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Threshold pump intensity effect on the refractive index changes in InGaN SQD: Internal constitution and size effects

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ABSTRACT

In the present paper, internal composition and size-dependent threshold pump intensity effects on on-center impurity-related linear, third-order nonlinear and total refractive index changes are investigated in wurtzite (In,Ga)N/GaN unstrained spherical quantum dot. The calculation is performed within the framework of parabolic band and single band effective-mass approximations using a combination of Quantum Genetic Algorithm (QGA) and Hartree–Fock–Roothaan (HFR) method. According to the results obtained, (i) a significant red-shift (blue shift) is obtained as the dot size (potential barrier) increases and (ii) a threshold optical pump intensity depending strongly on the size and the internal composition is obtained which constitutes the limit between two behaviors.

1. Introduction

In the few last decades, the wide band-gap III-nitrides semiconductor based on GaN, AlN, (In,Ga)N and (Al,Ga)N have attracted tremendous attention due to their extraordinary capacity and potential for device applications. These materials are most auspicious for high-power, high-temperature electronic devices, such as high-brightness blue–green light emitting diodes (LEDs) and laser diodes (LDs) which is due to their direct and large band-gap ranging from infrared to ultraviolet. Semiconductor quantum dot (QD) structures have attracted much attention due to their unique physical properties and their potential applications in micro- and optoelectronic devices. In zero-dimension structures, the free carriers are confined to a small region by a so called confinement potential providing the quantization of electronic energy states based on the size of the dots. Atom-like discrete energy-levels are occurred when confining the carriers in a nano-region. Photons with appropriate energy can cause the intersubband transitions involving large electric dipole moments. The optical properties such as refractive index, absorption coefficient, and absorption cross section can be easily calculated once the linear and nonlinear susceptibilities of the QD are known. Large electric dipole matrix elements along with small energy differences between subbands, enhance the nonlinear contribution of dielectric constant, so one expects the light intensity plays a crucial role in the optical properties of the dots. In this regard the dot sizes and the composition of the ternary alloy can alter the values of electronic eigen-energies and their corresponding envelope functions [1–7]. The third-order nonlinear optical properties of typical structures have attracted much attention for both theoretically researches and practically applications such as infrared photo detectors, far-infrared laser amplifiers, optical memory technology, light emitting diode, high-speed electro-optical modulators and so on [8–19].

Zhang et al. [17] have investigated the effects of QD radius, incident optical pump intensity and impurity on the linear and nonlinear optical properties of strained GaN/AlN QD. Kirak et al. [18] reported a detailed calculation of linear and nonlinear optical absorption coefficients (ACs) and refractive index (RI) changes for 1s–1p and 1p–1d transitions in parabolic QDs using a variational method under the electric field influence. Karabulut and Baskoutas [20] have proposed a systematic study of size, impurity, external applied electric field and optical intensity on linear and nonlinear ACs as well as RI changes in CdS QDs. For finite and infinite Si QDs, Anchala et al. [21] have reported the effects of the potential barrier on ACs and RI changes. Additionally, the effects of conduction band non-parabolicity, the impurity and the optical intensity on intersubband ACs and RI changes of a typical $GaAs/Al_xGa_{1-x}As$ spherical QD (SQD) are theoretically investigated by Rezaei et al. [22] using the Luttinger–Kohn effective-mass equation. Incidentally, RI changes associated with intersubband transition in SQD, $GaAs/Al_xGa_{1-x}As$, has been theoretically calculated by Cakir et al. [23] in the presence of an impurity. In the same sense, the optical

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properties of a SQD under the effect of constant effective-mass and position-dependent effective-mass have been studied by Khordad [24]. For this purpose, the intersubband optical absorption coefficient and the refractive index changes are obtained using both a constant and a position-dependent effective-mass. The second and the third-harmonic generation in a quantum wire with parallelogram cross section has also studied under the electric field effects [25]. In our previous works, the effects of the relaxation time and the impurity's position on linear and nonlinear RI changes in (In, Ga)N–GaN SQD have investigated [26].

To the best of our knowledge, no work has done to treat the effect of threshold pump intensity and its dependence as a function of internal composition and dot's radius. In the present paper, we will attempt to investigate the influence of dot's size, potential barrier, optical pump intensity and its threshold value on linear, third-order nonlinear and total RI changes in (In,Ga)N/GaN SQD.

2. Theoretical framework

Within the framework of single band effective-mass and parabolic band approximations, the Hamiltonian of the electron in the presence of an on-center shallow-donor impurity in wurtzite $In_xGa_{1-x}N$–GaN SQD of radius R can be expressed in term of effective units as

$$H = -\nabla^2 - \frac{2}{\varepsilon_r r} + V(r) \tag{1}$$

where ε_r is the relative dielectric constant and $V(r)$ is the finite potential barrier given as

$$V(r) = \begin{cases} 0 & r \le R \\ Q\Delta E_g(x) & \text{elsewhere} \end{cases} \tag{2}$$

where Q and $\Delta E_g(x)$ are respectively the conduction band off-set parameter and the In-dependent difference between the band gaps of GaN and $In_xGa_{1-x}N$ [6].

Notice that the expression of linear and third-order nonlinear RI changes and all used parameters are the same as those used in our previous works [26–28].

$$\frac{\Delta n^{(1)}}{n_r} = \frac{\sigma |M_{fi}|^2}{2\varepsilon_0 n_r^2 \hbar} \frac{\omega_{fi} - \omega}{(\omega_{fi} - \omega)^2 + \Gamma_{fi}^2} \tag{3}$$

$$\frac{\Delta n^{(3)}}{n_r} = -\frac{\sigma I |M_{fi}|^4}{c\varepsilon_0^2 n_r^3 \hbar^3} \frac{\omega_{fi} - \omega}{\left[(\omega_{fi} - \omega)^2 + \Gamma_{fi}^2\right]^2} \left[1 - \frac{|M_{ff} - M_{ii}|^2}{4|M_{fi}|^2(\omega_{fi}^2 + \Gamma_{fi}^2)} \left\{\omega_{fi}(\omega_{fi} - \omega) - \Gamma_{fi}^2 - \frac{\Gamma_{fi}^2(2\omega_{fi} - \omega)}{\omega_{fi} - \omega}\right\}\right] \tag{4}$$

where σ is the electron density in SQD expressed as $\sigma = N/V_{QD}$, N is the number of electrons in the dot and V_{QD} is its volume. ω is the incident photon angular frequency, Γ_{fi} $(i \ne f)$ is the non-diagonal matrix element called as relaxation rate of final and initial states defined as the inverse of the relaxation time (τ_{fi}). The difference of the energy between the final and initial states is defined as $E_{fi} = E_f - E_i = \hbar\omega_{fi}$. $n_r = \sqrt{\varepsilon_r}$ represents the relative refractive index of the semiconductor, c is the speed of the light in vacuum, ε_0 is the static electrical permittivity of the vacuum and $I\left(=2\varepsilon_0 n_r c |E|^2\right)$ is the incident pump intensity. Therefore, the total RIC can be obtained by the following expression:

$$\frac{\Delta n(I,\omega)}{n_r} = \frac{\Delta n^{(1)}(\omega)}{n_r} + \frac{\Delta n^{(3)}(I,\omega)}{n_r} \tag{5}$$

The results presented below are given in the effective units, i.e., the effective Rydberg energy $R^* = m^* e^4/2\hbar^2\varepsilon_0^2$ as the unit of the energy and the effective Bohr radius (EBR) $a^* = \varepsilon_0\hbar^2/m^* e^2$ as the unit of length.

3. Results and discussion

In the following, linear, third-order nonlinear and total RI changes are computed in $In_xGa_{1-x}N$/GaN SQD in the presence of on-center impurity. In Fig. 1, the linear, third-order nonlinear and the total RI changes are plotted as a function of the pump energy $(\hbar\omega)$. The internal constitution, the pump intensity and the relaxation time are set to be respectively 0.2, 30 MW m^{-2} and 0.2 ps. It can be seen that the RI changes are not monotonic functions of the pump energy for all dot radii. At the beginning, the linear RI change increases steadily versus $\hbar\omega$ until it reaches a maximum value. This behavior is happened in the normal dispersion corresponding to $dn/d\lambda < 0$. However, as $\hbar\omega$ approaches the threshold energy $(E_{fi} - \hbar\Gamma_{fi})$ the linear and the total terms decrease quickly for reaching a minimum value at $E_{fi} + \hbar\Gamma_{fi}$. Notice that the anomalous dispersion given by $dn/d\lambda > 0$ is observed. This domain corresponds to a strong absorption phenomenon as shown in Refs. [27,28]. The effect of dot's radius is also shown on the same figure. A significant red-shift is obtained with increasing the dot size. The reason is that as R increases the difference between the energy levels of implied states decrease. It can be seen that the amplitude of all terms are enhanced with increasing R.

It is clear that the linear term is more substantial in small dot radius while the nonlinear term becomes important in large dot radius. Therefore, the total RI change is significantly reduced. From the same figure, it is shown that the nonlinear contribution should be considered in the interpretation of experimental results especially for high optical pump intensity and in large dot radii. From

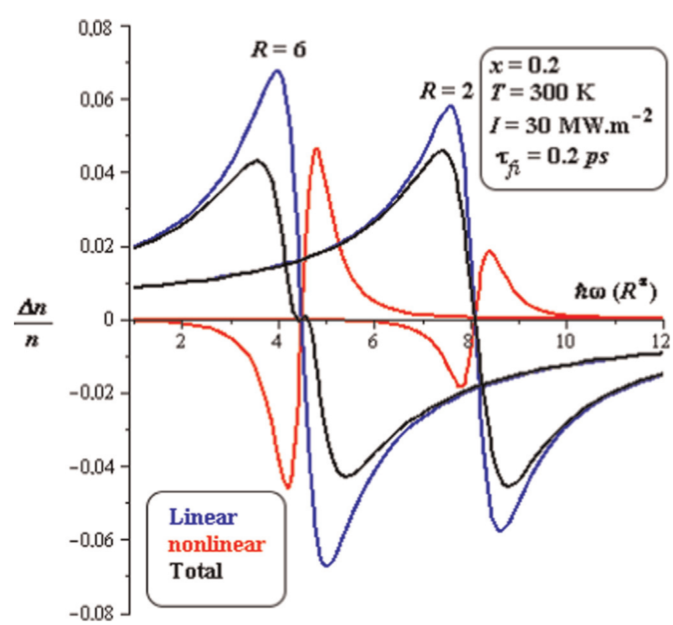

Fig. 1. Linear, nonlinear and total RI changes related to intra-conduction subband 1s–1p transition in (In,Ga)N–GaN SQD with the impurity as a function of the incident pump energy for two different values of the spherical dot radius.