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Peak position of the intersubband absorption spectrum of quantum wells with controlled electron concentrations

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We investigated the influence of electron concentration N_s on the peak position energy of intersubband absorption spectra in single modulation doped GaAs-$\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ quantum well structures of different thicknesses and doping profiles. We found experimentally very small shifts of peak position as a function of N_s. Also the sign of the energy shift is dependent on the well thickness. Findings were well explained by a compensation between depolarization shift and shift due to static Coulomb interaction of the electrons. The effect of the well width and the doping profile on the peak shift were also discussed.

Intersubband transitions (ISBT) in semiconductor quantum well (QW) structures have been successfully applied to novel infrared devices such as quantum well infrared photodetectors[1,2] and quantum cascade lasers.[3] The large oscillator strength of the transition and the controllability of the resonance by structural parameters of the QW, such as its width and its barrier height, facilitate the engineering of various functional possibilities of ISBT.

The dependence of the resonance energy on the electron concentration N_s is a key issue in ISBT. The electron-electron interaction affects the resonance energy in two ways. First, the energy difference E_{10} between the ground subband and the excited subband is shifted by the static Coulomb interaction of the electrons. Second, the resonance energy is shifted from E_{10} by the dynamical screening of the electrons. This effect is called the depolarization shift.

When electrons populate only the ground subband, the peak position energy E_p of the ISBT absorption spectrum is written as[4,5]

$$E_p=\sqrt{E_{10}^2+2E_{10}(\alpha-\beta)N_s}\simeq E_{10}+(\alpha-\beta)N_s, \qquad (1)$$

where αN_s in the second term of the right-hand side represents the depolarization shift and $-\beta N_s$ is the vertex correction. Although the explicit N_s dependence is only in the second term, the first term E_{10} and also the coefficient of N_s in the second term depend on N_s. E_{10} is conceptually written as $E_0+E_H+E_{XC}$. E_0 is the energy difference between the ground subband and the excited subband determined only by the structure parameters, E_H is the modification of E_0 by the direct Coulomb interaction of the electrons, and E_{XC} is its exchange-correlation (XC) correction. In the second term of Eq. (1), α (β) originates from the time dependent part of E_H (E_{XC}) under infrared light.[5] The nonparabolicity of the inplane dispersion contributes an additional shift of E_p (Ref. 6) by shifting E_{10} from the subband edge as a function of N_s. The balance of these terms gives the relation between N_s and E_p in real systems both for linear and nonlinear absorption regimes.[7,8] A detailed study of these contributions is of practical importance to design ISBT based devices, especially lasers, with high precision.

Previously, Pinczuk *et al.*[9] studied N_s dependence of the far-infrared intersubband excitation energy by measuring Raman scattering in a set of wide QW's with different N_s. Manasreh *et al.*[10] studied the relation between the peak position E_p of intersubband absorption spectrum and N_s using a set of samples with different doping concentration. Ernst *et al.*[11] employed Raman scattering in a wide wide QW's while controlling N_s by applying static pressure. Also far-infrared[7] and midinfrared[8] nonlinear intersubband absorption spectrum were studied in which depolarization effect is modulated by populating the excited states by intense infrared light while total N_s was kept constant.

In this work, we report an experimental investigation of the relation between N_s and E_p of the linear intersubband absorption spectrum in several single modulation doped QW's with different thicknesses and doping profiles. The N_s was controlled by gate voltage V_g to study the N_s dependence with a same sample, which is different from the previous studies.[9,10]

Six samples were grown by molecular beam epitaxy on (100) GaAs semi-insulating substrates. Each sample contains a single modulation doped GaAs QW cladded by $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ barriers. Three of these samples, B-1, B-2, and B-3, are modulation doped in the surrounding $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ layers. The structure of these samples are, from the top to the bottom, 10-nm-thick GaAs cap layer, 80-nm-thick *n*-type $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ with Si-doping density 5×10^{17} cm^{-3}, 10-nm $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ spacer layer, GaAs QW layer, 25-nm-thick $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ spacer layer, Si-δ doping layer at 10^{12} cm^{-2}, 0.2-μm-thick super lattice buffer with $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$(10 nm)/GaAs(3 nm), and 0.3-μm-thick GaAs buffer layer. Their respective QW thicknesses are 8.9 nm, 6.5 nm, and 4.9 nm. The remaining three samples, S-1, S-2, and S-3, are doped only on the surface side $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ layer. The structure of the samples are, from the top to the bottom, 10-nm-thick GaAs cap layer, 80-nm-thick *n*-type $\mathrm{Al}_{0.4}\mathrm{Ga}_{0.6}\mathrm{As}$ with Si-doping density 5×10^{17} cm^{-3}, 10-nm

TABLE I. Representative parameters of the samples. W is the width of the QW and N_s is the maximum electron concentration. W_{th} is the width used to fit the experimental result by the theory. E_p is the peak position energy of the intersubband spectrum, FWHM is the full width at half maximum of the spectrum, and E_p^{calc} is the calculated peak position energy. These are the values at the highest N_s. μ is the mobility measured at 77 K.

Sample	W (W_{th}) (nm)	N_s (10^{11} cm^{-2})	E_p (E_p^{calc}) (meV)	FWHM (meV)	μ (m^2 V^{-1} s^{-1})
B-1	8.9 (8.4)	11.0	114.4 (114.4)	3.5	3.6
B-2	6.5 (6.2)	13.2	159.7 (159.7)	6.8	2.0
B-3	4.9 (4.6)	9.3	199.1 (199.1)	7.9	1.8
S-1	10.2 (9.8)	6.9	95.6 (95.7)	4.7	9.3
S-2	7.4 (7.2)	7.2	138.6 (138.6)	6.1	4.8
S-3	5.5 (5.4)	5.7	180.2 (180.2)	13.4	3.1

$Al_{0.4}Ga_{0.6}As$ spacer layer, GaAs QW layer, 15-nm-thick $Al_{0.4}Ga_{0.6}As$ barrier layer, 0.2-μm-thick super lattice buffer, and 0.3-μm-thick GaAs buffer layer. Their respective thicknesses are 10.2 nm, 7.4 nm, and 5.5 nm. The representative parameters of these samples are listed in Table I.

The intersubband absorption spectra of these samples were measured in a 45° edges multi-pass waveguide geometry of 3 mm length and 0.3 mm thickness. On top of the devices, a Schottky electrode and Ohmic contacts were formed to control N_s. The samples were cooled at 4 K, and the measurements were performed with a rapid scan Fourier transform infrared spectrometer (FTIR) with a light polarized perpendicularly to the QW layer. The absorption spectrum at a given V_g was obtained as the ratio of the transmission spectrum at V_g to the transmission spectrum at a reference gate voltage V_{ref} at which electrons were completely depleted. We set V_{ref} at about 1.0 V below the threshold voltage V_{th}, which was measured by the in-plane electrical transport.[12]

In Fig. 1(a), the absorption spectra of a double-side doped sample B-1 at different V_g are shown. We observe that the absorption monotonically decreases when V_g is lowered. The electron concentration N_s labeling these spectra has been estimated from the integrated absorption by using an oscillator strength determined by calculation (see below). The value of N_s estimated in this way agreed well with the result of the Hall measurement in the V_g range where electrical transport is not quenched.[12]

Figure 1(b) summarizes the relation between N_s and E_p of sample B-1. When N_s is decreased from 11×10^{11} cm^{-2} to 5.6×10^{11} cm^{-2}, E_p shifts negatively from 114.4 meV by 0.36 meV, which is only 0.3% of E_p. When N_s is further decreased, E_p starts to increase, and then drops for $N_s<1.2\times10^{11}$ cm^{-2}. The full width at half maximum (FWHM) of the spectrum is 3.5 meV in the spectrum at the highest N_s. The FWHM increased from 3.5 meV to 3.6 meV when N_s decreased from 11×10^{11} cm^{-2} to 5.9×10^{11} cm^{-2}, then decreased to 2.1 meV by further decreasing N_s down to 0.8×10^{11} cm^{-2}. In the following, we concentrate on the relation between E_p and N_s.

The smallness of the observed shift in this sample indicates that the various contributions to the shift of E_p compensate each others. To understand the result quantitatively, we made a simulation of E_p. To find the dominant contribution to the peak shift, we employed a method based on the

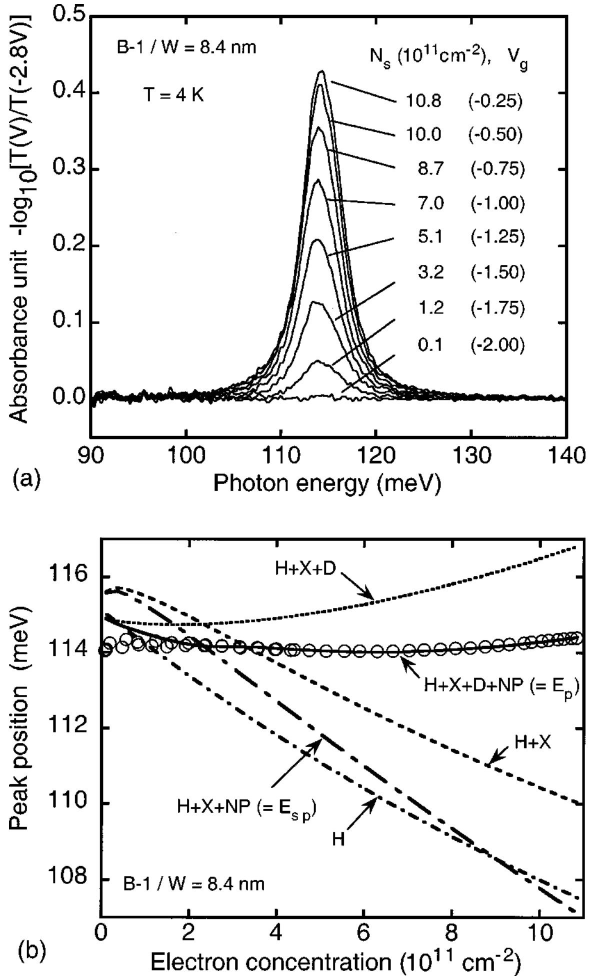

FIG. 1. (a) The intersubband absorption spectra of the sample B-1 at various gate bias voltage V_g. (b) The peak position energies E_p of the spectra shown in (a) are summarized as a function of N_s. N_s is estimated from the integrated absorbance. The curve denoted by (H+X+D+NP) shows the result of the theoretical calculation of E_p including the several contributions, H: Hartree self-consistent calculation; X: with exchange-correlation interaction in local density functional approximation; NP: nonparabolicity of the in-plane dispersion is considered; and D: depolarization effect considered. The different curves show the result of the calculations including the various contributions step by step.

local-density functional approximation (LDA) for exchange-correlation (XC) interaction, which gave a relatively good agreement in the thick (25-nm) GaAs QW between experiment and theory.[13] First, we calculated E_{10} at the bottom of the subbands by a self-consistent calculation including the effect of the conduction band nonparabolicity[14] and including the XC interaction by LDA.[15] Next, the single particle excitation (SPE) spectrum $G_0(\omega)$ was calculated including the effect of the different dispersion of the in-plane motion of both subbands. We neglected the k dependence of the XC energy for simplicity.[16,17] Then following Ref. 6, the absorption spectrum, including the depolarization effect, was calculated from $G_0(\omega)$. The parameters α and β were estimated according to Refs. 4, 5, and 18. The theoretical value of E_p was obtained as the peak position of this absorption spectrum, which was approximated well by Eq. (1) if one replaced E_{10} by the peak position E_{sp} of $\mathrm{Im}\, G_0(\omega)$. Then the theoretical E_p-N_s relation was calculated, using designed sample parameters, except the well width W_{th}, which was slightly (a few tenths of a nanometer) different from the designed value. The solid curve in Fig. 1(b), denoted as (H+X+D+NP), shows the result, where the letters denote, H: Hartree self-consistent calculation; X: with exchange-correlation interaction in local density functional approximation; NP: nonparabolicity of the in-plane dispersion is considered; and D: depolarization effect considered. The agreement with the experiment is good.

The steep peak shift for N_s smaller than 1.2×10^{11} cm^{-2} could not be reproduced by the theory. We consider this is due to the localization of the electrons in the dilute range, thus separate treatment is required.

To illustrate the physical meanings of various components contributing to determine E_p, we examine each of them step by step in the calculation. The curve (H) in Fig. 1(b) shows E_{10} without the XC interaction (Hartree approximation). Since we applied the electric field to control N_s, both the field-induced Stark shift of E_0 and the N_s-induced shift of E_H determine the curve (H). In sample B-1, these contributions cause a shift of 7.5 meV in E_{10}. The curve (H+X) is calculated with the XC interaction. The XC effect increases E_{10} by 2.5 meV at the maximum N_s and is proportional to $N_s^{1/3}$. The curve (H+X+D) in Fig. 1(b) shows E_p when the depolarization shift is added to E_{10} in (H+X) as shown in Eq. (1). The depolarization shift more than compensates the negative shift of the three previous contributions, resulting in a weak concave shape similar to the experiment. These results show that each of these contributions is important to determine the actual energy shift.

An effect of the nonparabolicity is to broaden the SPE spectrum toward lower energy, and therefore to shift the peak position slightly below E_{10} as shown by the curve (H+X+NP). We included this effect in the curve labeled (H+X+D+NP). We see that this effect does not change the result qualitatively.

We discuss next how the shift in absorption spectrum depends on the well thickness W. Figure 2(a) shows the result of the measurements and theoretical calculations for samples B-1 to B-3 and Fig. 2(b) for samples S-1 to S-3. The zeros of the peak shift are defined as the peak position at the maximum N_s of each sample (see Table I). The result shows that qualitative features of the peak shift change as W is decreased. The concave curve for sample B-1 becomes convex in B-3, and the peak energy increases with N_s in S-1 while it decreases in S-3. In intermediate samples B-2 and S-2, the shift is almost zero. We observe also that the shift is larger for samples doped only on the surface side. The theoretical peaks calculated including all the contributions discussed above are shown by plane curves and agree well with the experiment.

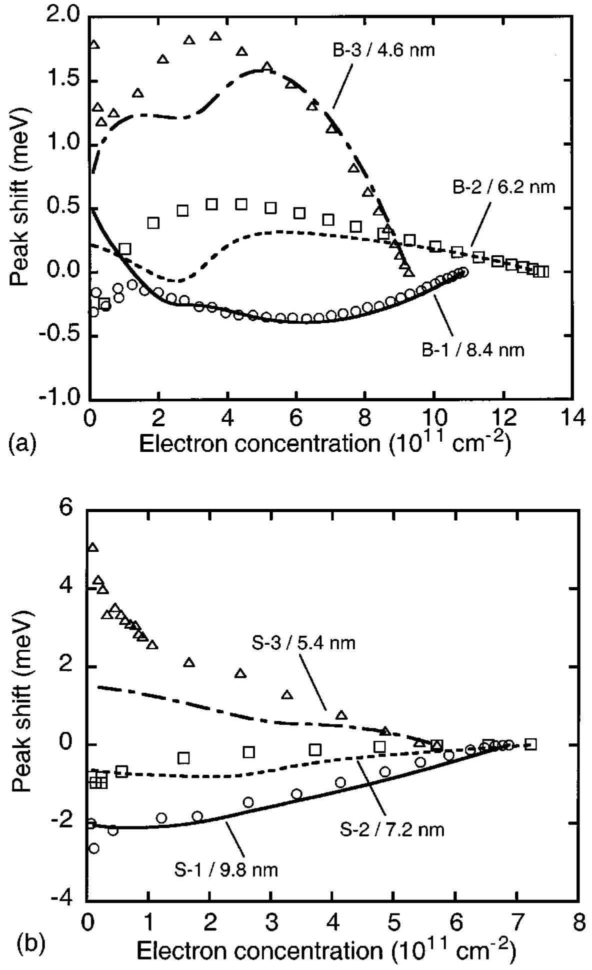

FIG. 2. The peak shift of the intersubband absorption spectra as a function of N_s (a) for the samples for B-1 to B-3, and (b) for the samples S-1 to S-3. The curves are the calculated shift (H+X+D+NP) for each sample. The zeros of the peak shift of both experiment and calculation are the experimental E_p at the maximum N_s for each sample.

When N_s and W are changed, both the shift ΔE_H and $\Delta(\alpha N_s)$ vary approximately proportionally to $\Delta(N_s W)$, because these originate from the electrostatic potential of electrons.[19] Note here that the Stark shift ΔE_0 is roughly proportional to $\Delta(N_s W)^2$, although this effect is smaller in the present case than in the QW without carriers due to the screening of the electric field by electrons. Therefore, the shift of E_p due to these factors is smaller in narrower QW's. The two other contributions, ΔE_{XC} and $\Delta(-\beta N_s)$, are proportional to $\Delta(N_s/W)^{1/3}$ within the local-density functional approximation[15] and are not sensitive to N_s and W. Therefore the shift of E_p is mainly determined by ΔE_0, ΔE_H, and $\Delta(\alpha N_s)$: this explains the very small shift observed in the narrower samples B-2 and S-2. In sample B-3 and S-3, the excited level approaches very close to the top of the barrier. Hence the behavior of E_{10} depends sensitively on the electric field and governs the shift of E_p, resulting in the convex shape as seen in the experiment.

The XC contributions are expected to become important as N_s and W are decreased, from the $(N_s/W)^{1/3}$ dependence. In the wide QW sample B-1, Fig. 1(b) shows that the peak position of the SPE spectrum (the curve H+X+NP) is higher than the peak position of the absorption spectrum for N_s smaller than 2.3×10^{11} cm^{-2}, because $(\alpha-\beta)N_s$ becomes negative in that region.[11,20] In narrow QW's, B-3 and S-3, as the result of the penetration of the excited state wave function into the barrier, XC terms are smaller than expected and are not important for the qualitative behavior of the shift of E_p in $N_s>5\times10^{11}$ cm^{-2} for B-3 and in $N_s>3.5\times10^{11}$ cm^{-2}. However, in lower N_s XC terms appears overestimated (in B-3, S-3, and also B-2). This observation suggests that the exchange-correlation interaction is overestimated in LDA theory, especially in narrow QW's and in the low electron concentration region, which may be resolved by a many-body calculation.[13,21,22] A recent theoretical analysis was done of the interplay of the Coulomb interaction and the subband dispersions using the semiconductor Bloch equation method. It was found that a large difference of the subband dispersions is necessary for the finite contribution of the exchange interaction,[21] which is not the case in the $\mathrm{GaAs/Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ QW system. This finding is consistent with our observation.

The larger shift of S-1 compared to B-1 manifests the effect of the different doping profiles on the shift of $\Delta(E_0+E_H)$, which inverts the sign of ΔE_0 while keeping the ΔE_H approximately the same. In sample S-1, when the electrons are depleted, the potential profile of QW is almost flat[23] and the increase of N_s by gate bias increases E_0, i.e., $\Delta E_0>0$, as expected from the Stark effect, while the negative contribution $\Delta E_H<0$ by the direct Coulomb potential of electrons cancels this shift, resulting in almost no shift of E_{10}. On the other hand, in sample B-1, when the electrons are depleted, there is a large electric field in the direction opposite to the gate field. Therefore, as the gate bias is increased, ΔE_0 is negative $(\Delta E_0<0)$ and the negative shift of E_H doubles the net shift in E_{10}. Hence, the depolarization shift stays uncompensated in S-1, while it is canceled by the shift of E_{10} in B-1.

In conclusion, we studied the shift of the peak position of the intersubband absorption energy when the electron concentration is controlled by a gate voltage. We found that the mutual cancellation of the depolarization shift and the single particle excitation energy shift results in an extremely small shift of energy. The observed shifts were understood and reproduced by a simple theory for various samples with different well widths and the doping profiles.

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