Assessment of Energy and Density of States of Three Dimensional Quantum Structure (Bulk)

J. Ilouno[1], Gesa, F. Newton[2], N.Okpara[3]

[1, 3]*Physics Department, University of Jos, Jos, Nigeria.*
[2]*Physics Department, Federal University of Agriculture, Makurdi, Benue State, Nigeria*

*Corresponding Author: *J. Ilouno, Physics Department, University of Jos, Jos, Nigeria.*

ABSTRACT

Quantum structures are integral part of optoelectronics devices e.g. lasers, modulators, switches etc. In three dimensional quantum structures (bulk), the particles move freely in all directions with zero confinement. 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 real solids were calculated. The results showed that energy increases with increase in the density of state. But, the density of state does not increase linearly with energy. The density of state has peaks when the energies are at 5eV, 7.5eV and 10eV. The highest peak occurred at 10eV and thereafter, the density of states kept increasing with increase in energy up to 25eV which is the maximum energy under investigation. The findings are in agreement with published literatures. Quantum structure technologies are applicable in measuring devices for IR photo detectors, optics for diode lasers, and micro-electronics for high electron mobility transistor devices.

Keywords: *Bulk, Confinement, Density of State, Energy of State, Quantum Structure*

INTRODUCTION

Quantum structure is a region of a semiconductor that has low energy where electrons and holes are trapped and whose properties are controlled by quantum mechanics [1]. The dimension of quantum structure is typically between 1-1000 nm [1, 2]. Quantum wells are vital building blocks for semiconductor devices such as 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 structure called the inter-sub band transitions. The inter-band and inter-sub band transitions have a smaller energy gap which enable them interact with light in the mid- to far- infrared part of the spectrum [3, 4].

A quantum confined structure is classified based on confinement direction as quantum bulk, quantum well, quantum wire, and quantum dots or nano-crystals as shown in Table 1 [5].

Table 1: *classification of quantum confined structures*

Structure	Quantum confinement	Number of free dimension
Bulk (real solid)	0	3
Quantum well	1	2
Quantum wire	2	1
Quantum dot	3	0

A narrow band-gap material is placed between wider band-gap materials as shown in Figure 1. 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].

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 1, 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 [6, 7].The simplest model for absorption between the valence and conduction

bands in a bulk semiconductor can be seen when an electron is raised from the valence band to a state of essentially the same momentum in the conduction band by the absorption of a photon.
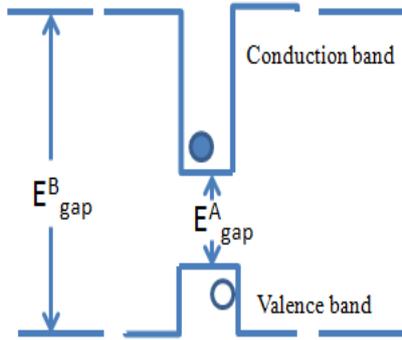
Figure 1: *Energy band diagram of quantum structure*

This simple model is presumed that all transitions have identical strength, although they will have different energies corresponding to the different energies for such vertical transitions [8, 9]. Hence, the optical absorption spectrum follows directly from the density of states in energy, and in bulk semiconductors the result is an absorption edge that rises as the square root of energy. In bulk semiconductors excitonic effect is neglected [10, 11]. Quantum structure could be finite, infinite or super lattice [12]. In finite quantum structure, the particle in the box exhibit tunneling penetration while in an infinite quantum structure the particle is seen in the box only. Whereas, in super lattice quantum structure the wells are so close that the wave-functions couple to give "mini bands" [9].

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

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

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 2 [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.
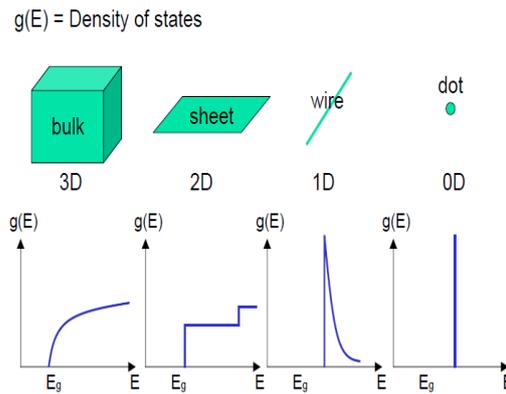
Figure 2: *Density of electron states of a semiconductor as a function of dimension*

RESEARCH METHODOLOGY

Energy and Density of States of 3-Dimensional Cubic Quantum Structure (Real Solid)

Let us consider a real semiconductor crystal as a cubic real solid in 3- dimensional system with sides of length l, using the Schrodinger equation;

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

But,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Thus, equation 3 becomes

$$\frac{\partial^2 \Psi \ (x,y,z)}{\partial x^2} + \frac{\partial^2 \Psi \ (x,y,z)}{\partial y^2} + \frac{\partial^2 \Psi \ (x,y,z)}{\partial z^2} + \frac{2m (E-V)}{\hbar^2} \Psi \ (x, y, z) = 0 \tag{4}$$

But for potential energy equal zero then,

Assessment of Energy and Density of States of Three Dimensional Quantum Structure (Bulk)

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

Also, $\frac{\partial\Psi}{\partial x} = \Psi(y)\Psi(z)\frac{d\Psi}{dx}$, $\frac{\partial\Psi}{\partial y} = \Psi(x)\Psi(z)\frac{d\Psi}{dy}$, and $\frac{\partial\Psi}{\partial z} = \Psi(x)\Psi(y)\frac{d\Psi}{dz}$

$$\left.\begin{array}{l} \frac{\partial^2\Psi}{\partial x^2} = \Psi(y)\Psi(z)\frac{d^2\Psi}{dx^2} \\[2mm] \frac{\partial^2\Psi}{\partial y^2} = \quad \Psi(x)\Psi(z)\frac{d^2\Psi}{dy^2} \\[2mm] \frac{\partial^2\Psi}{\partial z^2} = \quad \Psi(x)\Psi(y)\frac{d^2\Psi}{dy^2} \end{array}\right\} \qquad (6)$$

Putting equation 6 into equation 5, yields:

$$\Psi(y)\Psi(z)\frac{d^2\Psi(x)}{dx^2} + \Psi(x)\Psi(z)\frac{d^2\Psi(y)}{dy^2} + \Psi(x)\Psi(z)\frac{d^2\Psi(z)}{dy^2} + \frac{2mE}{\hbar^2}\Psi(x)\Psi(y)\Psi(z) = 0 \qquad (7)$$

Divide through by $\Psi(x)\Psi(y)\Psi(z)$ gives:

$$\frac{1}{\Psi(x)}\frac{d^2\Psi(x)}{dx^2} + \frac{1}{\Psi(y)}\frac{d^2\Psi(y)}{dy^2} + \frac{1}{\Psi(z)}\frac{d^2\Psi(z)}{dz^2} + \frac{2mE}{\hbar^2} = 0 \qquad (8)$$

Let $\frac{2mE}{\hbar^2} = K^2$, then $K = \sqrt{\frac{2mE}{\hbar^2}}$

$$\frac{1}{\Psi(x)}\frac{d^2\Psi(x)}{dx^2} + \frac{1}{\Psi(y)}\frac{d^2\Psi(y)}{dy^2} + \frac{1}{\Psi(z)}\frac{d^2\Psi(z)}{dz^2} + K^2 = 0 \qquad (9)$$

where K is a constant.

$$\frac{d^2\Psi(x)}{dx^2} + \frac{d^2\Psi(y)}{dy^2} + \frac{d^2\Psi(z)}{dz^2} + K^2\Psi(x)\Psi(y)\Psi(z) \qquad (10)$$

The solution to the equation 10 is given as:

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

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

$\Psi(z) = A\sin Kz + B\cos Kz$

Thus for a metal of length l along each axis; $\Psi(x) = 0$ at 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≠0

Sin Kl = 0   Thus, Kl = sin⁻¹(0) = nπ

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

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

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

$\Psi(z) = A\sin\frac{n_z\pi z}{l}$ and $K_z = \frac{n_z\pi}{l}$

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

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

Assessment of Energy and Density of States of Three Dimensional Quantum Structure (Bulk)

$$\Psi(x,y,z)=\sqrt{\frac{2}{l}}\ sin\ \frac{n_x\pi x}{l}\ \sqrt{\frac{2}{l}}\ sin\ \frac{n_y\pi y}{l}\ \sqrt{\frac{2}{l}}\ sin\ \frac{n_z\pi z}{l} \tag{11}$$

Thus, the wave function of such a system is given by: $\Psi(x,y,z)=\sqrt{\frac{8}{l^3}}\ sin\ \frac{n_x\pi x}{l}\ sin\ \frac{n_y\pi y}{l}\ sin\ \frac{n_z\pi z}{l}$

To obtain the energy of such a system we use the effective mass approximation model, such that

$$E=\frac{\hbar^2 K^2}{2m^*} \tag{12}$$

Thus, $K^2=\frac{2m^*E}{\hbar^2}=(\frac{n\pi}{l})^2$

The energy for a 3-dimensional system is therefore given as:

$$E=\frac{\hbar^2\pi^2}{2m^*l^2}(n_x{}^2+n_y{}^2+n_z{}^2) \tag{13}$$

Therefore,

$$n_x{}^2+n_y{}^2+n_z{}^2=\frac{2m^*l^2E}{\pi^2\hbar^2} \tag{14}$$

where

$n_1,n_2,n_3,n_4\ldots\ldots\ldots\ldots\ldots.n\ =1,2,3,4\ \ldots\ldots\ldots\ldots\ldots..$

But, $n_x{}^2+n_y{}^2+n_z{}^2$ is equivalent to the radius R for the K- space. $R^2=\frac{2m^*l^2E}{\pi^2\hbar^2}$

Hence,

$$R=(\frac{2m^*l^2E}{\pi^2\hbar^2})^{\frac{1}{2}}$$

But the volume of the sphere for 3-dimensional K-space $=\frac{4}{3}\pi R^3$ =V system (sphere),

$$V=\frac{4}{3}\pi R^3=\frac{4}{3}\pi(\frac{2m^*l^2E}{\pi^2\hbar^2})^{\frac{3}{2}} \tag{15}$$

Volume of the single state cubic in K-space $=(\frac{\pi}{a})(\frac{\pi}{b})(\frac{\pi}{c})=(\frac{\pi^3}{V})$ = V single state $=\frac{\pi^3}{V}$

Number of atom for a crystal at position (0,0,0) and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ in 3-dimension $=2\ x\ (\frac{1}{2}\ x\ \frac{1}{2}\ x\ \frac{1}{2})$

Hence, the number of state $\phi(E)=\frac{V\ system\ (sphere)}{V\ single\ -state}\ x\ Number\ of\ atoms$

$$\phi(E)=\frac{\frac{4}{3}\pi(\frac{2m^*l^2E}{\pi^2\hbar^2})^{\frac{3}{2}}}{\frac{\pi^3}{V}}\times 2\ x\frac{1}{2}\ x\frac{1}{2}x\ \frac{1}{2}\qquad but\qquad V=a\ x\ b\ x\ c=l^3$$

$$\phi(E)=\frac{\frac{4}{3}\pi(\frac{2m^*l^2E}{\pi^2\hbar^2})^{\frac{3}{2}}}{\frac{\pi^3}{l^3}}\ x\ \frac{1}{4}\ =\frac{\frac{4\pi l^3}{3\pi^3}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}}E^{\frac{3}{2}}}{\frac{\pi^3}{l^3}}\ x\ \frac{1}{4}=\frac{\frac{4\pi l^3}{3\pi^3}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}}E^{\frac{3}{2}}}{\frac{\pi^3}{l^3}}\ x\ \frac{1}{4}$$

$$\phi(E)=\frac{1}{3\pi^2}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}}\ E^{\frac{3}{2}} \tag{16}$$

Thus, the density of states is obtained as:

$$g(E)_{3D}=\frac{d\ \phi(E)}{dE}=\frac{3}{2}\ x\ \frac{1}{3\pi^2}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}}\ E^{\frac{3}{2}-1}\ =\frac{1}{2\pi^2}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}}\ E^{\frac{1}{2}}$$

$$g(E)_{3D}=\frac{1}{2\pi^2}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}}\ E^{\frac{1}{2}} \tag{17}$$

Equation 17 gives the expression for the density of state for a 3-dimensional system and shows that it is directly proportional to the square root of the energy E of the system.

Data Analysis

The following parameters were used in the calculations of the energy and density of states

of real solids in three dimensions and result tabulated in Table 2.

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

$\pi = 22/7 = 3.142$

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

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

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

RESULTS

Table2: *Results Data of the Energy and Density of States for Three Dimensional Energy Levels*

ENERGY LEVELS n_x, n_y, n_z	ENERGY (JOULES)	ENERGY (eV)	DENSITY OF STATES $(m^{-3}J^{-1})$	DENSITY OF STATES $(m^{-3}eV^{-1})$
1, 1, 1	1.8060×10^{-19}	1.12875	4.522×10^{46}	1.130×10^{56}
1, 1, 2	3.6120×10^{-19}	2.25750	6.395×10^{46}	1.599×10^{56}
1, 2, 2	5.4100×10^{-19}	3.38625	7.832×10^{46}	1.958×10^{56}
1, 2, 3	8.4280×10^{-19}	5.26750	9.768×10^{46}	2.442×10^{56}
2, 2, 3	1.0234×10^{-18}	6.39625	1.076×10^{47}	2.691×10^{56}
3, 1, 1	6.6220×10^{-19}	4.13875	8.658×10^{46}	2.165×10^{56}
3, 3, 3	1.6254×10^{-19}	10.1588	1.357×10^{47}	3.391×10^{56}
4, 2, 1	1.2642×10^{-18}	7.90125	1.196×10^{47}	2.991×10^{56}
4, 2, 2	1.4880×10^{-18}	9.03000	1.279×10^{47}	3.197×10^{56}
4, 2, 3	1.7458×10^{-18}	10.9113	1.406×10^{47}	3.515×10^{56}
4, 4, 4	2.8896×10^{-18}	18.0600	1.809×10^{47}	4.522×10^{56}
4, 1, 1	1.0836×10^{-18}	6.77250	1.108×10^{47}	2.769×10^{56}
4, 3, 1	1.5652×10^{-18}	9.78250	1.331×10^{47}	3.328×10^{56}
5, 1, 1	1.6250×10^{-18}	10.1588	1.357×10^{47}	3.391×10^{56}
5, 2, 1	1.8060×10^{-18}	11.2875	1.430×10^{467}	3.575×10^{56}
5, 3, 1	2.1070×10^{-18}	13.1688	1.544×10^{47}	3.860×10^{56}
5, 3, 2	2.2876×10^{-18}	14.2975	1.610×10^{47}	4.023×10^{56}
5, 3, 3	2.5886×10^{-18}	16.1788	1.712×10^{47}	4.280×10^{56}
5, 4, 1	2.5280×10^{-18}	15.8025	1.692×10^{47}	4.230×10^{56}
5, 4, 2	2.7090×10^{-18}	16.9313	1.751×10^{47}	4.378×10^{56}
5, 4, 3	3.0100×10^{-18}	18.8125	1.846×10^{47}	4.615×10^{56}
5, 4, 4	3.4314×10^{-18}	21.4463	1.971×10^{47}	4.927×10^{56}
5, 4, 5	3.9732×10^{-18}	24.8325	1.120×10^{47}	5.300×10^{56}

DISCUSSION

From Table 2 and Figure 3, it is clearly seen that the energy of state of quantum bulk increases with the density of states non-linearly. The density of state has peaks when the energy is at 5eV, 7.5eV and 10eV. The highest peak occurs at 10eV and after which the density of states kept increasing with increase in energy up to 25eV which is the maximum investigated. 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.
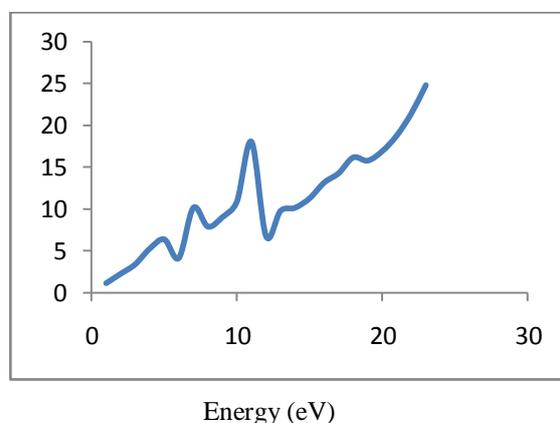
Figure3: *Variation of the density of states with energy of real solids*

CONCLUSION

The assessment of energy and density of states of quantum bulk has a tremendous impact in opto-electronics with diverse applications. In

this paper, the energy and density of states for a three dimensional cubic quantum structure were calculated and analyzed. The result showed maximum and minimum peaks for the non-linear relationship between energy and density of states of quantum bulk.

REFERENCES

[1] Paul, H. (2011). Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures. Wiley.

[2] Arthur, E. and Gabriel, K.O. (2015). Fundamentals of Solid State Physics. Department of Physics, Delta State University Abraka, Nigeria.

[3] Liu, H.C. (2000). Inter sub band Transitions in Quantum Wells: Physics and Device Applications II.vol.65 of Semiconductors and Semimetals, Academic press.

[4] Rosencher, E. and B. Vinter, B. (2002). Optoelectronics. Cambridge University Press.

[5] Alastair, R. (1998). Quantum Mechanics.3rd Ed, IOP Publishing.

[6] Vijay, A.S., Ranjan, V., & Manish, K. (1999). Semiconductor quantum dots: Theory & phenomenology. *Indian academy sciences*, (22)3, 563-569.

[7] Vijay, A.S., Ranjan, V., & Manish, K. (1999). Semiconductor quantum dots: Theory & phenomenology. *Indian academy sciences*, (22)3, 563-569

[8] Richard, D.T. (2008). Synthesis and applications of nano particles and quantum dots. *Chemistry in New Zealand*, pg 146-150.

[9] Bimberg, D. (1999). Quantum dot hetero structures. London, United Kingdom, Wiley-Blackwell.

[10] Brennan, K.F. (1997). The Physics of Semiconductors. New York, Cambridge University Press.

[11] Calvin R.K. (2005). Density of States: 2D, 1D, and 0D. Georgia Institute of Technology ECE 6451.

[12] Brennan, K.F. (1997). The Physics of semiconductors. New York, Cambridge University press.