Islamic Azad University

Journal of
Optoelectronical Nanostructures

Summer 2021 / Vol. 6, No. 3

Research Paper

The Effect of Ambient Temperature on the Linear and Nonlinear Optical Properties of InAs/GaAs Quantum Dot

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Received:
Revised:
Accepted:
Published:

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Keywords:
Quantum Dot
Linear and Nonlinear Susceptibility
Ambient Temperature
Finite Element Method
Intersubband Transition

Abstract :
In this work, we calculated the energy levels of truncated pyramidal-shaped InAs/GaAs QDs by using the finite element method by taking into account the ambient temperature, because the system under study is not symmetric, it is impossible to use the analytical method to find the wave functions and energy levels of the electron, and the finite element method is the solution to such problems. We showed that, with increasing the temperature, the energy level of both the ground state and the first excited state as well as S-to-P transition frequency increase. But the important point was that, increasing the temperature can shift linear and nonlinear susceptibility graphs to higher frequencies. For example, for a pyramid with a base length of 25 nm and a height of 5 nm, at zero and 500 K the maximum linear and nonlinear susceptibility values are shifted from 14 terahertz to the 18 terahertz. This ability can be effective in designing optical devices.

Citation: Mohammad Amin Zekavat Fetrat, Mohamma Sabaeian, Ghahraman Solookinejad. The effect of ambient temperature on the linear and nonlinear optical properties of InAs/GaAs quantum dot. **Journal of Optoelectronical Nanostructures. 2021; 6 (3): 81- 92. DOI:** 10.30495/JOPN.2021.29138.1240

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1. INTRODUCTION

In recent years, many studies have been conducted on the semiconductor quantum dots (QDs) structures [1]. These structures are used in the fields of diode lasers [2], quantum computing [3], quantum information [4, 5], solar cells [6-11], medicine and industry, etc. Due to the quantum confinement of electrons in three dimensions, the energy levels of electrons are similar to the energy levels of isolated atoms. Therefore, they have unique optical properties [12, 13]. The radiation of QDs in this case fall in the terahertz spectral range. These waves have many applications in imaging, space and defense industries, and medicine [14]. In general, two types of transitions occur at QDs: intersubband transitions and interband transitions. In the intersubband transitions, the energy difference of the subbands is of the order of meV. Sabaeian et al. were studied the optical properties of QDs with various dimensions and geometries [15-17]. One of the geometries which is very closed to the experimental shapes, is the truncated pyramidal shape [18]. In the growth of QDs, such as InAs/GaAs, by the famous method of Stranski-Krastanov (S-K) [19, 20], islands are created in various shapes (InAs) on a substrate (GaAs). The reason for this phenomenon is the difference between lattice constant of two materials used during the growth of the structure. In this growth method, a wetting layer is remained, which has very important role in the electronic and optical properties. Due to the asymmetry in these structures, analytical study of real QDs is not possible. This would be more complicated, when the effects of wetting layer and temperature are also taken into account in the calculations.

By exciting the QDs with use of external fields, radiations in the terahertz range can be observed. External factors such as temperature, pressure, and electromagnetic fields can change the energy levels; so the radiation of the QDs may also change. Therefore, by considering the external factors, the radiation of the QDs, which is important in the manufacture of optical devices, can be controlled. Therefore, it is necessary to study the optical properties of QDs by considering the temperature as an inevitable environmental parameter. So far, several studies have considered the effect of temperature and the pressure on the optical properties of QDs [21, 22]. In this work, the optical properties of a truncated pyramidal-shaped InAs/GaAs QDs are studied by considering the ambient temperature.

2. THEORY

According to Fig. 1, our system is a truncated pyramidal-shaped QD with a wetting layer (InAs) that is placed entirely in a matrix (GaAs). The wetting layer is a thin and flat layer with a thickness of 0.5 nm which is made of InAs and is attached to the truncated. Due to the difference between the QD material and the wetting layer (InAs) with that of the substrate (GaAs), a potential barrier is created at the boundaries of two substances due to the difference in the conduction band edge of the two materials. This confinement potential is 500 mV [23]. Therefore, by considering a single electron trapped in this potential, the eigenfunctions and eigenvalues of the electron can be found. For this purpose, we use the single-band effective-mass Schrodinger equation (given below) and consider the ambient temperature on the system [23]

$$-\frac{\hbar^2}{2m^*}\nabla^2\Psi\ (x,y,z)+V(x,y,z)\Psi\ (x,y,z)=\varepsilon\ \Psi\ (x,y,z) \qquad (1)$$

where m* is the effective mass of electron, with a value of $0.04m_0$ in InAs and $0.067m_0$ in GaAs [18]. V(x,y,z) is the confinement potential arising from the difference between the band gaps of InAs and GaAs and imposes a potential barrier of 500 meV which is affected by strain considerations [23]. In Fig. 1 (b), Dirichlet ($\Psi\ (\vec{r})=0$) and Neumann boundary conditions ($\partial\ \Psi\ (\vec{r})/\partial n=0$) have been shown, where n is a unite vector perpendicular to the boundaries. At the materials interface, i.e. InAs/GaAs interface, we use the boundary condition of $1/m^*_{InAs}[\partial\Psi_{InAs}(\vec{r})/\partial n]=1/m^*_{GaAs}[\partial\Psi_{GaAs}(\vec{r})/\partial n]$ [23].

The temperature-dependent effective mass for GaAs and InAs is given as follows [24]:

$$\frac{m_0}{m^*(P,T)}=1+2\gamma+[\frac{E_P^\Gamma(E_g^\Gamma+(\frac{2}{3})\Delta_{SO})}{E_P^\Gamma(E_g^\Gamma+\Delta_{SO})}] \qquad (2)$$

Where E_P^Γ is the energy related to the momentum matrix element, Δ_{SO} is the spin orbit splitting, E_g^Γ is the energy gap, and is the Kane parameter [24]. E_g^Γ is a function of hydrostatic pressure and temperature as follows [24]:

$$E_g^\Gamma(P,T)=E_g^\Gamma(0,0)-\frac{\alpha\ T^2}{\beta+T}+D\cdot P \qquad (3)$$

Where (α,β) and D are the temperature and pressure coefficients, respectively. $E_g^\Gamma(0,0)$ is the energy gap at pressure $P=0$ Kbar and temperature T=0 K .

The recommended parameters used in Eqs. (2) and (3) adopted in our alculations are listed in Table 1.

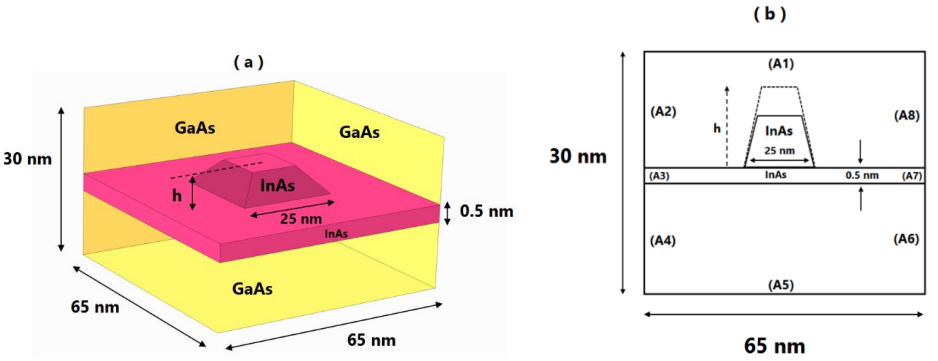

Fig.1. 3D schematic of our truncated pyramidal-shaped QD with wetting layer without graphene (a) with its distinct boundaries (b).

The above Schrodinger equation given by Eq. (1) cannot be solved analytically, because the geometry under study is asymmetric. We have solved Eq. (1) numerically with a finite element method. The details of this method are discussed in this reference [25].

Table 1

The recommended parameters used in Eqs. (2) and (3) and adopted in our calculations [24].

Parameters	GaAs	InAs
$E_g^{\Gamma}(0,0)(eV)$	1.519	*0.533*
$\alpha(\frac{meV}{K})$	0.5404	*0.276*
$\beta(K)$	204	*83*
$D(\frac{meV}{Kbar})$	10.8	*7.7*
$\Delta_{so}(eV)$	0.341	*0.39*
$E_p^{\Gamma}(eV)$	28.8	*21.5*
γ	-1.94	*-2.9*

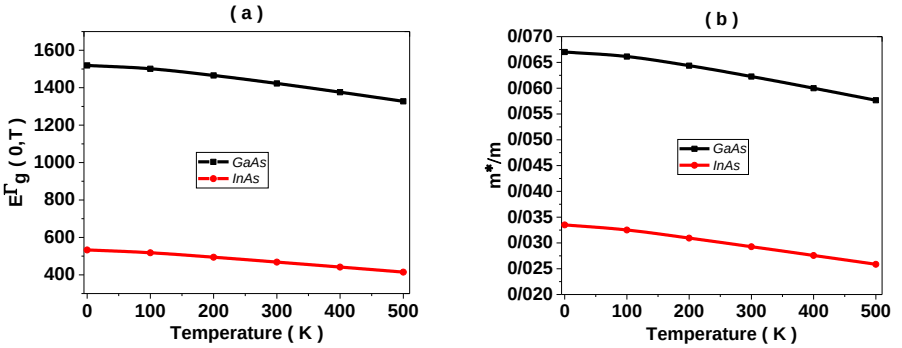

Fig.2. (a) The energy band gap at p=0 Kbar, (b) and the ratio of effective mass to electron mass as a function of temperature.

As can be seen in Fig. 2, the effective mass and energy band gap of GaAs and InAs decrease with increasing the ambient temperature, which is to be expected regarding relation given in Eqs. (2) and (3). Having found the eigenfunctions and eigenvalues of QDs, the linear and nonlinear susceptibilities can be calculated as follows[23]

$$\chi^{(1)}(\omega)=\frac{N}{\hbar\varepsilon_0}\frac{\left|M_{21}^2\right|}{(\omega_{21}-\omega-i\gamma_{21})} \tag{4}$$

$$\chi^{(3)}(\omega)=-\frac{N}{\hbar^3\varepsilon_0}\frac{\left|M_{21}^2\right|}{(\omega_{21}-\omega-i\gamma_{21})}$$

$$\times\{\frac{4\left|M_{21}^2\right|}{(\omega_{21}-\omega)^2+\gamma_{21}^2}-\frac{(M_{11}-M_{11})^2}{(\omega_{21}-i\gamma_{21})(\omega_{21}-\omega-i\gamma_{21})}$$

Where N is the carrier density, γ is the damping rate, and ω_{21} is the transition frequency. The values of $N=3\times10^{22}m^{-3}$ and $\gamma_{21}=5ps^{-1}$ are considered for the carrier density and damping rate, respectively [23]. In the formulas above $\mathbf{M}_{ij}=\langle\Psi_i|(-e\times\mathbf{r})|\Psi_j\rangle$

3.RESULTS

In this section, the results of the effect of ambient temperature on the eigenvalues energy and optical properties of our system are presented. In Fig. 3, the distribution of wave functions of ground state (S-state) and the first excited state (P-state) are shown. As the distribution of wave functions of ground state

and the first excited state are similar to hydrogen atom [26], we call them S- and P-state, respectively. In this figure, only the probability density of ground state and the first excited state of truncated pyramidal-shaped QD with height of 7 nm at T=0 K are plotted. Changing the temperature does not cause a noticeable change in the electron probability densities.

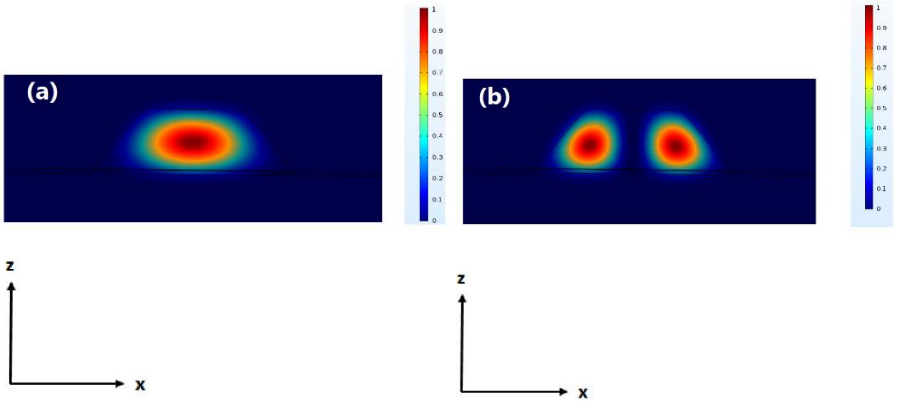

Fig.3. The probability density of (a) ground state (S-state) and (b) the first excited state (P-state) of a truncated pyramidal-shaped QD with the height of 7 nm and base length of 25 nm in T=0 K.

Figure 4 shows the energy eigenvalues of S- and P-state and S-to-P transition frequency as a function of the height of the pyramid and temperature. As shown in this figure, with increasing the temperature, the energy level of the both the ground state and the first excited state as well as S-to-P transition frequency increase, which, of course, is expected, because based on the effective mass approximation, the relationship between the effective mass and the second energy derivative is $\frac{1}{m^*}=\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$. In this formula it is well shown that, energy levels and effective mass are inversely related. In a particular case, if the effective mass is not dependent on the direction of the wave vector, then the above relation will be as follows :

$$E=\frac{\hbar^2 k^2}{2m^*} \tag{5}$$

In the above relation, the inverse relationship between energy and effective mass is quite clear. Because the effective mass decreases with increasing temperature, so the energy levels of the quantum dot increase with increasing temperature.

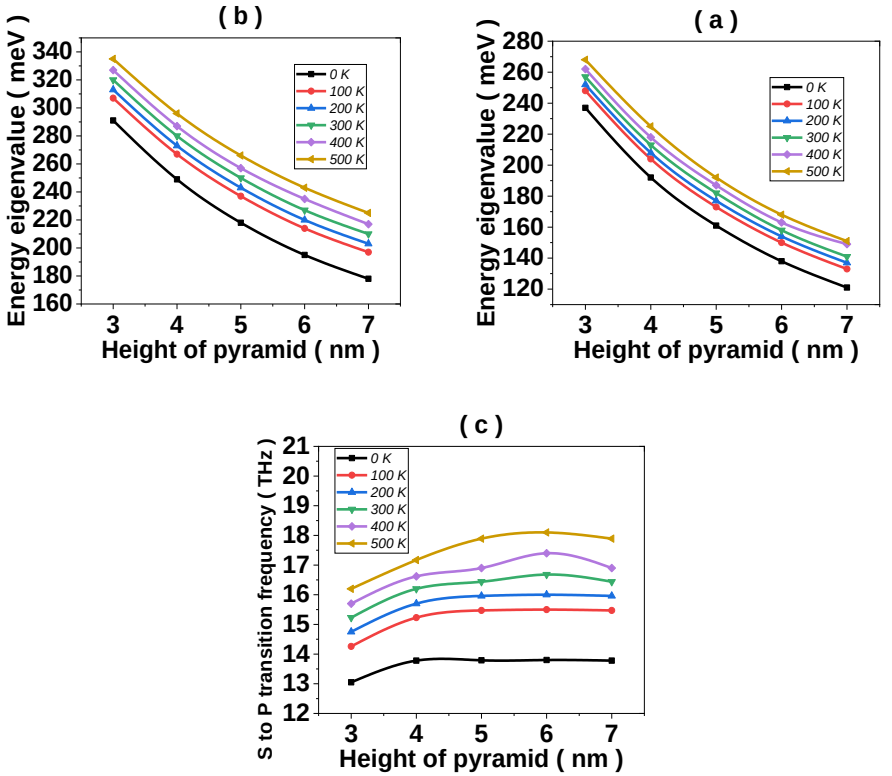

Fig.4 (a) Energy eigenvalues of S- and P-state and (b) S-to-P transition frequency as a function of temperature and height for a QD with the constant base of 25 nm.

Figure 5 shows the optical susceptibilities of our QD system, with a height of 5 nm and a base length of 25 nm for pyramid as a function of temperature. According to figure 4, as the temperature increases, the frequency of the transition also increases. On the other hand, in Eq (4), the transition frequency appears at the denominator of the fraction (ω_{21}). Therefore, as the transition frequency increases, the linear and nonlinear susceptibility graphs are shifted to higher frequencies. In fact, by changing the temperature, the QD finds the ability to express its linear and nonlinear optical properties at any frequency.

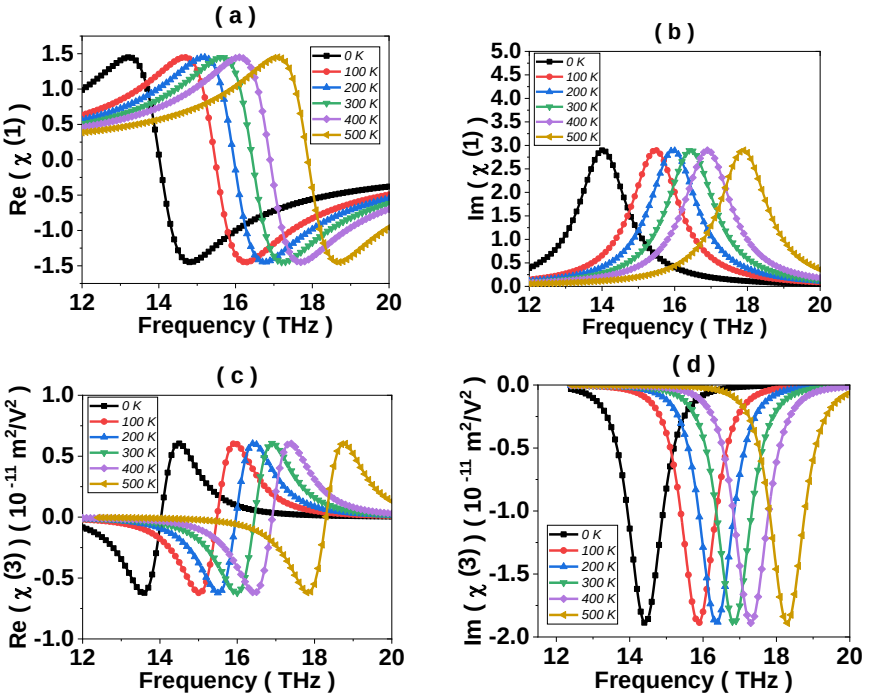

Fig.5. Linear susceptibility (a, b) and nonlinear susceptibility (c, d) for a pyramid with a height of 5 nm and a base length of 25 nm as a function of frequency for different temperatures.

3.CONCLUSIONS

In summary, we have studied the linear and third-order susceptibilities of pyramidal-shaped InAs/GaAs QDs by taking into account the ambient temperature. The effective mass and energy band gap of GaAs and InAs is decreased with increasing the ambient temperature. As a result, with increasing the temperature, the energy level of both the ground state and the first excited state as well as S-to-P transition frequency increase. But the important point was that, increasing the temperature can shift linear and nonlinear susceptibility graphs to higher frequencies. This ability can be effective in designing optical devices.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest regarding the publication of this manuscript.

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