Intersubband dipole electron transitions involving donor resonant states in quantum wells

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***Abstract*—The intersubband dipole electron transitions involving resonant states of shallow donors in a AlGaAs/GaAs quantum well heterostructure have been considered theoretically. We used the donor electron wave function expansion in terms of the electron wave function inside a quantum well without a donor to calculate the energies, lifetimes and probability of transitions for resonant states belonging to the second subband.**

Index Terms— quantum well, resonant state, intersubband transitions.

I. Introduction

The resonance states of shallow impurities in semiconductors are a very promising object from the point of view of laser generation in the far infrared region. Stimulated light emission has been observed for hole transitions between the resonant and localized states of shallow acceptors in axially stressed bulk *p*-Ge [1]. It is well known that the properties of the shallow impurity state in a quantum well (QW) are more flexible compared with these in a bulk semiconductor. So far the resonant states of shallow donors in QW systems have not been adequately studied both experimentally and theoretically. The ionization energies and resonant levels width for donor in QW were calculated in works [2,3]. But phonon scattering processes were not heretofore taken into account for electro in resonant state.

In this paper we carried out a theoretical investigation of the properties of the shallow donor resonant states ($2p_0$) in quantum well AlGaAs/GaAs heterostructures. The dependencies of the resonance width on impurity location for the resonant states belonging to the second subband are calculated. Since the resonance states are often detected experimentally by measuring the photocurrent spectrum, we calculated the latter for electron transitions from the ground donor state to the states of the second subband including the resonant states.

II. Model For Calculation the States Of A Shallow Donor

To calculate the shallow donor states localized in a quantum well AlGaAs/GaAs heterostructure we used the method suggested in [4] and developed in [5]. Note that the *z*-projection of the angle momentum L_z (axis *z* is the normal to the QW plane) is the integral of motion. The electron wave function corresponding to $L_z = \hbar m$ in used model is represented in the following form:

$$\Psi^m(\rho,\varphi,z) = \exp(im\varphi) \times \sum_{n,k} \int_0^{2\pi} \frac{\sqrt{2}a_n^m(k)}{\sqrt{k}\pi^{1/4}S^{3/4}} \exp(ik\rho\cos\theta + im\theta)\psi_n(z)d\theta \quad (1)$$

here ρ, φ are the polar coordinates in the QW plane, k is the wave vector value, S is the QW square, $\psi_n(z)$ is the wave function corresponding to the electron state on the bottom of the *n*-th subband, which is derived from the solution of the Schrödinger equation with the Hamiltonian

$$\hat{H}_0 = \hat{\vec{p}}^2 / 2\mu + U(z),$$

where μ is the effective electron mass, U(z) is the quantum well potential due to the Al content and p_z is the *z*-component of the momentum operator. Substituting (1) in the Schrödinger equation with the Hamiltonian

$$\hat{H} = \hat{H}_0 - \frac{e^2}{\kappa\sqrt{\rho^2 + (z - z_{im})^2}},$$

where κ is the dielectric constant, z_{im} is the donor *z*-coordinate and *e* is the electron charge, we found the integral equation for the coefficients $a_n^m(k)$. It is clear that for localized and the resonant shallow donor states the functions $a_n^m(k)$ are small for large k when $1/k << r_B$, where r_B is the Bohr radius of the donor state in the QW plane. So we use finite difference method (with step Δk) and reduce solution of integral equation to the diagonalization of the real symmetrical matrix A^m:

$$A^m_{n,i;n',j} = \left(\varepsilon_n + \frac{\hbar^2 k_i^2}{2\mu}\right)\delta_{n',n}\delta_{i,j} - \Delta k \cdot I^m_{n,n'}(k_i, k_j), \quad (2)$$

$$I^m_{n,n'}(k,k') = \frac{q^2}{2\pi\kappa}\int_0^{2\pi} d\theta \frac{\sqrt{kk'}\cos(m\theta)}{\sqrt{k^2 + k'^2 - 2kk'\cos\theta}} \times \int_{-\infty}^{\infty} dz \cdot \exp\{-|z - z_{im}|\sqrt{k^2 + k'^2 - 2kk'\cos\theta}\}\psi^*_n(z)\psi_{n'}(z)$$

The eigenvalues and eigenvectors of A^m describe the energies and the wave function of both localized and delocalized electron states.

III. Dipole Transitions Of Electrons

The total resonant level width is determined by the departure of an electron from the resonant state due to the

Manuscript received March 16, 2007.

interaction of subbands via the Coulomb potential of the donor (decay width) and due to PO phonon scattering (PO phonon width).

The resonance width dependences on donor location in QW are presented in Fig. 1 (for calculation details see [6]). A comparison of Fig. 1a and 1b shows that the main contribution to the total resonant level width comes from the scattering by PO phonons for not very broad QWs.

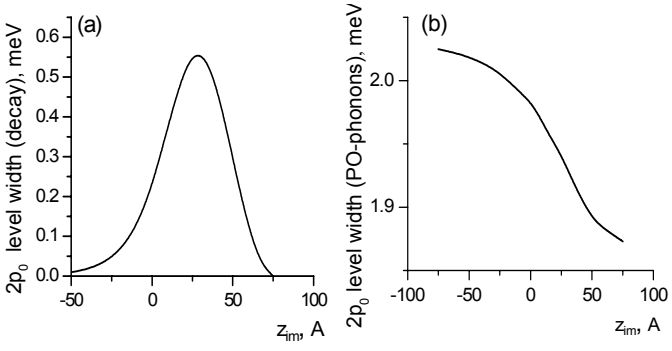

Fig.1 Resonant level ($2p_0$) width in $GaAs/Al_{0.2}Ga_{0.8}As$ QW 150 Å wide determined by decay processes (a) and PO phonon scattering (b) as a function of donor position z_{im} (z_{im}=75 Å corresponds to the QW center, $z_{im}>0$ and $z_{im}<0$ correspond to well and barrier, respectively).

The wave functions of the localized and resonant states are formed mainly by the states of the nearest upper subband. Therefore, the selection rules for the dipole electron transition between the ground donor state and the resonant states are similar to those for the transitions between the first subband and subband which forms resonance state. It means that the electron transitions to the resonant states belonging to the second subband are allowed for *z*- light polarization. Since the wave functions of the donor states contain small parts of other subbands components, the dipole transitions with the *x,y*-polarizations are also allowed, but strongly suppressed. On the contrary, in the case when the initial and the final states belong to the same subband, the transitions for *x,y*-polarizations are allowed and for *z*-polarization are suppressed. Further we discuss *z*- polarized light only.

The expression for the rate of the electron dipole transitions from the ground donor state to the second subband is

$$W(\hbar\omega) = \frac{2\pi}{\hbar} e^2 E^2 \left| z_{if} \right|^2 G(\hbar\omega - \varepsilon_{1s}), \qquad (3)$$

here E is the electric field amplitude of light, $\hbar\omega$ is the photon energy, $z_{i,f}$ is the intersubband matrix element of *z*-operator, and $G(\varepsilon)$ is the density of states, ε_{1s} is the energy of the ground donor state. The dimentionless absorption coefficient spectrum is proportional to $W(\hbar\omega)$:

$$\beta(\hbar\omega) = \frac{2\pi W(\hbar\omega)\hbar\omega N}{cE^2 n}. \qquad (4)$$

Here c is the light velocity, $N=3\cdot10^{10}$ cm^{-2} is the surface impurity concentration, n is the refractive index.

Figure 2 shows the comparison of absorption spectra (4) taking into account and disregarding PO phonon scattering (for the donor position z_{im}=50 Å). The large peak on the spectra is due to the electron transition into the lowest resonant state of the second subband.

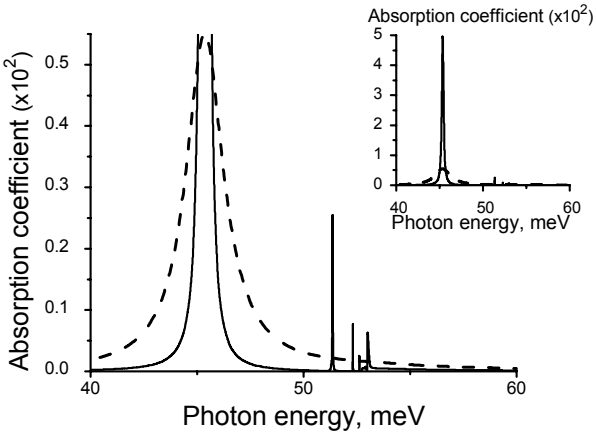

Fig. 2. Absorption coefficient spectrum calculated disregarding scattering (solid curve) and taking into account PO phonon scattering (dashed curve).

Since the density of states determining the peak of the Lorentz line is $G_{max}= 2/\pi\Gamma$ (Γ is a final state width), the absorption peak amplitude is inversely proportional to the width of level to which transition takes place.

It should be noted that the shape of the main peak in Fig. 2. is Lorentzian. This is a consequence of the fact that the intresubband part of z-operator matrix element is equal to zero. Otherwise, the absorption spectrum would have more complicated shape [7].

IV. Conclusion

The absorption linewidth is mainly determined by the interaction of electrons with PO phonons if scattering processes are allowed by energy conservation law.

Acknowledgment

This work was financially supported by the RFBR (Nos 04-02-17178, 07-02-00549 and 05-02-17341) and the Dynasty Foundation (Grant for L.V. Gavrilenko).

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