Theoretical Study of Dependence of Wavelength on Size of Quantum Dot

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Abstract— In this paper CdS, CdSe, ZnO, GaAs and CdTe semiconductor materials are used for studies. Using the effective mass approximation (EMA) method Quantum confinement effect on semiconductor quantum dots (QD's) has been studied. Effect of Size of Quantum Dot on wavelength is observed .The result shows that wavelength is directly proportional to the size (radius) of quantum dot. Thus, as one increases the radius (size), the wavelength increases. It means the biggest quantum dots produce the longest wavelengths, while the smallest dots make shorter wavelengths It also shows that wavelength can be tuned by changing the size of quantum dots (QDs) based on the quantum confinement effect which plays a fundamental role in electrical and optical properties of QDs. In addition, our results indicate that the after 1-4 nm, the effect of size of quantum dot on wavelength is very less for different semiconductor materials.

Key words: Quantum confinement effect, wavelength, Quantum dot, Effective mass approximation

I. Introduction

Today quantum dot structures are widely used as gain material for semiconductor laser. The atom like state density in quantum dot associated with three dimensional confinement of electrons and holes would cause an increase of optical gain and limit thermal carrier distribution.[1]

Quantum dots are minuscule semiconductor nanostructures that limit electron movement in all three spatial directions, confining them to a tiny area around the dot. These dots can range in size from 2 nanometers to 10 nanometers in diameter, with the entire dot encompassing 100 to 100,000 individual atoms. Because quantum dots are semiconductor materials, their conductivity changes in relation to external stimuli. The conductivity of a material depends primarily on the band gap, which scientists define as the space between the conduction band and the valence band of an atom where electrons cannot propagate. The band gap determines how much energy is required to elevate an electron from the valence band into the conduction band. Because quantum dots are semiconductors, the concepts of energy levels and bandgap energy apply. Quantum dots have distinct energy levels, much like individual atoms. For this reason, quantum dots are sometimes called artificial atoms or pseudo-atoms.[2]

The existence of discrete energy levels around quantum dots can be explained by the exciton Bohr radius, which is the average distance between an electron and the hole it leaves behind when it enters the conduction band. Different materials have different exciton Bohr radii. As a semiconductor crystal becomes smaller than its exciton Bohr radius, its energy levels will become discrete. By definition, a quantum dot must be smaller than the exciton Bohr radius of the material with which it is made out of. The existence of discrete energy levels around a quantum dot, called quantum confinement, has important repercussions on the absorptive and emissive behavior of the semiconductor material. One special property of quantum dots is that they emit light at very specific wavelengths depending on several factors including shape, the material makeup, and most importantly the size of the dot. Thus, a larger dot requires less energy to create an exciton and will release less energy when the electron returns to the valance band, corresponding to a longer wavelength of light. Thus, scientists can control the wavelength and energy of the light emitted by a quantum dot by tuning its size. Studies show that quantum dots have a high quantum yield, which means that they produce many excitons for each high-energy photon that they absorb. [2]

II. Theory

The smaller the dimensions of the quantum dot, the larger the separation between adjacent energy levels. As the band gap increases, excited electrons occupy higher energy levels, and can decay to a greater number of lower state values. As a result of size tunable band gaps within the quantum dot.Effective Mass Approximation Model approach, based on the 'Particle-in-Box Model', is the most widely used model to predict quantum confinement. It was first proposed by Efros [3] in 1982 and later modified by Brus [4]. It assumes a particle in a potential well with an infinite potential barrier at the particle boundary.

Hence according to effective mass approximation (EMA) the effective band gap is given by

$$E_g^*(QD) = E_g(bulk) + \frac{\hbar^2\pi^2}{2r^2}\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right) - \frac{1.80\,e^2}{4\pi\varepsilon\varepsilon_0 r} - 0.25E_{Ryd}^*$$

The second term of the Eq.(1) represents a relation between 'particle-in-a-box' quantum localization energy or confinement energy and the radius of the quantum dot (r), whereas the third term shows the Columbic interaction energy with a r-1 dependence. The Rydberg energy term is size independent and is usually negligible, except for semiconductors with small dielectric constant [5]. Based on Equation (1), the first excitonic transition (i.e., the band-gap) increases as the quantum dot radius (r) decreases (quantum localization term shifts to higher energy with lower r value (r-2) and Columbic terms shifts excited electronic state to lower value (r-1)). After neglecting the fourth term, effective band gap can be written as-

$$E_g^* = E_g^{bulk} + \frac{\hbar^2\pi^2}{2r^2}\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right) - \frac{1.80\,e^2}{4\pi\varepsilon\varepsilon_0 r}$$

$$E_g^* = E_g^{bulk} + \frac{h^2}{8r^2}\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right) - \frac{1.80\,e^2}{4\pi\varepsilon\varepsilon_0 r} \qquad 2$$

Where e is the charge of electron.$E_g^*$is the band gap energy of the quantum dots. $E_g^{Bulk}$is band gap energy of the bulk material at room temperature. h is Planck's Constant, r is the radius of quantum dot , m_e is the mass of a free electron, m_e^* is the effective mass of a conduction band electron , m_h^* is the effective mass of a valence band hole , ε is the relative permittivity of quantum dot .

The wave length of the light obtained by a quantum dot will be-

$$\lambda^* = \frac{C}{\nu^*} = \frac{C}{E_g^* / h}$$

After substituting the value of E_g^*,

$$\lambda^* = \frac{hc}{E_g^{bulk} + \frac{h^2}{8r^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) - \frac{1.80\, e^2}{4\pi\varepsilon\varepsilon_0 r}} \qquad 3$$

III. RESULT AND DISCUSSION

Variation in λ^* have been calculated for five different semiconductors Quantum dots CdS, CdSe, ZnO, GaAs and CdTe. In arriving at the results, several parameters were used, for CdS, CdSe, ZnO, GaAs and CdTe as in **Table 1** below.

Figure (1) shows the graph between the wavelength and quantum dot radius. For CdS, CdSe, ZnO, GaAs and CdTe semiconductor quantum dots, the wavelength vary in a range from (282.05)nm to (519.24)nm, (242.35)nm to (729.64)nm, (246.88)nm to (372.64)nm , (164.04) nm to (869.23) nm and (222.72) nm to (819.14) nm respectively. It is clear from the Figure (1) that as the size of quantum dots are increased a sudden increment in wavelength occurs and then it becomes constant for large values of quantum dots size.. It means as dots become larger, the wavelength of light emitted becomes longer, causing the color to move towards the red end of the visible light spectrum. As dots become smaller, the wavelength becomes shorter and the coloration shifts towards the blue end of the spectrum. This is because as a quantum dot grows larger, its energy levels move closer together

PARA-METERS	Values for following Quantum dots				
	CdS	**CdSe**	**ZnO**	**GaAs**	**CdTe**
Eg (in eV)	2.4	1.7	3.35	1.42	1.51
h (in J-sec)	6.6×10^{-34}	6.6×10^{-34}	6.6×10^{-34}	6.6×10^{-34}	6.6×10^{-34}
e (in C)	1.6×10^{-19}	1.6×10^{-19}	1.6×10^{-19}	1.6×10^{-19}	1.6×10^{-19}
m_e^* (in Kg)	$0.19\times9.1\times10^{-31}$	$0.13\times9.1\times10^{-31}$	$0.24\times9.1\times10^{-31}$	$0.067\times9.1\times10^{-31}$	$0.096\times9.1\times10^{-31}$
m_h^* (in Kg)	$0.80\times9.1\times10^{-31}$	$0.45\times9.1\times10^{-31}$	$0.45\times9.1\times10^{-31}$	$0.45\times9.1\times10^{-31}$	$0.84\times9.1\times10^{-31}$
C (in nm/sec)	3×10^{17}	3×10^{17}	3×10^{17}	3×10^{17}	3×10^{17}
ε	5.7	10.0	3.7	12	10.39

Table 1: Values of parameter used in the calculations

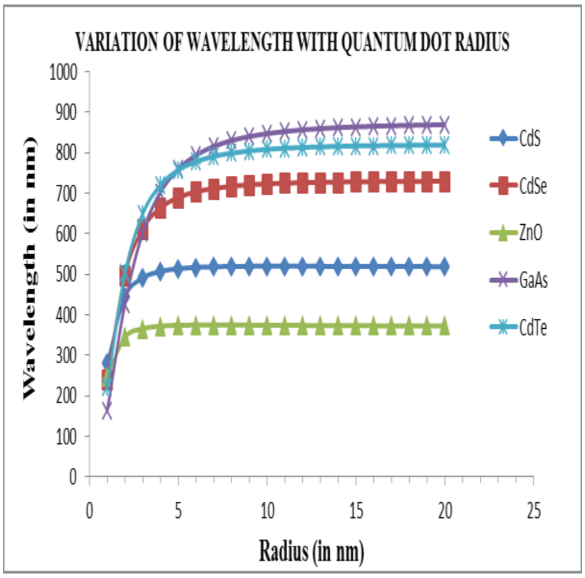

Fig. 1: Variation of wavelength with quantum dot radius for different semiconductor materials

IV. CONCLUSION

In this paper Effective mass approximation method is used for investigations. Due to quantum confinement effect, the band gap increases as the size of QD decreases. Relation between the wavelength of light and quantum dot radius has been shown. Graph between wavelength and radius of quantum dot of different semiconductor materials like CdS, CdSe, ZnO, CdTe, GaAs is plotted. From above it is concluded that wavelength of light obtained by semiconductor QD depends on the size of QD. Altering the size of a quantum dot will change the distances between energy levels, changing the band gap and thus the energy required for an electron to cross it.

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