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Thresholds and Delimitations of Quantum Confinement in Spherical Gallium Nitride and Gallium Arsenide Quantum Dots.

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ABSTRACT

Quantum dots (QDs) composed of gallium nitride (GaN) and gallium arsenide (GaAs) have captivating prospects in the field of nanotechnology. This paper explores the complicated confinement regimes in GaN and GaAs quantum dots, highlighting the critical thresholds and subtle boundaries that characterise the confinement regime and regulate their behaviour at the quantum level. Understanding the specific limits and boundaries of the quantum confinement effect is crucial due to factors like form and material composition. To fully exploit the potential of GaN and GaAs quantum dots in many fields, such as optoelectronics and quantum computing, it is imperative to address these challenges.

Keywords: Quantum confinement, confinement regime, confinement energy, de Broglie wavelength, exciton.

I. Introduction

Transistors, diodes, solar cells, and a plethora of other technologies are all built on semiconductor materials, which constitute the foundation of contemporary electronic devices (Gupta, 2014). At the macroscopic level, these materials display well-defined electrical characteristics as determined by classical physics. However, as technology advances towards the nanoscale, tbe behaviour of electrons within semiconductors becomes drastically different, principally due to the phenomenon known as quantum confinement (Shchukin *et al.*, 2009).

Quantum confinement refers to the limitation of electron mobility to dimensions equivalent to or less than their characteristic wavelength, as specified by the laws of quantum mechanics. This confinement introduces discrete quantization of energy levels, substantially changing the electronic structure of semiconductors at the nanoscale. The effects become increasingly evident as the size of the semiconductor structure approaches the de Broglie wavelength of the charge carriers or the exciton bohr radius of the respective semiconductor (Chukwuocha *et al*., 2012).

Quantum confinement occurs in semiconductors when the material's physical dimensions match or decrease the electron's wavelength, resulting in quantized energy levels and discrete electronic states. This is due to the wave-particle duality of electrons, which exhibit both particle-like and wave-like features. Confinement energy is the energy corresponding to the quantum confinement of charge carriers in semiconductor nanostructures, like quantum dots. When the dimensions of these structures approach or equal the de Broglie wavelength of electrons, quantized energy levels are produced. Based on effective mass approximation and assuming an ideal spherical quantum dot in which excitons are confined in spherical confining potential, Harry and Adekanmbi (2020) gave the confinement energy for a spherical quantum dot as:

$$E_{conf} = \frac{\hbar^2}{2d^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)X_{n,l}^2 \qquad \text{Equation 1}$$

Where m_h^* = effective mass of hole, m_e^* = effective mass of electron, d = diameter of sphere,

$X_{n,l}$ = nth zero of the lth order spherical Bessel function (for ground state , it is $X_{1,0}$ = 3.142 (Oliver *et al*, 2010).

The effects of quantum confinement are particularly visible in reduced-dimensional semiconductor such as quantum dots, quantum wells, and quantum wires. In these nanostructures, the three-dimensional mobility of electrons is limited, leading to the development of discrete energy levels. The confinement-induced changes in the electronic band structure, density of states, and other material characteristics have important consequences for the performance of nanoscale electronic and optoelectronic devices (Semonin, Luther, and Beard, 2012; Nurmikko 2015) . Figure 1 shows an increase in bandgap due to quantum confinement.

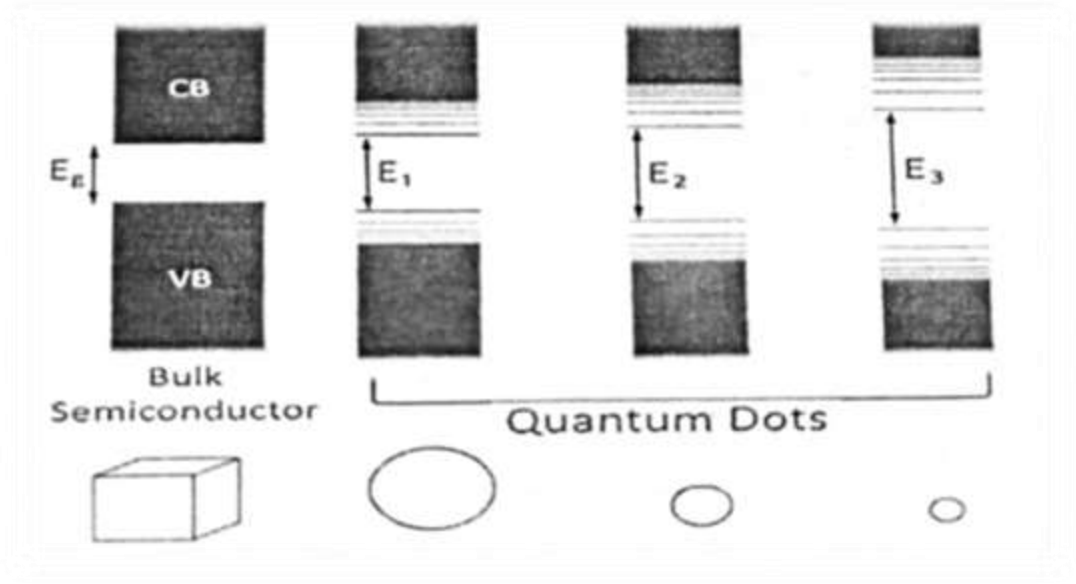

Figure 1: Increase in band gap due to quantum confinement as size is gradually reduced (Harry *et al*, 2023)

Transmission electron microscopy and scanning tunneling microscopy are two experimental techniques that have provided direct visual verification of quantum confinement events. These methodologies enable scientists to investigate the size-dependent changes in the electronic structure of semiconductor nanostructures, thereby validating quantum mechanics' theoretical predictions (Murphy and Coffer, 2002).

The research on quantum confinement in semiconductors is not just a theoretical goal but also a practical undertaking with substantial technological ramifications. Harnessing the unique electrical and optical features offered by quantum confinement has led to the creation of innovative technologies, including quantum dot-based LEDs, nanowire transistors, single-electron transistors, and lasers based on quantum wells, wires, and dots (Davies, 2005; Hornyak *et al*, 2008; Subannajui *et a*l, 2011; Cress and Datta, 2013; Lu *et al*, 2019). Quantum dots are semiconductor nanoparticles in which excitons are confined in all three dimensions. They are sometimes referred to as zero dimensional materials due to the zero degree of carriers in them. Quantum dots are the ultimate limits of quantum confinement and represent the utmost challenge for novel device fabrication. These improvements not only push the boundaries of existing technology but also offer up new paths for the design and deployment of next-generation electrical, electronic, and photonic devices.

The size regime or limit in which quantum confinement events take place is referred to as the confinement regime. Different semiconductor materials have different exciton Bohr radii affecting how small a quantum needs to be to exhibit quantum confinement. These confinement regimes, are crucial in determining their electronic and optical properties. Depending on the strength of confinement, it is divided into strong, intermediate, and confinement regimes. The shift between these regimes is determined by the size, form, and material composition of the quantum dot, offering a rich playground for designing their behavior and enabling diverse uses in fields such as quantum computing, photonics, sensors, and optoelectronics. Understanding and controlling these confinement conditions is important for engineering quantum dots with tailored features for specific technological uses. Quantitatively, these size regimes are dictated by the exciton-bohr radius of electrons and holes in the respective semiconductors. In this paper, an attempt is made to define the thresholds for quantum confinement and transitions from one regime to another in spherical-shaped gallium nitride and gallium arsenide quantum dots.

The quest to understand quantum confinement limits in GaN and GaAs quantum dots will bring about unprecedented technological breakthroughs (Peng *et al*, 1998). Applications ranging from efficient light-emitting diodes (LEDs) to quantum information processing and solar cells stand to benefit from the ideas gained through this study.

1.1 Quantum confinement in GaN quantum dots

Gallium Nitride (GaN), known for its wide bandgap and exceptional electronic qualities, takes the forefront in the world of quantum confinement. As the dimensions of GaN nanostructures, such as quantum dots, shrink to the size of the de Broglie wavelength of electrons, an interesting quantum dance unfolds. The confinement energy, a crucial parameter in this dance, appears as a witness to the quantized energy levels of electrons and holes within the nanostructure.

The beauty of GaN quantum dots lies in their ability to contain electrons and holes in three dimensions, leading to separate energy states. The size of these quantum dots influences the amount of the confinement energy, a key factor affecting the performance of optoelectronic devices. GaN quantum dots find uses in cutting-edge technologies such as light-emitting diodes (LEDs) and lasers, where the controlled confinement of charge carriers results in improved performance and spectral purity (Ramval *et al*, 2000).

1.2 Quantum confinement in GaAs quantum dots

The size-dependent confinement energy in GaAs quantum dots unlocks a multitude of opportunities for tailoring electronic properties and designing novel devices, from high-electron-mobility transistors (HEMTs) to laser diodes (Krishan and Garg 2015). Researchers delve into the nuances of confinement energy in GaAs nanostructures, exploring the interplay between size, shape, and crystal structure to engineer devices with unprecedented performance. Meanwhile, Gallium Arsenide, with its narrower bandgap, exhibits its own mesmerizing quantum confinement effects (Leandro *et al*, 2020).

2. Methodology:

Size regime for quantum confinement effects are influenced by the de Broglie wavelength and exciton bohr radius of semiconductors. The minimum size for these effects in any semiconductor material is obtained by a mixture of classical and quantum physics.

De Broglie wavelength:

Every particle has characteristics similar to waves, which are indicated by its de Broglie wavelength. For electrons and holes in a semiconductor, their de Broglie wavelength is governed by their momentum (Shchukin, 2009). In quantum confinement, when the dimensions of the semiconductor become similar to or smaller than the de Broglie wavelength of the carriers within it, the confinement takes place which affect the behavior of these carriers. For example, at a tiny enough semiconductor structure, the quantization of energy levels becomes visible, and electrons and holes exhibit wave-like behaviors such as quantum tunneling or discrete energy states . In terms of momentum of particle p, the de Broglie wavelength λ_b is given as (Aruldhas, 2014).

$$\lambda_b = \frac{h}{p} \qquad \text{Equation 2}$$

Where h is the planck's constant

Excitons:

Frenkel excitons found in semiconductors are pairs of an electron and a hole (an empty space where an electron can live) that are linked together in semiconductors. They are made when an electron is excited from the valence band to the conduction band. The extent to which apart the electron and hole are on average in an exciton pair is called the exciton Bohr radius. In quantum confinement, the size of the semiconductor is the same as or smaller than the exciton Bohr radius. This is especially true in nanoscale shapes of semiconductors like quantum dots, wires, or wells. When this happens, the confinement changes the way excitons behave in significant ways. One example is that the energy levels and emission qualities can change because excitons are confined in these smaller structures. The de Broglie wavelength and exciton bohr radius, r are equivalent forms of each other and their equivalence is given as (Kuno, 2005).

$$r = \frac{\lambda_b}{2\pi} \qquad \text{Equation 3}$$

Quantitatively, the exciton bohr radius a_b and the bohr radius a_0 are related as (Aruldhas, 2014):

$$a_b = a_0 \left(\frac{\varepsilon}{m^*_{ex}}\right) \qquad \text{Equation 4}$$

Where m^*_{ex}, and ε are effective exciton mass and dieletric constant of semiconductor respectively.

Minimum size (diameter) of spherical quantum dot for quantum size effect

For minimum size, the heterostructure must be such that it can confine at least a single electron. This means, for stability both ends must be a node as shown in Figure 2**.**

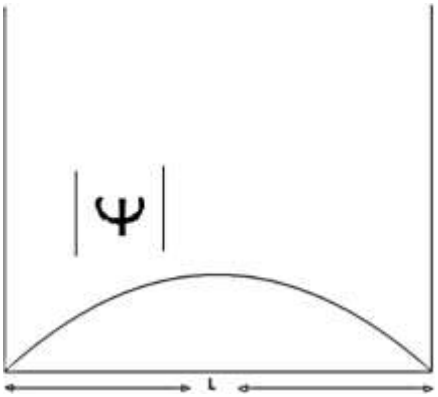

Figure 2: minimum length L for quantum confinement (Aruldhas, 2014).

Using classical physics, This corresponds to :

$L = \frac{\lambda_b}{2}$ Equation 5

Where λ_b = de Broglie wavelength of electron (particle).

Using classical physics and following Harry *et al*, (2023), minimum size, L

is given as:

$L = \frac{h}{2\sqrt{2m^* E_K}}$ Equation 6

Where m^* = effective mass m^*, h = the planck's constant,

E_k = kinetic energy of particle (electron) which is about 26 Mev (Kuno, 2005)

3 Results

Parameters of Gallium Nitride (GaN) and constants used are: bulk bandgap , E_{bulk} at 300k = 3.36eV , a_B(exciton bohr radius) = 4.2nm, electron rest mass $m_0 = 9.11 \times 10^{-31}$kg Effective mass of electron in GaN, $m^*_{ne} = 0.19m_0$, Effective mass of hole in GaN, $m^*_{nh} = 0.60m_0$, h = 6.63 x 10^{-34} Js.

Parameters of Gallium Arsenide (GaAs) and constants used are: bulk bandgap , E_{bulk} at 300k = 1.42eV , a_B(exciton bohr radius) = 6nm,

Effective mass of electron in GaAs, $m^*_{ae} = 0.067m_0$, Effective mass of hole in GaAs, $m^*_{ah} = 0.50m_0$.

Using Equations 4 and 5, de Broglie wavelengths of electrons and holes in Gallium Nitride and Gallium Arsenide are as follows:

De Broglie wavelength of electrons in Gallium Nitride $\lambda_{ne} = \frac{h}{\sqrt{2\, m^*_{ne} E_K}} = 17.5$nm

De Broglie wavelength of holes in Gallium Nitride $\lambda_{nh} = \frac{h}{\sqrt{2m^*_{nh}{}^* E_K}} = 9.8$nm

De Broglie wavelength of electrons in Gallium Arsenide $\lambda_{ae} = \frac{h}{\sqrt{2\, m^*_{ae} E_K}} = 30nm$

De Broglie wavelength of hole in Gallium Arsenide $\lambda_{ah} = \frac{h}{\sqrt{2\, m^*_{ah} E_K}} = 10.6$nm

Following Equation 3, exciton bohr radius of electrons and holes in Gallium Nitride and gallium arsenide are computed to be:

Exciton bohr radius of electron in Gallium Nitride, $r_{ne} = 2.78$nm

Exciton bohr radius of hole in Gallium Nitride, $r_{nh} = 1.56$nm

Exciton bohr radius of electron in Gallium Arsenide, $r_{ae} = 4.77$nm

Exciton bohr radius of hole in Gallium Arsenide, $r_{ah} = 1.69$nm

4. Discussion

Ground state is usually considered for thresholds. The lower threshold is the minimal size limit of quantum (forceful) confinement. This dictates the cluster and magic size limit for the nanocrystal. Confinement regimes were established for the two quantum dots by comparison with Bohr radius for the exciton, electrons and holes of the respective quantum dots. In Gallium Nitride, confinement regime is between 1.41 nm and 19.00 nm while in Gallium Arsenide, it ranges from 2.46 nm to 30.00 nm. In Gallium Nitride (GaN), the lower threshold is about 1.41nm in diameter(size). The associated confinement energy is determined using equation 1 to be 1.3138 eV. The transition from strong to intermediate confinement regime happens at a size (diameter) of around 3.12nm. This equates to a confinement energy of roughly 0.2683 eV. Transition from an intermediate to a weak confinement regime happens with a size of around 5.56nm. The associated confinement energy is 0.0845 eV. The limit for the weak confinement regime (upper threshold) is around diameter, d = 17.5 nm, which equates to a confinement energy of 0.0085 eV . Beyond the size limit of 17.5nm, quantum confinement effects in Gallium Nitride become insignificant.

Similarly, with Gallium Arsenide (GaAs), the minimal size which represent the lower threshold for quantum confinement effects is about 2.37nm in diameter. This equates to a confinement energy of roughly 1.1357 eV. The transition from strong to intermediate confinement is around 3.38nm in diameter. The confinement energy at this scale is roughly 0.5584 eV. The transition from intermediate to weak happens at a size of around 9.54 nm, which corresponds to a confinement energy of about 0.0701 eV. The size limit for the weak confinement regime is roughly 30 nm . The confinement energy at this scale is 0.0071 eV.

5. Conclusion

Quantum confinement in semiconductors is a fascinating phenomenon with significant implications for electrical, photonic, and optoelectronic technology. In the realm of GaN and GaAs quantum dots, knowing the thresholds and delimitations of confinement regimes is important for maximizing their full potential. As researchers triumph over the challenges faced by size, shape, and material-related issues, the applications of these quantum wonders

continue to develop. The voyage into the quantum world is replete with opportunities and discoveries, opening the way for a new era in nanotechnology and semiconductor research.

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