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Polaron effect on absorption coefficient in $Al_xGa_{1-x}As$/ GaAs modulation doped single quantum well

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Abstract. The barriers of a single quantum well fabricated using $Al_{0.3}Ga_{0.7}As$/GaAs heterojunctions is doped by donors which get ionized at finite temperature. The ionized electrons flow into the well region which enhance the carrier density in the well. The strong electron-electron interaction gives rise to Hartree and exchange-correlation potential due to many-body effects. The effective mass equation including confining potential, the Hartree potential and the exchange-correlation potential are solved iteratively using the Fourier series method for different dopant densities. The energies and envelope functions are perturbed by the electron-phonon interaction in the Frohlich form. The calculated dipole matrix elements and the relaxation rates are used to calculate absorption coefficients. The absorption coefficients are enhanced by the increased dipole matrix elements due to electron-phonon interaction. The absorption coefficients are also enhanced when the strength of doping is increased.

Keywords: Quantum well, electron-phonon interaction

1. Introduction

In a non-degenerate QW the electronic structure of the subbands are described by in the single particle formalism where the electron energy subbands and corresponding envelope functions are completely decided by Al composition, well width and barrier height [1].In a modulation doped single QW the barriers are doped by donors. At a finite temperature the donors get ionized and then the ionized electrons flow from the barrier regions into the well in bringing the system to equilibrium. As a result of the higher electron density in the well, the system becomes degenerate. The Coulomb interaction between electrons become significant needing a complete many-body approach to address the situation. Density functional theory (DFT) is a popular method for solving the many-body problem [1].

In this method the ground state energy of the interacting electrons is described

by the charge density of the non-interacting electrons. The many-body effects are taken in the exchange-correlation potential treated in the local density approximation (LDA). The single particle subband energies and envelope functions are calculated using the self-consistent Kohn-Sham equation [2]. Different numerical methods have been applied to solve the self-consistent Kohn-Sham equation in a modulation doped QW. The linear and nonlinear optical absorptions considering the weak-coupling electron-LO phonon interaction in asymmetric semi parabolic QWs are theoretically investigated in [3] they found that the theoretical values of the optical absorptions are more than a factor of 2-3 higher than the one in the structure without considering the electron-LO-phonon interaction by calculating.

In this work the Fourier series method is used to solve the Kohn-Sham equation. The Fourier series method has been employed to solve effective mass equation for single QWs with different confining potentials [4]. We have used the same method for solving the Hartree equation.

2. Method of Calculation

The electronic states in a modulation doped single QW fabricated using $Al_{0.3}Ga_{0.7}As/GaAs$ heterojunctions is studied by the Fourier series method. Since the carrier density becomes high in the QW, both Hartree and exchange-correlation potentials become significant in the QW due to enhanced electron-electron interaction. The effective mass equation for the modulation doped single QW is written in the DFT with LDA as [2]

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z}+V(z)+V_H(z)+V_{xc}(z)\right]\Psi_n(z)=E_n\Psi_n(z) \tag{1}$$

where E_n and $\Psi_n(z)$ are the *nth* energy level and the corresponding envelope function, respectively. Here V(z) is the confining potential,$V_H(z)$is the Hartree potential and$V_{xc}(z)$ is the exchange-correlation potential

The Hartree potential is obtained from the Poisson's equation as

$$\frac{d}{dz}\left[\epsilon_b(z)\frac{d}{dz}V_H[n(z)]\right]=4\pi e^2[N_D^+(z)-n(z)] \tag{2}$$

where $N_D^+(z)$and $n(z)$ are dopant density and carrier density, respectively. $\in_b$ is the bulk dielectric constant.

The exchange-correlation potential in the LDA is written as [5]

$$V_{xc}(z) = -\frac{e^2}{8\pi\epsilon_0\epsilon_b(z)a_0(z)}\left\{1+\frac{0.7734r_s(z)}{21}ln\left[1+\frac{21}{r_s(z)}\right]\right\}\left[\frac{2}{\pi\alpha r_s(z)}\right] \quad (3)$$

where

$\alpha = (4/9\pi)^{1/3}, a_0(z) = 4\,\pi\epsilon_0\epsilon_b(z)\hbar^2/m^*(z)e^2 \;\; and \;\; r_s(z) = \{4\pi a_0^3(z)n(z)/3\}^{-1/3}\, n(z)$ is the 2D carrier density.

An expression for the absorption coefficient is obtained from the density matrix formalism as[6]

$$\alpha(\omega, I) = \frac{\omega}{n_r c\epsilon_0}\sigma_{21}|M_{21}|^2\frac{\hbar\Gamma_{21}}{E_{21}^2+\hbar^2\Gamma_{21}^2}\left[1-\omega\frac{4|M_{21}|^2 I}{(E_{21}-\hbar\omega)^2+\hbar^2\Gamma_{21}^2}\right] \quad (4)$$

where$E_{21} = E_2 - E_1$ I is the optical intensity ,$\hbar\Gamma_{21}$ is the line shape. $\sigma_{21}$is 2D density of states[6]. The dephasing rate using eq.(25) and eq.(26) of ref.[4]we obtained as

$$\Gamma_i(k_t) = \frac{m^*(0)\omega_{LO}e^2}{\hbar}\left(\frac{1}{\in_\infty}-\frac{1}{\in_0}\right)\sum_{j\neq i}^{2}\int_0^\infty dq_z\,|G_{ji}(q_z)|^2$$

$$\left[\frac{n_B(\hbar\omega_{LO})}{\sqrt{q^4{}_z+2q^2{}_z(2k^2{}_t-\Delta_{ij}^-)+(\Delta_{ij}^-)^2}}+\frac{n_B(\hbar\omega_{LO})+1}{\sqrt{q^4{}_z+2q^2{}_z(2k^2{}_t-\Delta_{ij}^+)+(\Delta_{ij}^+)^2}}\right]$$

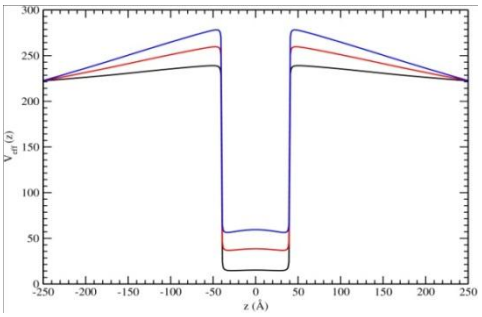

Figure1(Confining potential of modulation)

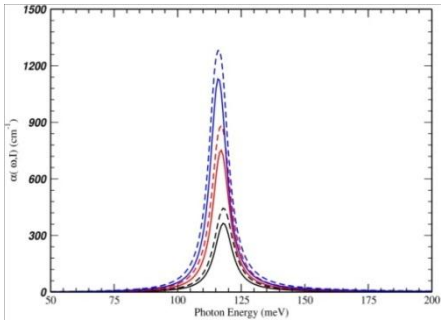

Figure.2.(Absorption Coefficients) (Doped AlGaAS/GaAS QW)

3. Results and Discussions

The barrier height is given as$V_0(x) = 0.6(1.155x + 0.37x^2)$meV, where the factor 0.6 is due to band offset. With Al composition *x*=0.3, we find$V_0(x)$*=278* meV. The effective mass is taken as $m^*(x) = (0.0632 + 0.856x + 0.0231x^2)m_0$, where m_0 is the electron rest mass. The bulk dielectric

constant is taken as$\epsilon_b(x) = 10.89 - 0.73x$The temperature *T=100* K. We have solved Eqs.(l) and (3) iteratively to achieve convergence of 0.1 meV, The effective potential including confining, Hartree and exchange-correlation potentials for different donor concentrations are shown in Figure 1. For dopant densities $1\times$,$2\times$ and 3×10^{17}cm^{-3}, the ground state energy levels are found as 55.9, 78.7 and 98.9 meV, respectively, whereas, the first excited energy levels have been foundas 173.9, 195.6 and 214.9 meV, respectively i.e. On increasing doping concentration, the ground state energy level and first excited energy level increase. However, for these dopant densities, the energy separation between first excited energy levels and ground state energy levels decreases as 117.9, and 116.9 and 115.9 meV, respectively.

The absorption coefficient curves are represented in Fig.2.The dipole matrix element for different dopant densities $1\times$,$2\times$ and 3×10^{17}cm^{-3}arefound as -21.9×, -21.7× and -42.5× 10^{-8} cm, respectively. Thus the dipole matrix element increases with increasing dopant densities. Absorption coefficients are enhanced by the increased dipole matrix elements due to electron-phonon interaction. Since the Fermi energy increases with doping, the absorption coefficients are enhanced with increasing in doping. The dephasing rates for different above dopant densities are found to be 3.6, 3.2 and 3.1meV, respectively.

4. Conclusion

Using DFT the energy levels and corresponding envelope function are solved in modulation doped $Al_{0.3}Ga._{0.7}As/GaAs$ single QW. The energy levels are found to increase with increasing doping concentration. The dipole matrix elements and absorption coefficients calculated. Absorption coefficients are enhanced by the increased dipole matrix elements due to electron-phonon interaction. The confining potential Hartee potential and exchange–correlation potential are solved iteratively.

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