrm{~X10^{-28}}$	$0.7 ext{ x10}^{5}$
$0.662 \ \mathrm{X10^{-28}}$	$0.6 ext{ x10}^{5}$
$0.602 \ \mathrm{X10^{-28}}$	$0.5 \ \mathrm{x10^5}$
0.552 X10 ⁻²⁸	$0.5 \text{ x}10^5$

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Phenomena such as the rate of absorption or emission and the distribution of electrons and holes within a solid, the number of available states per unit volume energy are turned by the responses of crystal momentum and wave number. Optical state properties of a semiconductor are affected by the increase in crystal momentum and decrease in wave number. The response of the calculated crystal momentum within the IR region for some existing values of wave number tabulated in Table 3 is plotted in Fig. 3. The bulk germanium crystal momentum greatly enhanced as the wave number decreases.



Fig. 3 Absorption coefficient (α) against extinction coefficient (k).

Conclusion

The influences of wavelength, frequency and crystal momentum on the optical properties of germanium semiconductor were investigated using some developed models. It is observed that the variable state of wavelengths, the corresponding frequencies and crystal momentum of the optical germanium change exponentially even at the infrared region, thereby affecting the absorption and emitted energy in the same aspect. The effect of extinction coefficient on the absorption rate on the optical germanium is also examined theoretically. Increase in extinction coefficient leads to optimum optical absorption in the infrared region of the Ge material. This shows that the photons with energy above the bandgap depend strongly on the wavelength and have constant absorption coefficient.

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