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Temperature shift of intraband absorption peak in tunnel-coupled QW structure

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ABSTRACT

An experimental study of the intersubband light absorption by the 100-period GaAs/$Al_{0.25}Ga_{0.75}As$ double quantum well heterostructure doped with silicon is reported and interpreted. Small temperature redshift of the 1–3 intersubband absorption peak is detected. Numerical calculations of the absorption coefficient including self-consistent Hartree calculations of the bottom of the conduction band show good agreement with the observed phenomena. The temperature dependence of energy gap of the material and the depolarization shift should be accounted for to explain the shift.

1. Introduction

Electron transitions between size-quantized subbands of the conduction band of semiconductor nanostructures provide one of the most popular bases for the optical devices such as photodetectors, modulators and lasers in infrared and terahertz spectral ranges. Starting almost 30 years ago from the first quantum well infrared photodetectors [1] and later with quantum cascade laser [2] the intersubband optics in quantum wells is still an intensively developing area with many existing and perspective applications [3,4]. One of the main challenges for the effective implementation of quantum well structures as a basis for optoelectronic devices is to control the band structure and subband positions to a high extent. Practically independent control of electron level positions in each of tunnel-coupled quantum wells provides the possibility to set exact values of intersubband transition energies in such structures. A number of unique properties of these structures related to the effect of electron redistribution between subbands under various external factors [5] can boost the performance of the devices based on them.

Here we report and interpret an experimental study of the intersubband light absorption in the 100-period GaAs/AlGaAs heterostructure, namely the temperature shift of the absorption peak. We perform Hartree self-consistent calculations of the energy structure of the double quantum wells and reproduce numerically the observed phenomenon with a good agreement to the experimental data. We outline the set of factors that should be accounted for in order to describe the shift numerically with a proper precision. Also we estimate the intersubband electron lifetimes and discuss the results.

2. The object

The object under study is the MBE-grown multiple double quantum well GaAs/$Al_{0.25}Ga_{0.75}As$ structure doped with a shallow donor impurity (silicon). It is grown on the semi-insulating GaAs substrate with silicon-doped cap and buffer layers. The period consists of two GaAs wells of different widths (66 Å and 45 Å) with an $Al_{0.25}Ga_{0.75}As$ 30 Å - wide barrier between them. The wider well contains an intensively doped with silicon layer in the middle (layer width is 25 Å, impurity concentration $N = 1.6 \times 10^{18}$ cm^{-8} that corresponds to the sheet concentration $N_{2D} = 4 \times 10^{11}$ cm^{-2}). The double quantum wells periods are separated from each other as well as from the cap and buffer layers by the $Al_{0.25}Ga_{0.75}As$ barriers

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wide enough to neglect quantum coupling effects. The configuration of the experiment (described in more details in Ref. [6]) implies four-pass geometry so the light crosses 400 double QW periods on its way. Only the absorption of light polarized in plane of QW has been taken into account (with a part of absorption equal to the one of the light polarized in the direction of structure growth being subtracted) to allow for only the absorption of the 2-dimensional electron gas inside the wells.

3. Theoretical framework

The electron bound state positions and wave functions were found within the Hartree self-consistent calculations framework, which leads to the iterative process involving consecutive numerical solving of Schrödinger, Poisson and electroneutrality equations.

The Schrödinger problem in case of quantum well structures has one dimension, namely the direction of the structure growth (here z coordinate) perpendicular to the quantum well containing (quasi) 2-dimensional electron gas. Here we allowed for conduction band only that is good enough approach for a shallow donor-doped GaAs/AlGaAs heterostructures. So the Schrödinger equation in our case takes form

$$\left(\frac{-\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + V(z) + V_H(z)\right)\varphi(z) = E\varphi(z),$$

where $V(z)$ is a quantum well potential including conduction band energy positions for the materials of the structure with a discontinuities at the edges of the well, $V_H(z)$ is a Harteree potential formed by the ionized donor centers and electrons bound to the size-quantized subbands in the quantum well, $\hbar$ is the Planck's constant, m^* is an effective electron mass. The results of the solution of the equation above are bound energy levels E_j and corresponding bound wave functions $\varphi_j(z)$, j denotes a number of a bound subband.

The electroneutrality equation:

$$\sum_j n_j = n_I$$

Here n_I is the sheet concentration of the ionized donor centers. In our case it was taken equal to the total donor sheet concentration N_{2D} assuming full impurity ionization (grounded in the next section), n_j is a sheet concentration of electrons in j-th subband according to Fermi statistics:

$$n_j = \frac{m^* k_B T}{\pi\hbar^2}\ln\left(1 + \exp\left(\frac{E_F - E_j}{k_B T}\right)\right)$$

where E_F is a Fermi energy, k_B is a Boltzmann constant, T is a temperature.

The result of the solution of this equation is the Fermi energy.

And the Poisson equation:

$$\frac{\partial^2 V_H(z)}{\partial z^2} = \frac{e}{\varepsilon\varepsilon_0}\left[N_D^+(z) - N(z)\right],$$

where $N_D^+(z)$ is a concentration of ionized impurity centers, ε is a dielectric constant of the material and ε_0 is a vacuum permittivity, e is the unit charge. $N(z)$ is the negative charge density:

$$N(z) = \sum_j n_j|\varphi_j(z)|^2,$$

The result of solution of Poisson equation is $V_H(z)$.

The self-consistent procedure starts by solving Schrödinger equation with $V_H(z) = 0$. Then obtained energy levels are used in the solution of the electroneutrality equation and the resulted Fermi energy together with wave functions of the subbands are used to obtain Hartree potential from the Poisson equation. The above repeats iteratively until the key values from the two last iterations converge with good precision.

Numerically the method was implemented following the nonuniform mesh discretization method described in Ref. [7] within parabolic and effective mass approach.

The temperature-dependent bandgap of GaAs was calculated as (formula 2.13 in Ref. [8]) : $E_{g,GaAs}(T) = E_{g,GaAs}(T=0) - \frac{\alpha T^2}{T+\beta}$, with $E_{g,GaAs}(T=0) = 1517$ meV, $\alpha = 0.55$ meV/K, $\beta = 225$ K [9]. The bandgap of the $Al_{0.25}Ga_{0.75}As$ was assumed to be proportional to the bandgap of GaAs as $E_{g,AlGaAs}(T) = E_{g,GaAs}(T)\frac{E_{g,AlGaAs}(T=300)}{E_{g,GaAs}(T=300)}$ with $E_{g,AlGaAs}(T=300) = 1.424 + 1.247x = 1.736$ eV ($x = 0.25$ is Al content). The band offset ratio was considered constant $\Delta E_c/\Delta E_v = 62\%/38\%$ [10]. The electron effective masses and relative permittivity in wells and barriers are: $m_w^* = 0.67m_0$, $m_b^* = (0.67 + 0.083x)m_0$, $\varepsilon_w = 13.1$, $\varepsilon_b = 13.1 - 3x$.

The absorption coefficient $\alpha_{2D,\,ij}(\omega)$ provided by the transitions from i-th to j-th subbands was calculated from Fermi golden rule with Dirac delta function replaced by the Lorenzian spectral line broadening as [11,12]:

$$\alpha_{2D,ij}(\omega) = \frac{\omega\mu_0 c}{\chi}|M_{ji}|^2\frac{\sigma_{2D,ij}\Gamma_{ji}}{\left(E_{ji} - \hbar\omega\right)^2 + \Gamma_{ji}^2} \quad (1)$$

where ω is the angular frequency of the photon, μ_0 is the vacuum permeability, χ is the refractive index of the material, $E_{ji} = E_j$-E_i is the energy difference between i-th and j-th subbands, $\Gamma_{ji} = \hbar/\tau_{ji}$ is the broadening of the absorption peak, where τ_{ij} is the intersubband nonradiative relaxation time. $\sigma_{2D,ij}$ is the electron sheet concentration difference between i-th and j-th subbands,

$$\sigma_{2D,ij} = \frac{m^* k_B T}{\pi\hbar^2}\ln\left\{\frac{1 + e^{(E_F - E_i)/k_B T}}{1 + e^{(E_F - E_j)/k_B T}}\right\},$$

The dipole matrix element

$$M_{ji} = \int \varphi_j^*(z)|e|z\varphi_i(z)\mathrm{d}z.$$

As soon as the concentration of carriers is high enough we took into account the depolarization shift, which is a many body effect. The energies of each transition are recalculated according to [13]:

$$\tilde{E}_{ji}^2 = E_{ji}^2 \times (1 + \kappa_{ij}),$$

where $\tilde{E}_{ji}$ is the actual value of transition energy,

$$\kappa_{ij} = \frac{2e^2\sigma_{2D,ij}}{\varepsilon\varepsilon_0 E_{ji}}S,$$

where

$$S = \int_{-\infty}^{\infty} dz\left[\int_{-\infty}^{z} dz'\varphi_j\left(z'\right)\varphi_i\left(z'\right)\right]^2.$$