

A New Model for the Estimation of Energy Gap for GaAs and AlGa

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Summary: The photoacoustic spectrum was obtained on GaAs and AlGa. A unique formula for the determination of energy gap is developed for these materials, the numerical values of which are found to be in conformity with other results. The energy gap formula is established on the basis of self-conjectured relationship, which follows the peak frequency of the photoacoustic spectrum. The frequencies of the optical and acoustic mode of phonons have also been calculated and reported the very first time. The Debye Waller factor was also calculated to categorize the properties of these materials.

Introduction

During the last decade photoacoustic spectroscopy (PAS) techniques became well established for investigating the optical, thermal and structural properties of materials including semi-conductors, metals, alloys and insulators [1]. Furthermore it has also been applied for direct verification and quantification of optical properties of semi-conductors [2], thin films [3], semimetals, microstructures [4-8], structural relation, thermal diffusivity in amorphous metal alloys [9], internal cavitation in the superplastic alloys [10], the deformation and development of layered structure in glasses [8]. When photoacoustic spectroscopy is used as a scanning technique, it reveals the possibility of examining the subsurface cracking and the development of flaws in the metals and ceramic materials [11].

Metal oxide continuous vapor deposition (MOCVD), heterostructure and multiple quantum well structures (MQWS), exhibit an enhancement of exciton binding energy and the exciton resonance even at room temperature because of quantum confinement effect [12-13].

We have in the present work, focused on the study of the optical properties of GaAs and AlGa experimentally and derived certain theoretical expressions to justify our work. The energy gap formula, which we have developed, provides numerical values of gap energies in conformity to the values obtained by other methods. Our conjecture establishes some of the most exciting observations, which shall indeed help resolve the unattended areas of research. The photoacoustic spectrometer (Model OAS-400) was used in the present study. Surprisingly

enough, our experimental results on GaAs and AlGa are in agreement with the results of Massimo Gurioli et al [Phys. Rev. letters. Vol.78, 3208(1997)] and J.H.Chu et al [Appl. Phys. Letters. 64, 746(1994)], respectively.

Results and Discussion

Fig. [1 & 2] show photoacoustic spectrum of GaAs and AlGa materials, whereas tables # 1 & 2 show our calculations on theoretically derived parameters.

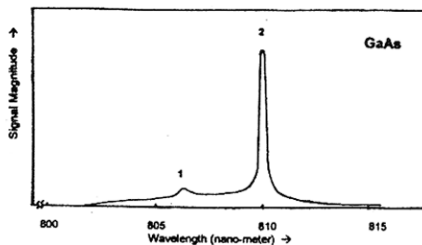


Fig 1. Emission spectra of GaAs QW. Reproduced from Massimo Gurioli, Franco Bogani, Simeone Coccherini and Marcello Colocci. *Phy.Rev.letters*, vol.78, P.3208 (1997). Our experimental results are exactly the same on photoacoustic spectrometer (Model OAS-400).

Table-1

Sample	N/V 10^{24} (m ⁻³)	k _F 10^{10} (m ⁻¹)	k _D 10^{10} (m ⁻¹)	v _D 10^3 (ms ⁻¹)	v _F 10^6 (ms ⁻¹)	θ _{ext} (K)	E _F (eV)	E _G (eV)
GaAs	2.443	0.89	1.12	8.90	1.03	736	3.0	1.325
AlGa	2.680	0.927	1.167	8.56	1.07	764	3.279	1.604

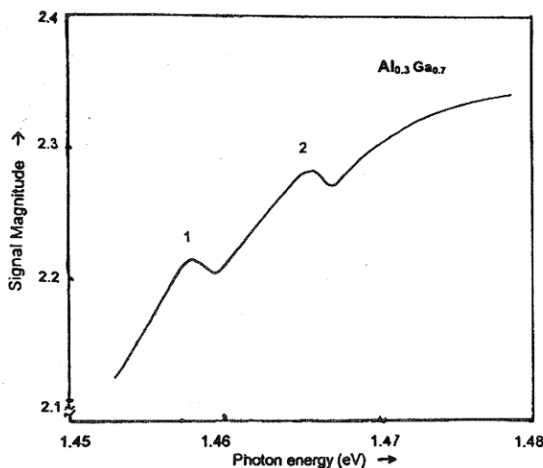


Fig. 2. PA Amplitude Spectrum of $Al_{0.3}Ga_{0.7}$ at room temperature. Reproduced from J. H. Chu, Y. H. Bak, J. H. Kim, H.L.Park. S. H. Park, U. Kim, J. G. Choi and I. J. Kim. Applied Phys. Letters. 64, P.7 46, (1994). Our experimental results are exactly the same on photoacoustic spectrometer (Model OAS-400).

Table -2

Sample	Peak	f	ΔE 10^{-19} (J)	m^* 10^{-34} (kg)	B 10^{-14}	DWF 10^{-14}	v_D 10^{14} (Hz)	v_{est} 10^{14} (Hz)
GaAs	1	1.95	0.0006	0.189	339	1.04	0.16	3.559
	2	1.95	0.0004	0.284	226	0.99	0.16	3.540
AlGa	1	2.238	0.001	0.430	0.14	0.9961	0.16	3.60
	2	2.249	0.009	0.390	0.16	0.9955	0.16	3.61

We tried to develop a model using self-conjectured formula for fractional filling of the excited mode of phonons. The electronic concentration N/V of the sample at room temperature and at atmospheric pressure was calculated by multiplying the atomic concentration [14] of the element with its valency as well as by finding the percentage composition of the sample as

$$\frac{\text{Atomic Wt. of the element}}{\text{Atomic Wt. of the Sample}} \times 100 \quad (1)$$

Then multiplying this by the atomic concentration of this element, we get the atomic concentration of the sample.

For N primitive cells, the total number of acoustic phonons mode is $3N$, then the cutoff frequency ω_D can be written,

$$k_D = \frac{\omega_D}{v} = \left\{ 6\pi^2 N/V \right\}^{1/3} \quad (2)$$

where k_D is Debye wave vector and v is the velocity of sound, with the assumption of constant velocity of sound if $v = 5 \times 10^3 \text{ms}^{-1}$ & $N/V = 10^{29}$ atoms m^{-3} then ω_D is nearly 1×10^{14} rad s^{-1} for which k_D is $2 \times 10^{10} \text{m}^{-1}$.

In our calculations as in Table-1, the value is nearly in agreement with assumed values. The Debye temperatures were estimated by the relation,

$$\theta_{est} = \left[\frac{\hbar v_D / k_B}{\left[6\pi^2 N/V \right]^{1/3}} \right] \quad (3)$$

where $\hbar = h/2\pi$ and k_B is Boltzman's Constant.

The electron velocity at Fermi surface k_F is given by

$$v_F = \frac{\hbar k_F}{m}$$

In our calculations, we used

$$k_F = \left[3\pi^2 N/V \right]^{1/3} \quad (4)$$

$$v_F = \frac{\hbar \left[3\pi^2 N/V \right]^{1/3}}{m}$$

We found from our table that $k_D > k_F$ & $v_F > v_D$, the reason of which is ascribed separately for each sample. The absolute reason for $v_F > v_D$, would have far reaching consequences in dealing with the theoretical estimated cutoff velocity at ω_D , where the Fermi surface would have to be modified for Heisenberg interaction, i.e., preferably for s-d interaction. Pseudo Fermi surfaces or screened Fermi surfaces were expected to be produced and that would be possible only at room temperature. This possibility, in our case, for the photoacoustic spectrum at room temperature is overruled.

The values of N/V , k_F , k_D , v_D , θ_{cut} and v_F are shown in table #1. From this table the value of v_D , i.e., the Debye velocity for most of the samples, changes from a constant value of $5 \times 10^3 \text{ ms}^{-1}$ at $\omega_D = 1 \times 10^{14} \text{ rad s}^{-1}$, which suggests that electrons acquire energy due to intermittent heating of the samples. This shows that some of the electrons are at Brillouin zones, which should not, in the case where s-d interaction to occur or J^{s-d} coupling to occur, electron should remain isolated from taking thermal energies in the Brillouin zones otherwise the density of the state would be modified at $\omega < \omega_D$. In our calculation the cutoff wave vector is less than the Debye wave vector, for most of the samples. The density of the mode will oscillate with the energy equal to $k_B T$. With our assumption $v_D \cong v_F$ the density of state for this ω_D would change due to the change in v_D in such a manner that curvature on the left side of the figure (3) will be modified [15]

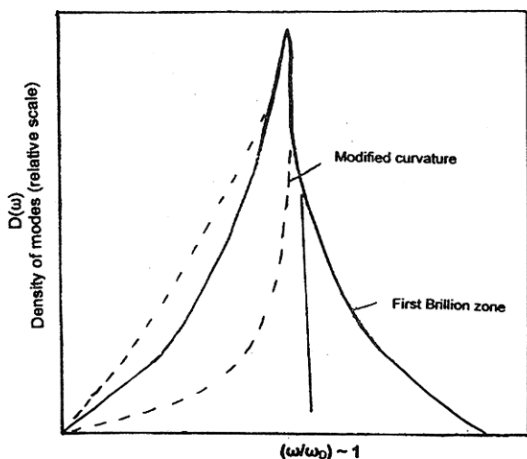


Fig 3. Arbitrary diagram showing the density of modes $D(\omega)$ (relative scale) versus frequency ω with assumed constant phonon velocity, and with modified curvatures at $\omega \leq \omega_D$.

As we know that Fermi energy

$$E_F = \frac{mv_F^2}{2} \quad (5)$$

The effective mass of electron at different peaks will be different because the photons which are chopped at different frequencies, when interact with sample, cause intermittent heating. This in fact

excites the phonons of different modes. We calculated the effective mass m^* of electrons in the lattice by using photoacoustic spectra by,

$$m^* = \frac{m}{\left[1 + 4E_F / \Delta E\right]} \quad (6)$$

where E_F is the fermi energy and ΔE is the energy difference calculated at the peak valley area of each peak. Photoacoustic signal generation is a two stage process, i.e., heat production and generation of acoustic waves. An absorbed phonon may excite a molecule or atom from its ground state energy E_1 to the excited state energy E_2 , so that,

$$E_2 - E_1 = \Delta E \quad (7)$$

The Debye Waller factor, to our opinion, plays an important role for describing either the presence or absence of s-d interaction as well as oscillating effect of the phonons within Brillouin zones.

Debye Waller factor is,

$$\text{DWF} = \exp \left[\frac{-2B \sin^2 \theta}{\lambda^2} \right] \quad (8)$$

where λ is the chopping wavelength and B is the temperature factor,

$$B = \left[\frac{6\hbar^2}{k_B} \right] \left[\frac{T}{\theta_D} \right] \left[\Phi_X + \frac{X}{4} \right] \quad (9)$$

where $X = \frac{\theta_D}{T}$ and Φ_X is the wave function, we can choose Φ_X as the asymptotic value at high value of $\frac{T}{\theta_D}$ which is 24.943 J/mole K

Thus equation (8) is modified at $\theta = 90$; $\sin^2 \theta = 1$

$$\text{DWF} = \exp \left[\frac{-2B}{\lambda^2} \right] \quad (10)$$

DWF values are shown in table-1, which shows an oscillating effect. This is an indication that there exist s-d interaction due to effective masses of

the electrons at different phonon frequencies which helps induced hybridized orbital state electrons. This is another proof that there exists an electron-phonon coupling. The s-d interaction under discussion is quite different than Heisenberg interaction at low temperatures. The s-d interaction in one case manifests itself due to hybridized orbital state in which s-p leads s-d interaction. Different bonding orbitals are excited such as J and π bonding orbital at different frequencies. Nevertheless, the s-d interaction although not very much pronounced, plays a significant role.

We have used self-conjectured relationship, i.e.,

$$f = \frac{E_F}{h\nu_{peak}} = \frac{E_F}{E_{photoacoustic}} \quad (11)$$

where 'f' is the fractional filling of energy gap, 'h' is the Planck's constant and ν_{peak} is the combined frequency for optical and acoustic mode of phonons.

DWF is compared with the fractional filling 'f' which we have conjectured to see whether electron-phonon coupling exists or not. Equation (11) is found good enough, showing the presence of electron-phonon coupling.

Now we develop another relationship using self conjectured formula for the fractional filling 'f' of excited mode of phonons. Thus the electronic concentration $N/V = n$ due to electron-phonon coupling and also due to the effective mass of the electron is given by,

$$n = f \exp\left(\frac{E_F - E_g}{k_B T}\right) \quad (12)$$

$$\ln n = \ln f + \left(\frac{E_F - E_g}{k_B T}\right)$$

$$\ln\left(\frac{n}{f}\right) = \left(\frac{E_F - E_g}{k_B T}\right)$$

$$E_g = E_F - k_B T \ln\left(\frac{n}{f}\right) \quad (13)$$

Using this relation we calculated the energy gaps which are nearly the same as expected. Thus our self conjectured formula works well for most of the samples [26].

Now we discuss the results of each individual sample in view of the interpretations as mentioned in the above paragraph. The parametric calculations, the calculations and the formula for the energy gap, to our knowledge, have not yet been found anywhere in the previous literature.

Conclusions

Galium Arsenide

From the photoacoustic spectra, we get Fermi energy $E_F = 3\text{eV}$ and then calculated the energy gap $E_g = 1.325\text{ eV}$, by using our self determined formula, as in Table -1

We infer the following conclusions:

- The quantum well structure of GaAs has a direct energy gap of 1.325 eV.
- The quantum well structure of GaAs has a Fermi energy of 3 eV.
- Our self conjectured relationship of fractional filling of the excited mode of phonons works quite satisfactorily for other samples, too [2].
- The energy gap formula which is developed in equation (13), works nicely for all other samples [2], and the magnitude of energy obtained for all samples is commensurate and in close agreement with other studies.
- The acoustic frequencies of phonons in quantum well structure of GaAs helps electrons to make a direct jump.
- The arsenic modifies the position of Fermi energy in gallium and does not produce localized region.
- The quantum structure of GaAs shows a metallic behavior.
- Debye frequency is localized to Brillouin zones in GaAs quantum well structure.

- From the table # 2, it is observed that the Debye Waller factor is high at peak frequencies of the photoacoustic spectrum of GaAs corresponding to a low fractional filling of the excited mode of phonons.

$$v_{\text{opt}} \gg v_{\text{acoustic of phonons}}$$

Aluminium Gallium

From the photoacoustic spectra, we get Fermi energy $E_F = 3.279$ eV and then calculated the energy gap $E_g = 1.604$ eV.

From these mathematical results we conclude that $k_D > k_F$ which shows that the acoustic frequency of phonons helps electrons to hop the energy gap due to excitation behavior. As $E_f \gg E_g$ leads to a metallic behavior. It seems to have a behavior like a deep level semiconductor.

From Table-2 we observed that the frequency of optical mode of phonons is much greater than the acoustic mode of phonons, v_{opt} for phonons are extended, v_D is localized to the Brillouin zones. As $v_{\text{opt1}} \cong v_{\text{opt2}}$ therefore there is no indirect gap. At higher frequency, Debye's Waller factor decreases corresponding to an increase in $f = E_f / E_{\text{peak}}$.

We infer the following conclusions:

- Aluminium Gallium has the direct gap of 1.6 eV.
- Aluminium Gallium has a Fermi energy of 3.279 eV.
- Fermi energy being greater than the energy gap leads to a metallic behavior of the sample.
- Aluminium Gallium seems to have a behavior like a deep level semiconductor.
- Frequency of optical mode of phonons for peak one is nearly equal to the frequency of optical mode of phonons. Peak two shows that there is no indirect gap in Aluminium Gallium.
- The acoustic frequency of phonons help electrons to hop the energy gap due to excitation behavior.

- Debye frequency is localized to Brillouin zones.
- Frequency of optical mode of phonons is much greater than the acoustic mode of phonons.
- Debye Waller factor decreases at high frequency corresponding to an increase in fractional filling of excited mode of phonons.

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