EVALUATION OF ENERGY AND DENSITY OF STATES OF TWO DIMENSIONAL QUANTUM STRUCTURE (QUANTUM WELL)

Abstract

Quantum structures (e.g. quantum wells) are critical part of optical system designs (lasers, modulators, switches etc.). In quantum well, the motion of the particle is quantized in one direction while the particle moves freely in other two directions. The density of state of quantum structure is the possible number of state an excited electron can occupy per unit volume. The density of state depends on the energy at which the electron moves when excited. In this paper, the energy and density of states of two dimensional quantum structure (quantum well) were calculated. The results obtained revealed the density of state increases with the energy but exhibited maximum and minimum peaks. Maximum peaks occurred at 4eV and 7.5eV while the minimum peaks occurred at 5eV and 8eV. These show that energy of state for quantum wells neither varies linearly nor exponentially with density of state because of high energy level. The findings are in agreement with published literature. Some applications of quantum wells include: bioconjugates, solar cells, photovoltaic, photo and electrochromic devices etc.

Keywords: Confinement, Density of State, Energy of State, Quantum Structure, Quantum Well

1.0 Introduction

One of the most significant nanostructures required for the design and building of nanoelectronic devices is quantum well [1]. Quantum well is referred to a semiconductor region that possesses lower energy where electrons and holes are trapped and whose properties are governed by quantum mechanics (where specific energies and band gaps are allowed). The typical nanoscale dimension of quantum well is between 1-1000 nm [1, 2]. Quantum wells are practical vital semiconductor devices used in many applications (e.g. LEDs, lasers, detectors etc.). Their optical transitions are very strong with the capability of tuning the energy. However, they also rely on optical transitions between the valence and conduction bands called inter-band transitions [3]. There are also optical transitions between the different electron levels within the quantum well called the inter-subband transitions. The inter-band and inter-subband transitions have a smaller energy gap which enable them interact with light in the mid- to far- infrared part of the spectrum [3, 4].

In quantum wells, electrons are confined in one direction and free to move only in the other two directions as seen in Figure 1. So, the electronic energy level bands are less crowded when compared with bulk materials [5].

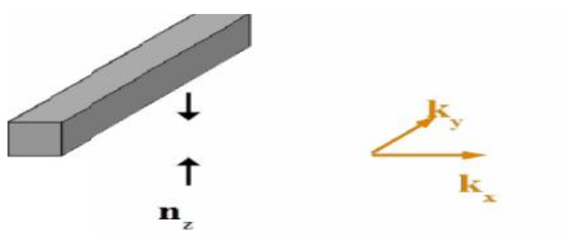

Figure 1: One dimension quantization in quantum well

A narrow band-gap material is placed between wider band-gap materials as shown in Figure 2. The decrease of the thickness of the well layer results to decrease in the electron and hole waveforms in the quantum well by the surrounding layers [6].

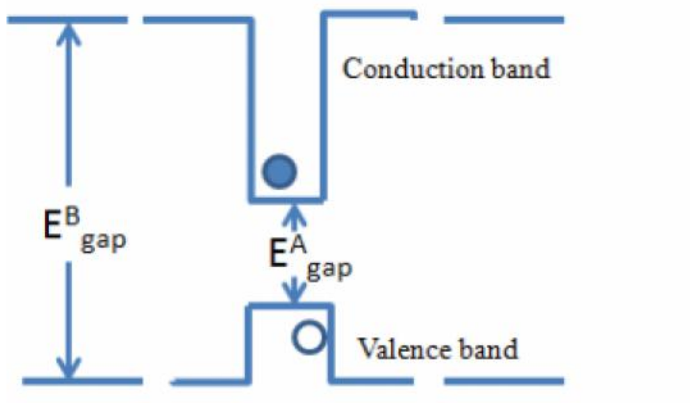

Figure 2: Energy band diagram of quantum well

The band gaps of two different semiconductors can be joined to form a hetero-junction. A potential well can be formed from the discontinuity in either the valence or conduction band. From Figure 2, if a thin layer of a narrower-band gap material 'A' is sandwiched between two layers of a wider-band gap material 'B', then a double hetero-junction is formed. A single quantum well can also be formed if layer 'A' is sufficiently thin for quantum properties to be exhibited.

As a result of confinement of extcitons in layers with thickness less than the exciton Bohr diameter, the oscillator strength and binding energy of the exciton increase [7]. The excitonic states become more stable and more visible at room temperature which is an impossible phenomenon in bulk structures. It is thinner and gets smaller in all directions. The holes and the electrons are closer to each other which results to larger Coulomb binding energy, faster classical orbit time, and greater optical absorption strength. Quantum confinement allows quantum structure to be tailored to specific incident energy levels based on particle size. Quantum confined structure is categorized based on the conferment direction into quantum well, quantum wire and quantum dots [8]. Quantum well could be finite, infinite or superlattice. In finite quantum well, the particle in the box exhibit tunneling penetration while in an infinite quantum well the particle is seen in the box only. Whereas, in superlattice quantum well the wells are so close that the wave-functions couple to give “minibands” [9].

The number of states attained by a quantum system is the possible number of available states. It is given mathematically as [2]:

$$\varphi(E) = \frac{V\ system}{V\ single{-}state}\ x\ \boldsymbol{N} \tag{1}$$

where

$\varphi(E)$ is number of states, V_{system} is volume of whole system (sphere, circle, line), V_{single} is volume of single state of that system, and N is the number of atoms in the crystal. Each quantum state has unique wave function.

Density of state is the possible number of state an electron when excited can occupy per unit volume [10]. The density of state depends on the energy at which the electron moves when excited. It is the first derivative of the number of state with respect to the energy. It is given mathematically as [11].

$$g(E) = \frac{d\ \phi(E)}{dE} \tag{2}$$

where

g(E) is the density of state and ϕ is number of states.

Density of electron states in bulk, 2D, 1D and 0D semiconductor structure is shown in Figure 3 [2, 12]. 0D structures has very well defined and quantized energy levels. The quantum confinement effect corresponding to the size of the nanostructure can be estimated via a simple effective-mass approximation model.

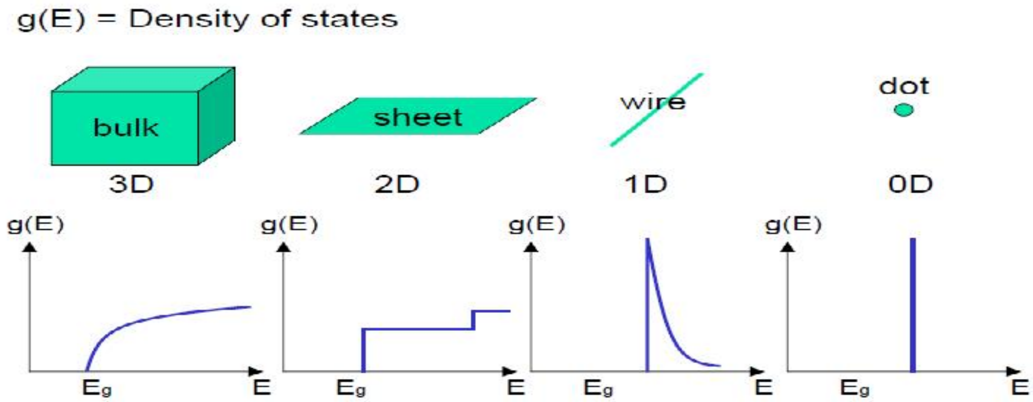

Figure 3: Density of electron states of a semiconductor as a function of dimension

2.0 Research Methodology

Energy and Density of State of Quantum Well

In this case, a semiconductor is modeled as quantum well (2D) with each side equal to l. Electron of mass m* are confined in the well. Setting the potential energy (P.E) = 0, and solving the Schrodinger equation yields;

$$\nabla^2\Psi\,(x,y,z) + \frac{2m(E-V)}{\hbar^2}\Psi\,(x,y,z) = 0 \qquad (3)$$

But for 2D,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \qquad (4)$$

Since potential energy is zero, then equation 3 becomes:

$$\frac{\partial^2\Psi\,(x,y)}{\partial x^2} + \frac{\partial^2\Psi\,(x,y)}{\partial y^2} + \frac{2mE}{\hbar^2}\Psi\,(x,y) = 0 \qquad (5)$$

But,

$$\frac{\partial\Psi}{\partial x} = \Psi(y)\Psi(z)\frac{d\Psi}{dx} \text{ and } \frac{\partial\Psi}{\partial y} = \Psi(x)\Psi(z)\frac{d\Psi}{dy} \qquad (6)$$

Also,

$$\frac{\partial^2\Psi}{\partial x^2} = \Psi(y)\frac{{}^2\Psi}{x^2} \text{ and } \frac{\partial^2\Psi}{\partial y^2} = \Psi(x)\frac{{}^2\Psi}{y^2} \qquad (7)$$

Putting equations 6 and 7 into equation 5 gives:

$$\Psi(y)\frac{\partial^2\Psi(x)}{\partial x^2}+\Psi(x)\frac{\partial^2\Psi(y)}{\partial y^2}++\frac{2mE}{\hbar^2}\Psi(x)\Psi(y)=0 \qquad (8)$$

Divide through equation 8 by $\Psi(x)\Psi(y)$ and Let $\frac{2mE}{\hbar^2}=K^2$ then,

$$\frac{1}{\Psi(x)}\frac{\partial^2\Psi(x)}{\partial x^2}+\frac{1}{\Psi(y)}\frac{\partial^2\Psi(y)}{\partial y^2}+\frac{2mE}{\hbar^2}=0 \qquad (9)$$

Or,

$$\frac{1}{\Psi(x)}\frac{\partial^2\Psi(x)}{\partial x^2}+\frac{1}{\Psi(y)}\frac{\partial^2\Psi(y)}{\partial y^2}+\frac{1}{\Psi(z)}\frac{\partial^2\Psi(z)}{\partial z^2}+K^2=0 \qquad (10)$$

where

K is a constant.

$$\frac{\partial^2\Psi(x)}{\partial x^2}+\frac{\partial^2\Psi(y)}{\partial y^2}+K^2\Psi(x)\Psi(y)=0 \qquad (11)$$

The solution to the equation 11 is given as:

$\Psi(x)=A\sin Kx+B\cos Kx$

$\Psi(y)=A\sin Ky+B\cos Ky$

At the point $\Psi(x)=0$ and $x=0$

$0=A\sin(0)+B\cos(0)$ Therefore, $B=0$

Hence, $\Psi(x)=A\sin Kx$

Taking the boundary conditions at $\Psi(x)=0$; $x=l$

$0=A\sin Kl$ But $A\neq 0$

Since $Kl=0$ then,

$Kl=\sin^{-1}(0)=n\pi$

Therefore, $K=\frac{n\pi}{l}$

Substituting back gives:

$\Psi(x) = A \sin \frac{n_x \pi x}{l}$ and $K_x = \frac{n_x \pi}{l}$

$\Psi(y) = A \sin \frac{n_y \pi y}{l}$ and $K_y = \frac{n_y \pi}{l}$

Thus, $K = K_x + K_y = \frac{n_x \pi}{l} + \frac{n_y \pi}{l}$

Normalizing the wave function,

$$\int \Psi(x)\,\Psi(x)^* = \int A^2 \sin^2 \frac{n_x \pi}{l} = 1$$

Therefore, $A = \sqrt{\frac{2}{l}}$ and

$$\Psi(x, y) = \sqrt{\frac{2}{l}} \sin \frac{n_x \pi x}{l} \sqrt{\frac{2}{l}} \sin \frac{n_y \pi y}{l}$$

(12)

Thus, the wave function of such a system is given by:

$$\Psi(x, y, z) = \sqrt{\frac{4}{l^2}} \sin \frac{n_x \pi x}{l} \sin \frac{n_y \pi y}{l}$$

(13)

Using the principle of effective mass approximation,

$$E = \frac{\hbar^2 K^2}{2m^*}$$

(14)

But, $K^2 = \frac{2m^* E}{\hbar^2} = (\frac{n\pi}{l})^2$ and $n = n_x{}^2 + n_y{}^2$

(15)

Substituting for K into E gives

$$E = \frac{\hbar^2 \pi^2 n^2}{2m^* l^2}$$

$$E = \frac{\hbar^2 \pi^2}{2m^* l^2}(n_x{}^2 + n_y{}^2)$$

(16)

The equation 16 is the energy of a 2-dimensional quantum well.

K-space volume for a single state = $\left(\frac{\pi}{a}\right)\left(\frac{\pi}{a}\right) = \frac{\pi^2}{V} = \frac{\pi^2}{l^2}$

K-space volume for the 2-dimensional system (circle) = V circle = πR^2

But,

$$R^2 = (n_x{}^2 + n_y{}^2) = \frac{2m^* l^2 E}{\hbar^2 \pi^2} \text{ and } R = \left(\frac{2m^* l^2 E}{\hbar^2 \pi^2}\right)^{1/2} \quad (17)$$

$$V_{circle} = \pi \text{ x } \left(\frac{2m^* l^2 E}{\hbar^2 \pi^2}\right)^{1/2} \quad (18)$$

Number of atoms for a crystal at position (0, 0) and (1/2,1/2) is = 2 x ½ x½

So,

$$\phi(E) = \frac{\pi \text{ x } \left(\frac{2m^* l^2 E}{\hbar^2 \pi^2}\right)^{1/2}}{\frac{\pi^2}{l^2}} \text{ x 2 x ½ x ½} = \frac{\cancel{\pi} l^2}{a \cancel{\pi}^2}\left(\frac{2m^* l^2 E}{\hbar^2 \pi^2}\right)^{1/2} \text{ x } \cancel{2} \text{ x} \frac{1}{\cancel{2}} \text{ x } \frac{1}{2}$$

$$\phi(E) = \frac{l^2}{\pi}\left(\frac{2m^* l^2 E}{\hbar^2 \pi^2}\right)^{1/2} \text{ x } \frac{1}{2} = \frac{l^3}{2\pi\hbar}\left(\frac{2m^* E}{\pi}\right)^{1/2} E^{\frac{1}{2}} \quad (19)$$

The density of state is therefore given as:

$$g(E)_{2D} = \frac{d\phi(E)}{dE} = \frac{1}{2} \text{ x } \frac{l^3}{2\pi\hbar}\left(\frac{2m^* E}{\pi}\right)^{1/2} E^{\frac{1}{2}-1} = \frac{1}{2} \text{ x } \frac{l^3}{\pi\hbar}\left(\frac{2m^* E}{\pi}\right)^{1/2} E^{-\frac{1}{2}} \quad (20)$$

Thus, the density of state per unit volume V is:

$$g(E)_{2D} = \frac{\frac{1}{2} \text{x} \frac{l^3}{\pi\hbar}\left(\frac{2m^* E}{\pi}\right)^{1/2} E^{-\frac{1}{2}}}{V} = \frac{\frac{1}{2} \text{x} \frac{l^3}{\pi\hbar}\left(\frac{2m^* E}{\pi}\right)^{1/2} E^{-\frac{1}{2}}}{l^3}$$

$$g(E)_{2D} = \frac{1}{2\pi}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{1}{2}} E^{-\frac{1}{2}} \quad (21)$$

Equation 21 gives the density of state for a 2-dimensional infinite potential well.

Data Analysis

The following parameters were used in the calculations of the energy and density of states of quantum dots in one dimension and result tabulated in Table 1.

$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34}$ J.S

$\pi = 22/7 = 3.142$

L = dimension of well and line assumed =10 $A^0 = 10 \times 10^{-10}$ m

m^* = mass of the electron = 9.11×10^{-31} kg

e = charge of electron = 1.6×10^{-19} C

3.0 Results

Table 1: Results Data of the Energy and Density of States for Two Dimensional Energy Levels

ENERGY LEVELS n_x, n_y	ENERGY (JOULES)	ENERGY (eV)	DENSITY OF STATES ($m^{-3}J^{-1}$)	DENSITY OF STATES ($m^{-3}eV^{-1}$)
1, 1	1.204×10^{-19}	0.75250	5.873×10^{27}	2.349×10^{18}
1, 2	3.0100×10^{-19}	1.88125	3.7147×10^{27}	1.48587×10^{18}
1, 3	6.0200×10^{-19}	3.76250	2.6267×10^{27}	1.051×10^{18}
1, 4	1.0234×10^{-18}	6.39625	2.0146×10^{27}	8.0583×10^{17}
2, 2	4.8160×10^{-19}	3.01000	2.939×10^{27}	1.1747×10^{18}
2, 3	7.8260×10^{-19}	4.89125	2.3040×10^{27}	9.215×10^{17}
2, 4	1.2040×10^{-18}	7.52500	1.857×10^{27}	4.429×10^{17}
3, 3	1.0836×10^{-18}	6.77250	1.9580×10^{27}	7.831×10^{17}
3, 4	1.5050×10^{-18}	9.40625	1.6610×10^{27}	6.645×10^{17}
4, 4	1.9264×10^{-18}	12.0400	1.4680×10^{27}	5.873×10^{17}
5, 1	1.5652×10^{-18}	9.78250	1.6290×10^{27}	6.516×10^{17}
5, 2	1.7458×10^{-18}	10.91125	1.5420×10^{27}	6.1697×10^{17}
5, 3	2.0468×10^{-18}	12.79250	1.4250×10^{27}	5.698×10^{17}
5, 4	2.4682×10^{-18}	15.42625	1.2970×10^{27}	5.189×10^{17}
5, 5	3.0100×10^{-18}	18.81250	1.1750×10^{27}	4.699×10^{17}
6, 1	2.2270×10^{-18}	13.92125	1.3660×10^{27}	5.462×10^{17}
6, 2	2.4080×10^{-18}	15.05000	1.31330×10^{27}	5.253×10^{17}
6, 3	2.7090×10^{-18}	16.93125	1.238×10^{27}	4.9529×10^{17}
6, 4	3.1300×10^{-18}	19.56500	1.1520×10^{27}	4.6075×10^{17}
6, 5	3.6722×10^{-18}	22.95125	1.0635×10^{27}	4.254×10^{17}
6, 6	4.3344×10^{-18}	27.09000	9.789×10^{26}	3.916×10^{17}

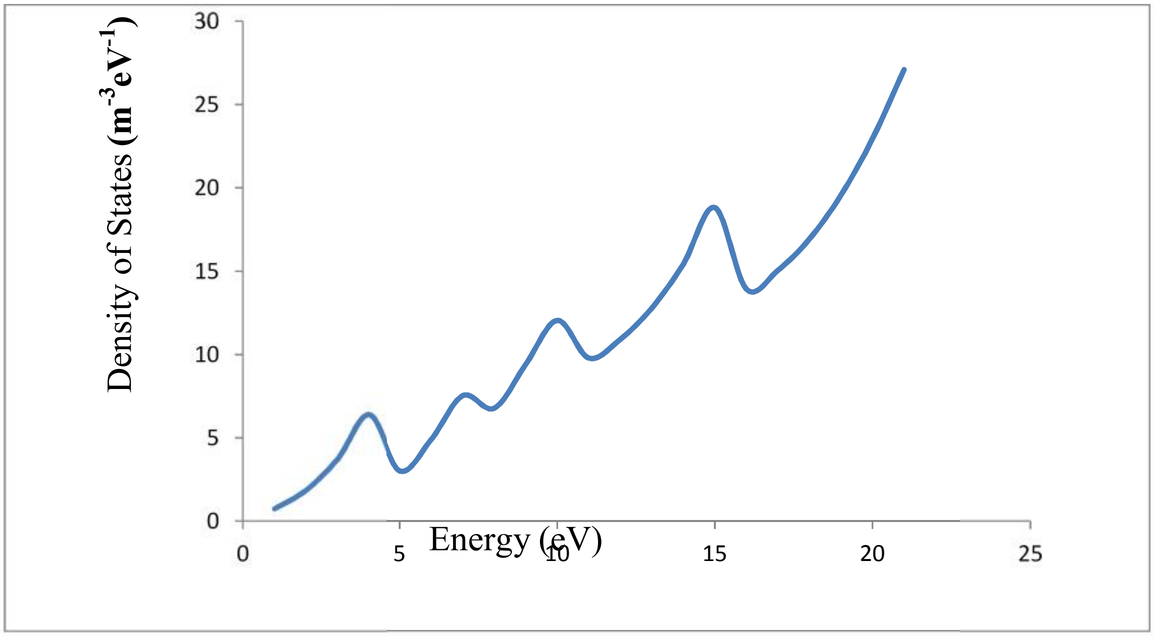

Figure 4: Variation density of state with energy for a 2D quantum well.

4.0 Discussion

From Figure 4 and Table 1, it shows that the density of state increases with the energy but exhibit maximum and minimum peaks. Maximum peaks occurred at 4eV and 7.5eV while the minimum peaks occurred at 5eV and 8eV. The energy continues to increase up to 12eV, for the first different levels investigated. These show that energy of state for quantum wells neither varies linearly nor exponentially with density of state because of high energy level. Also, this is a proof that density of state of quantum wells depends on other factors apart from energy. The findings are in agreement with published literature. The results obtained in this work may slightly differ from real life situations because of the following reasons:

I. In the calculation, the electronic mass of the electron was used throughout and not the effective mass of the electron, which varies in the reciprocal space lattice of the solid.

II. The dimension of the well was kept constant at a value of 10 A^0 irrespective of the dimension under consideration. Changes with the dimension of the box will certainly cause a change in the energy level and hence the density of state of the system studied.

5.0 Conclusion

The assessment of energy and density of states of quantum well has a tremendous impact in nano-technology which may revolutionize technology. However, clear understanding of energy and density of states of quantum wells is necessary for it. In this paper, the energy and density of states for a quantum well in two dimensions were calculated and analyzed. The result showed maximum and minimum peaks for the relationship between energy and density of states of quantum well indicating non-linearity of variations.

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