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Non-linear Study of Zinc Oxide Quantum Dot for Optoelectronics Applications

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ABSTRACT

The nanostructures are being used for the various nonlinear optical devices. In this paper we have studied the few nonlinearities of ZnO quantum dots considering susceptibility as the nonlinear parameter and the equation for the second order nonlinearity of quantum dots have been developed and simulations have been performed for second order susceptibility in terms of dot size, photon energy, and electric field. We found that the second order coefficient gets a higher value for a particular value of length L only. If the value of length L gets above or below that, a lower value of susceptibility is obtained. These effects will be useful for the applications in photonics devices like lasers, solar cells, resonators etc.

1. Introduction

Semiconducting quantum dots, whose molecule sizes are in the nanometer extent, have extremely uncommon properties. The quantum dots have band gaps that depend in a complicated manner upon various factors, depicted in the articles [1, 2]. Transforming structure-properties-execution connections are audited for compound semiconducting quantum dots [3]. Different systems for incorporating these quantum dots are examined, and additionally their subsequent properties [4, 5]. Quantum states and control of their excitons may move their optical absorption and emission energies [6, 9, 10]. Such impacts are vital for tuning their radiance animated by photons (photoluminescence) or electric field (electro-luminescence) [7, 8].

In the field of electronics and optoelectronics devices the nonlinearities play a very important role and it is interesting to know how the parameters of quantum dots varying or being affected by various parameters. Here in this paper we are going to model an equation for second order nonlinear susceptibility and we will show how the susceptibility is varying with the size and photon energy. And we are also trying to show the variation of susceptibility with respect to other parameters. Here we are going to show the SHG for cubical ZnO quantum dots with the applied electric field using the compact density matrix approach and iterative method. The result will show the maximum susceptibility for a specific length or size of the quantum dots. More importantly we will show that the SHG coefficient is not a monotonic function of length L and the applied electric field E. If we select a suitable value for E and L, we can achieve a higher value of susceptibility (SHG coefficient).

2. Mathematical Formulation

2.1 Coordination System for Quantum Dot

The charge carrier motions in a quantum dot are restricted in all three spatial directions and that can be represented by a three dimensional spherical mechanical system model as shown in the figure.

The excitons of the quantum dots will confine inside this system and will follow the quantum mechanical principles for the above mentioned three dimensional spherical co-ordinate system.

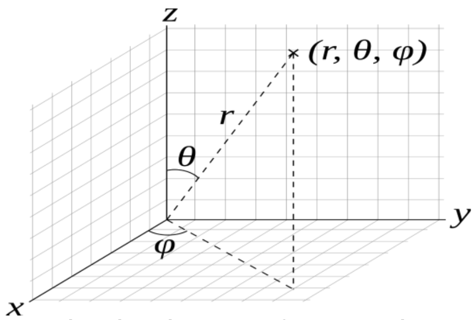

Fig. 1 Showing 3D spherical coordinate system for a quantum dot

2.2 Hamiltonian Operator

Hamiltonian is the operator which corresponds to the total energy of the system and it is usually denoted by 'H' and its spectrum is the set of possible outcomes when one measures the total energy of the system.

$$H = T + V \quad (1)$$

where, T = kinetic energy of the system, V = potential energy of the system. The expression for Hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m^*} + e\,\vec{F}.\,\vec{k} + V(x, y, z) \quad (2)$$

$$\text{Where, } V(x,y,z) = \begin{cases} 0, & |x||y| \text{ and } |z| < \frac{L}{2} \\ \infty, & \text{otherwise} \end{cases}$$

where, $\vec{F}$ is the electric field vector, $\vec{k}$ is the radial direction of electric field vector, e is electronic charge, L is length of the quantum dots and V(x, y, z) is the confining potential.

In spherical coordinates, the external electric field can be written as

$$\vec{F} = F(\sin\theta\cos\emptyset\,\widehat{k_1} + \sin\theta\sin\emptyset\,\widehat{k_2} + \cos\theta\,\widehat{k_3}) \quad (3)$$

Since we have chosen an infinite potential well the electron movement will be limited within cubic quantum dot. Therefore, the Hamiltonian can be rewritten as

$$H = -\nabla^2 + \eta(x\,\sin\theta\cos\phi + y\,\sin\theta\sin\phi + z\,\cos\theta) \quad (4)$$

where, $\eta = \frac{e\,a^* F}{R^*}$ is dimensional measure of electric field. The numerical method for solving the Schrodinger equation is given in the reference [3]. Using same method we can give corresponding solution for the wave function ψ.

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Consider now the system is excited by electromagnetic field

$$\overrightarrow{E(t)} = \widetilde{E}\, e^{j\omega t} + \widetilde{E}\, e^{-j\omega t} \quad (5)$$

Then the evolution of density matrix is given by time dependent Schrodinger equation and it is also known as Liouville's equation [11, 12].

$$\frac{\partial \rho_{ij}}{\partial t} = \frac{1}{i\hbar}[H_0 - qz\overrightarrow{F(t)}, \rho]_{ij} - \Gamma_{ij}(\rho - \rho^0)_{ij} \quad (6)$$

where, H_0 is Hamiltonian for the system without electric field, ρ_{ij} is the relaxation rate .We are selecting $\Gamma_{ij} = \Gamma_0 = \frac{1}{T_0}$ when i ≠ j for simplicity. The equation [6] is calculated by the following iterative method:

$$\rho(t) = \sum_n \rho^{(n)}(t) \quad (7)$$

With

$$\frac{\partial \rho_{ij}{}^{(n+1)}}{\partial t} = \frac{1}{i\hbar}\{[H_0 - \rho^{(2n+1)}]_{ij} - i\hbar\, \Gamma_{ij}\rho_{ij}{}^{(n+1)}\} - \frac{1}{i\hbar}[qz, \rho^n]_{ij}\overrightarrow{E(t)}. \quad (8)$$

The electric polarization of the quantum dot due to electric field $\overrightarrow{E(t)}$ can be expressed as

$$P(t) = \left(\epsilon_0\, \chi_\omega^{(1)} \widetilde{E}\, e^{j\omega t} + \epsilon_0\, \chi_{2\omega}^{(2)} \widetilde{E}^{\,2} e^{2j\omega t}\right) + \epsilon_0\, \chi_0^{(2)} \widetilde{E}^{\,2}$$

where, $\chi_\omega^{(1)}, \chi_{2\omega}^{(2)}$ *and* $\chi_0^{(2)}$ are the linear susceptibility, second harmonic generation and optical rectification susceptibility and ϵ_0 vacuum dielectric constant. The electronic polarization of nth order is given by, [10]

$$P^{(n)}(t) = \frac{1}{V}\, Tr(\rho^{(n)}\, ez) \quad (9)$$

where, V is the volume of interaction and Tr denotes the summation over the diagonal elements of the matrix $\rho^{(n)}\, ez$.

The Second order nonlinear equation for the susceptibility per unit volume is given by

$$\chi_{2\omega}^{(2)} = \frac{3e^3\rho}{5\varepsilon_{0\hbar^2}} \frac{M_{01}M_{12}M_{20}}{(\omega - 2\omega_{10} - i\Gamma_0)(2\omega - 5\omega_{20} - i\Gamma_0)}$$

where, ρ is the density of electron in the system and e is the electronic charge. $\omega_{ij} = \frac{(E_i - E_j)}{\hbar}$ is the transition frequency. $M_{ij} = |\langle \Psi_i | z | \Psi_j \rangle|$ is the off diagonal matrix element and $M_{01}M_{12}M_{20}$ is the matrix element's product. From equation of $\chi_{2\omega}^{(2)}$, we can get a peak value of SHG coefficient when the double-resonant condition can be met, i.e., $\hbar\omega \approx E_{10} \approx \frac{E_{20}}{2}$ and it can be obtained by

$$\chi_{2\omega\, max}^{(2)} = \frac{3e^3\rho}{7\varepsilon_{0\hbar^2}} \frac{M_{01}M_{12}M_{20}}{\Gamma_0{}^2} \quad (10)$$

The above equation is developed for a ZnO quantum dot by using the compact density matrix to solve the Hamiltonian. The various factors affect the susceptibility which can be seen by the second harmonic nonlinear equation for susceptibility.

3. Results and Discussion

Numerical calculations are carried out for ZnO cubical quantum dots with the external electric field. The parameters adopted in our calculations are as follows: $m^* = 0.027\, m0$, $R^* = 5.83\, meV$, $a^* = 98$ Å, $\epsilon_0 = 8.85\text{x}10^{-12}\, Fm^{-1}$, $T_0 = 0.2\, ps$ *and* $\rho = 5\text{x}10^{24} m^{-3}$.

In the figures given below (Figs. 2-6), the second order nonlinear susceptibility as a function of photon energy is shown for length of quantum dot as L= 13 nm, 14 nm, 16 nm, 18 nm and 20 nm.

In the simulation results as shown in figures, we have considered the dot size of different length and have obtained results for the photon energy and its susceptibility. For a particular quantum dot size and at particular photon energy, we have a peak value of susceptibility as shown in the resulting graphs.

The value of nonlinear SHG coefficient as a function of photon energy for an applied electric field is found as shown in the figure. The SHG coefficient gets a higher value for a particular value of length L only. If the value of length L gets above or below that value is gets a lower value of susceptibility as shown in the figures.

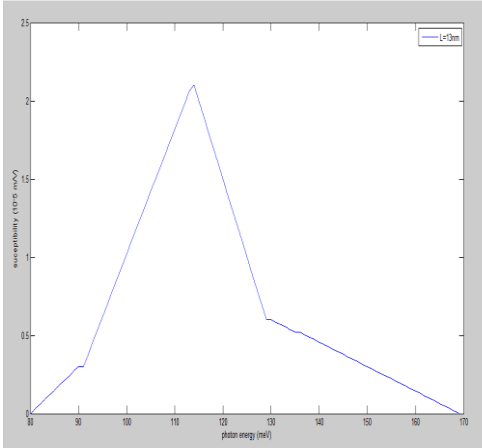

Fig. 2 Susceptibility as a function of incident photon energy for the length of quantum dot L= 13 nm

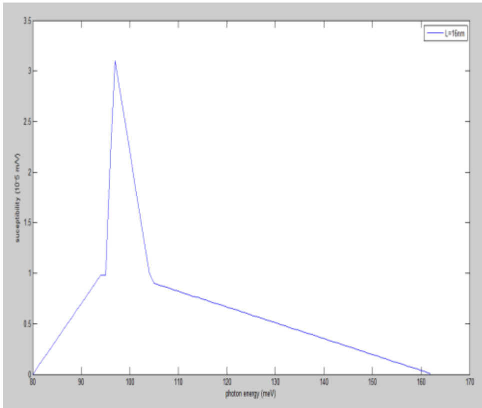

Fig. 3 Susceptibility as a function of incident photon energy for the length of quantum dot L= 16 nm

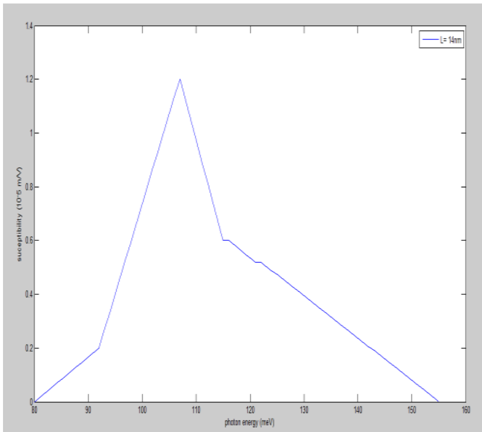

Fig. 4 Susceptibility as a function of incident photon energy for the length of quantum dot L= 14 nm

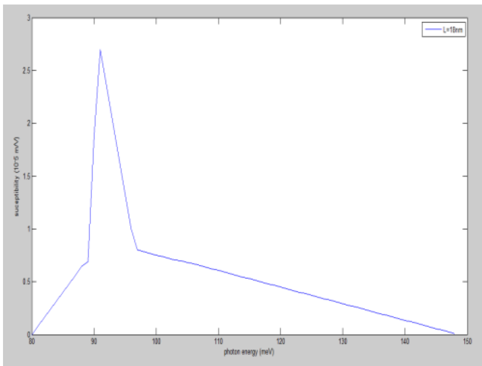

Fig. 5 Susceptibility as a function of incident photon energy for the length of quantum dot L= 18 nm

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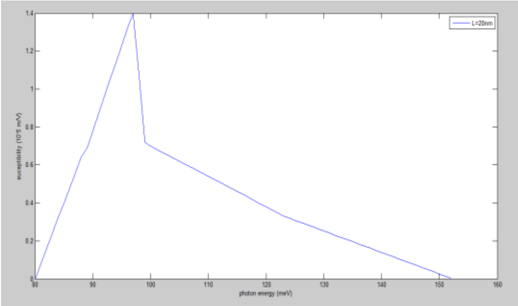

Fig. 6 Susceptibility as a function of incident photon energy for the length of quantum dot L= 20 nm

In our results, we can see that we get a higher value for the SHG coefficient (susceptibility) for length of the quantum dot L= 16 nm for a fixed applied electric field and for all other values of the length of the quantum dots we get a lower value of second order nonlinear susceptibility for an applied electric field.

At L= 16 nm, we found a peak value of susceptibility as 3.2 x 10^{-5} m/V and at L= 14 nm minimum value of susceptibility. Thus we can say that by varying the value of L and electric field E, We can get a higher value for susceptibility as to get it for particular applications.

Susceptibility is a dimensionless proportionality constant that indicates the degree of polarization of a dielectric material in response to an applied electric field. The greater the electric susceptibility, the greater the ability of a material to polarize in response to the field, and thereby reduce the total electric field inside the material (and store energy).

4. Conclusion

Thus we can say that if we see the behavior of a material in response to the applied electric field, we must have to know about the susceptibility which an important parameter when the designers select a material for a particular optoelectronics application. By tuning the size of the material we can get a desired value of nonlinear parameters such as susceptibility, magnetization and others.

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