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Tailoring the terahertz absorption in the quantum wells

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ABSTRACT

In this paper the optical properties of an inverse parabolic quantum well mixed with a square quantum well has been investigated. The Schrödinger equation has been solved using the numerical method and all the eigen-energies and wave functions are obtained. Furthermore, using the density matrix approach and perturbation method, the absorption coefficients and refractive index changes have been calculated and analyzed. The results show that for appropriate values of quantum well parameters the absorption coefficient peak lies in the terahertz frequency range. Also, the stability of the absorption peak due to small random defects in quantum well is investigated.

1. Introduction

In the last few years the great attention has been devoted to the quantum structures and their properties [1–5]. By progress in the high technological nanomaterial fabrication methods like Molecular Beam epitaxy (MBE), laser ablation, sputtering systems, etching techniques and so on, the selective synthesis of a quantum device is possible [6–8]. By manipulation of the semiconductor details the optical properties can be engineered and adjusted for desired applications. Among all the quantum structures, quantum dots and wells, and the investigation of their optical properties have been subject of many academic works recently [5,9–25]. The energy differences between the electronic bands in the usual quantum dots or wires are in the range of a few tenth of an electron volt that make them suitable for sensors application in the infrared frequency region [5,11,13,14]. It is well known that the potential details of the quantum structures, especially the shape of the quantum well plays an important role in the optical properties [5,11,15–19]. One of the reasonable models for the quantum dots or wells is the parabolic quantum well that was interesting for many groups in the resent years [11,13,20–25]. In the other hand, the terahertz (THz) frequency range due to the many different applications and also the lack of suitable high-performance chips has been intensively investigated in recent years [26–29]. The usual solid state devices (quantum dot, thin film sensors . . .) because of its energy gap that are in the range of infrared or higher frequencies could not operate in the terahertz region [13,14,30]. In this paper a quantum well is proposed so that its absorption peak lies in the THz range of frequency. The key idea here is to select a potential with appropriate symmetry, so that the pseudo degenerate states could be formed. As it is discussed in the context the lower part of an inverse parabolic potential (Fig. 1) is appropriate to meet this purpose. Also, the optical properties of this proposed potential are numerically calculated and investigate. As it is discussed latter, these kind of the quantum wells are very sensitive to any disordered in the potential, therefore the stability of the THz absorption is also investigated.

2. Theoretical model and numerical calculations

A quantum well inside the electric field is described by following equation of motion [31].

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}\left[\frac{p^2}{2m^*} + V(x) - qxE, \rho\right] - \frac{1}{2}(\Gamma\rho + \rho\Gamma), \tag{1}$$

where ρ is the density operator, p is the momentum operator, m^* is the electron effective mass, $V(x)$ is the potential as a function of the position operator (x), q is the electric charge, E is the electric field where its time dependency is considered as the exponential of ($i\omega t$) and Γ is the loss operator where the matrix elements are the relaxation rates of transition between two different states.

By enhancing the perturbation expansion of the density matrix, the following recurrence relation could be obtained [31]:

$$\rho = \sum_{n=1}^{\infty}\rho^{(n)} \Rightarrow \left(\frac{\partial \rho^{(n+1)}}{\partial t}\right) = \frac{1}{i\hbar}\left(\left[H_0, \rho^{(n+1)}\right] + \left[-qxE, \rho^{(n)}\right]\right) - \frac{1}{2}\left(\Gamma\rho^{(n+1)} + \rho^{(n+1)}\Gamma\right). \tag{2}$$

Using Eqs. (1) and (2), the matrix elements of the density operator in the first order of perturbation can be expressed as below:

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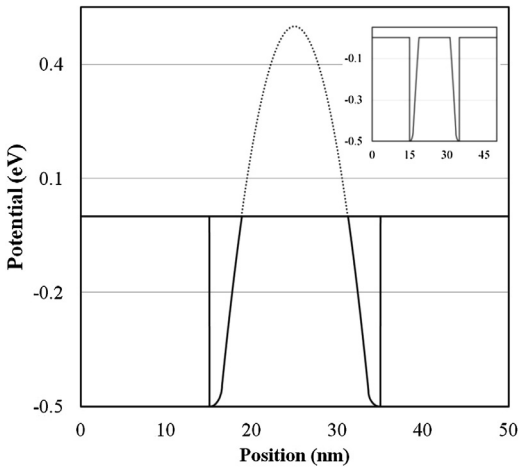

Fig. 1. Schematic diagram of the proposed quantum well. The solid line is the potential and dotted line is plotted for comparison with parabolic potential. The inset is also the real potential well.

$$\rho_{ij}^{(1)}(\omega)=\frac{\langle\psi_i|\,qEx\,|\psi_j\rangle}{\hbar\omega-E_{ij}+i\hbar\Gamma_{ij}}\left(\rho_{jj}^{(0)}-\rho_{ii}^{(0)}\right), \tag{3}$$

in which, the ij indices of the operators ρ and Γ are the ith row and jth column of the corresponding matrices, ψ_i is the ith quantum level wave function and $E_{ij}=E_j-E_i$. This iteration process can be continued straightforwardly to calculate the higher order density matrix elements that are dependent on the higher powers of external field intensity. Because the field intensity for the case of the sensors is weak enough, here the optical properties are calculated in the first order of perturbation. Using Eq. (3) and definition of the electric susceptibility this quantity is easily obtained as:

$$\chi^{(1)}(\omega)=\frac{q}{\varepsilon_0 V}\frac{\left|\langle\psi_i|\,x|\,\psi_j\rangle\right|^2}{\hbar\omega-E_{ij}+\hbar\Gamma_{ij}}. \tag{4}$$

By using the above equation and the following relations for optical properties in term of the electric susceptibility, expressions for the absorption and refractive index of quantum system could be calculated as:

$$\frac{\Delta n(\omega)}{n}=Re\left(\frac{\chi}{2n}\right),\quad \alpha(\omega)=\omega\sqrt{\frac{\mu}{\varepsilon_R}}Im(\varepsilon_0\chi)\Rightarrow$$

$$\frac{\Delta n^{(1)}(\omega)}{n}=\frac{1}{2n\varepsilon_0}\frac{\left|\langle\psi_1|\,x|\,\psi_2\rangle\right|^2\sigma(\hbar\omega-E_{12})}{(\hbar\omega-E_{12})^2+(\Gamma_{12})^2}, \tag{5}$$

$$\alpha^{(1)}(\omega)=\omega\sqrt{\frac{\mu}{\varepsilon_R}}\frac{\left|\langle\psi_1|\,x|\,\psi_2\rangle\right|^2\sigma\hbar\Gamma_{12}}{(\hbar\omega-E_{12})^2+(\Gamma_{12})^2},\quad \sigma=\frac{q}{V}.$$

In Eq. (5) it is supposed that the electron transition between ground state and the first exited state is the dominant transition and the other transitions is ignored.

The Schrödinger equation is solved using the Finite Difference Method (FDM) and all of the required allowed energies and the corresponding wave functions are derived.

The random potential is considered similar to the real situations so it is not just a white noise. This potential is produced using random algorithms so that the correlation length of randomness is approximately 5 nm. The diagrams of the random potential are represented in the paper. After calculation of the wave functions and the eigenenergies, the optical properties of the sample are obtained and analyses.

3. Results and discussion

The diagram of the quantum well potential has been illustrated as Fig. 1. As it is shown, the potential is an inverse parabola that cut the x axis, and the upper section is eliminated. Furthermore for more coincident with real state the lowest part of the potential is smoothed. Such a configuration could be artificially fabricated by epitaxial growth of some semiconductor into another host material [32]. The values of the physical parameters are typically chosen as follow: The minimum of potential is selected as -0.5 eV, also the optical absorption and the refractive indices are calculated for different well widths between 12 nm and 25 nm. The other parameters are chosen as: the relaxation time 5 ps, the relative refractive index 4, the electron effective mass 0.06 of electron mass, relative permittivity 13 and the particle density 10^{20} electron per cubic centimeters. It should be noted that this parameters do not change the operating frequency of the absorber, but they could change the maximum absorption or the absorption shape, the frequency of peaks that are determine the operating region is only depend on the eigenenergies and therefore the quantum well shape.

The absorption coefficient versus frequency of the incident photon for different well widths is plotted in Fig. 2. This figure represents the absorption for the large and small well size, respectively. This figure shows that by increasing the quantum well size, the absorption peaks shift to the lower frequencies which are desired for THz applications. In Fig. 2a, the absorption spectrum for quantum wells with sizes more than 20 nm are presented. The operating frequency range for such quantum well sensors is less than 4 THz. Fig. 2b, represents the same spectrum for the smaller size quantum wells, it is clear that the absorption peaks are shifted to the large frequencies remarkably.

The peak frequencies versus size of the system are drawn in Fig. 3a, also in the inset, the quantum well with frequency peaks lower than 10 THz is depicted. The increasing trend of the operating frequencies by decreasing the size of the quantum well is clear.

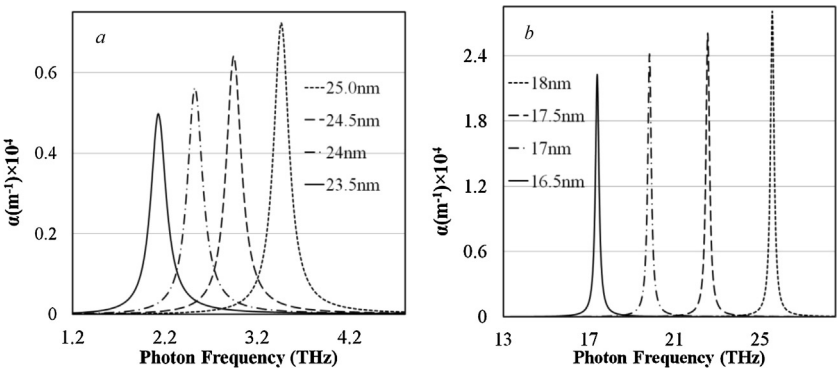

Fig. 2. Absorption coefficient spectrum for (a) larger size and (b) smaller size of quantum well.