Intraband optical absorption in semiconductor superlattices

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Absorption coefficients are calculated for intraband (intersubband in the conduction band) optical transition in semiconductor superlattices. The absorption line broadening is introduced by taking the fluctuation of well thickness into account. The selection rule is quite different for two kinds of transitions: transitions from the ground state to states below and above the conduction-band offset. The former follows the usual selection rule, whereas the latter does not. The calculated results well explain the experiments for $In_{0.53}Ga_{0.47}As/In_{0.53}Al_{0.47}As$ superlattices.

The conduction band and the valence band of bulk materials are quantized into several smaller subbands by making a superlattice (SL) structure, which consists of alternating layers of two semiconductors. So far, extensive studies have been focused on the optical transition between the subbands created in different bands (interband transition),[1] the wavelength of which corresponds to the absorption edge of the SL. Recently, another optical transition has attracted considerable attention (intraband transition), which occurs between the subbands that are created within the same band (for example, in the conduction band): its wavelength ranges mostly from near to far infrared. This latter transition suggests the possibility of a whole new field of applications and related physics. This follows from the unusual features which the above transition is thought to possess: (1) large absorption coefficient,[2] (2) narrow absorption linewidth,[3] (3) large optical nonlinearity,[4] (4) fast intraband relaxation,[5] and (5) reduced Auger effect.[6] These features could all be readily exploited to enhance the performance of optoelectronic devices such as lasers, detectors, and optical switches. Another advantage of this transition is (6) tunability for wavelengths in the infrared region by adjusting the SL structure. Moreover, if strained-layer SL's were used, this wavelength would be extended to the 1–2-μm region which is more attractive for optical-fiber communication. So far, a number of theoretical studies have reported on the optical absorption due to this intraband transition.[7–9] These reports have mostly considered isolated quantum wells instead of SL's: although Ando and Mori[7] did treat a SL structure, they did not calculate the absorption coefficient. In actual experiments, however, a SL structure must be employed instead of an isolated quantum well in order to enhance the absorption efficiency. Moreover, the above reports have neglected to pursue the origin of the absorption linewidth by treating it as an adjustable parameter.

This Brief Report reports the absorption coefficients due to intraband optical transition in semiconductor SL's. The effect of line broadening is taken into account assuming that it comes from the fluctuation of well thickness. We have compared the calculated results with the experiments reported for $In_{0.53}Ga_{0.47}As/In_{0.53}Al_{0.47}As$ SL's, which is thought to be the most promising material system for the present purpose owing to its large conduction-band offset.

In the effective-mass approximation,[10] the matrix element between the two subband states (ψ_n and ψ_0) in a SL can be expressed as follows:

$$\langle \psi_n | H' | \psi_0 \rangle = \frac{m}{m^*} \langle F_n | H' | F_0 \rangle \tag{1}$$

where index 0 denotes the ground state and H' is the interaction Hamiltonian between a free electron with mass m and a radiation field. Then, F_n and F_0 are the envelope functions, and m^* is the effective mass. Equation (1) indicates that the problem of intraband optical transition is converted to the problem of transition between envelope states with the bulk Bloch state being unchanged. The envelope functions are given by

$$F_n(\mathbf{r}) = \chi_n(\boldsymbol{\rho})\varphi_n(z) . \tag{2a}$$

Here, $\mathbf{r} = (\boldsymbol{\rho}, z)$ is the coordinate of the electron, where $\boldsymbol{\rho}$ and z correspond to the motion parallel and perpendicular, respectively, to the SL plane, and

$$\chi_n(\boldsymbol{\rho}) = (L_x L_y)^{-1/2} e^{i\boldsymbol{\kappa}_n \cdot \boldsymbol{\rho}} , \tag{2b}$$

$$\varphi_n(z) = L_z^{-1/2} e^{iK_{zn}z} \phi_n(z) \tag{2c}$$

are Bloch functions for free space (in the $\boldsymbol{\rho}$ direction) and for SL (in the z direction), respectively: ϕ_n is the periodic part of the SL Bloch function. Here, $\mathbf{K}_n = (\boldsymbol{\kappa}_n, K_{zn})$ is the wave vector. Envelope functions are orthonormalized in a box with volume $L_x L_y L_z$, and can be obtained after a somewhat complicated but straightforward calculation by imposing appropriate boundary conditions.[11]

Let us focus our attention on the transition $0 \to n$ and exclude other possible transitions such as $1 \to n$, etc. Let the occupancy of electrons be $f_0(K_0)$ and $f_n(K_n)$ for these states before irradiation. The transition rate is approximately given by

$$W(\hbar\omega)=\frac{2\pi}{\hbar}\sum_n\sum_{\substack{K_n,\\K_0}}|\langle\psi_n|H'|\psi_0\rangle|^2[f_0(K_0)-f_n(K_n)]$$

$$\times\delta(E_{n0}-\hbar\omega)\ ,\qquad(3)$$

where $E_{n0}=E_n(K_n)-E_0(K_0)$. The matrix element in Eq. (3) requires the conservation of the wave vector during this transition: $K_n=K_0$ $(=K)$. Here, we assume a parabolic band: $E_n(K)=\hbar^2\kappa^2/2m^*+\varepsilon_n(K_z)$, where $\varepsilon_n(K_z)$ is the SL dispersion relation. This assumption makes the δ function in Eq. (3) independent of κ, which allows us to integrate it over κ separately. The absorption coefficient is given by

$$\alpha(\hbar\omega)=\frac{8\pi^2e^2\hbar}{c}\frac{\cos^2\zeta}{n_r(m^*)^2}\frac{1}{L_p^2}\frac{1}{\hbar\omega}$$

$$\times\sum_n N_{n0}(K_z)|\langle\varphi_n|p_z|\varphi_0\rangle|^2$$

$$\times|D_1(\varepsilon_n(K_z))^{-1}-D_1(\varepsilon_0(K_z))^{-1}|^{-1}\ .\qquad(4)$$

Here n_r is the index of refraction, ζ is the angle between the electric vector of light and the normal to the SL plane and was made zero in the following calculations, $L_p=L_w+L_b$ is the period of SL where L_w and L_b are the thickness of well and barrier layers, respectively. Then, $\langle\varphi_n|p_z|\varphi_0\rangle$ is the matrix element of the z component of the momentum and $D_1(\varepsilon)$ is the one-dimensional density of states for SL. $N_{n0}(K_z)$ is given by

$$N_{n0}(K_z)=\frac{D_2}{\beta}\ln\left[\frac{1+e^{\beta[\mu-\varepsilon_0(K_z)]}}{1+e^{\beta[\mu-\varepsilon_n(K_z)]}}\right]\ ,\qquad(5)$$

where $D_2=m^*/2\pi\hbar^2$ is the density of states for a two-dimensional system, μ is the Fermi energy, and $\beta=1/kT$. The meaning of Eq. (5) can be elucidated by making the temperature (T) zero: when the electron concentration is such that μ locates between the two subband states (0 and n), then $N_{n0}(K_z)$ tends to $D_2(\mu-\varepsilon_0(K_z))$ which is the sheet electron concentration in the ground subband state. From this, it is clear that $N_{n0}(K_z)$ can be regarded as the effective sheet concentration of electrons which are involved in this optical transition. The optical transition for a given photon energy $(\hbar\omega)$ occurs at the K_z value which satisfies the relation $\varepsilon_n(K_z)=\varepsilon_0(K_z)+\hbar\omega$. Here, we assume that $\varepsilon_0(K_z)$ is independent of K_z and we write it as ε_0. This is generally true, since the ground state has a very sharp band unless the barrier layer is extremely thin. The above assumption implies that $D_1(\varepsilon_0(K_z))$ is infinite, which simplifies Eq. (4) to some extent. The Fermi energy (μ) for a given electron concentration (N) is determined using the standard expression,

$$N=\int_0^\infty g(E)D_3(E)dE\ ,\qquad(6)$$

where $g(E)$ is the Fermi distribution function and $D_3(E)$ is the three-dimensional density of state for a SL.

Throughout the above calculation, we have not considered any absorption line broadening except for the broadening due to the subband width which is a natural result of using a SL structure. In actual SL's, however, several factors may contribute to this line broadening: (1) carrier lifetime, (2) nonparabolicity of the conduction band, and (3) fluctuation of the thickness of well and barrier layers. Excited electrons are relaxed by scattering mechanisms due to LO phonon, acoustic phonon, intrasubband and intersubband processes, etc. The relaxation time calculated for these scattering processes, however, is of the order of 1 ps:[12] this leads to broadening of the order by only 1 meV. Hence these scattering processes are not sufficient to explain the absorption linewidth of 10–20 meV.[13,14] The nonparabolicity of the conduction band in the direction parallel to the SL plane might have some effects on widening the absorption line when the ground state is densely populated with electrons. This effect requires a complicated calculation when we apply it to a SL structure. Moreover, the nonparabolicity parameter values are not known for the SL materials we are primarily concerned with. For these reasons, we concentrate our attention to the next point. In the following calculations, the L_w thickness fluctuation is assumed as the main cause of the absorption line broadening:[15] the L_b thickness fluctuation seems to have less influence on the linewidth and was therefore neglected. We have assumed that our SL possesses the L_w fluctuation by a monolayer and the probability of finding the monolayer fluctuation (monolayer increase or decrease in L_w) is half that of finding no fluctuation. This discrete probability function can be approximated by the continuous Gaussian distribution function with the standard deviation of 2.3 Å. The actual absorption coefficient was obtained by averaging Eq. (4) over the entire well thickness with the weight of this Gaussian distribution function. Parameter values used are as follows: the conduction-band offset (ΔE_c) is 500 meV, $m^*=(m_w^*L_w+m_b^*L_b)/(L_w+L_b)$ where $m_w^*=0.042m$ and $m_b^*=0.076m$, and $n_r=(n_wL_w+n_bL_b)/(L_w+L_b)$ where $n_w=3.43$ and $n_b=3.10$.[16]

Figure 1(a) shows the absorption coefficient spectrum for an $In_{0.53}Ga_{0.47}As/In_{0.53}Al_{0.47}As$ SL at room temperature with $L_w=50$ Å, $L_b=100$ Å, and $N=1\times10^{18}$ cm^{-3}. The arrow indicates the photon energy (ΔE_c-E_0) which corresponds to the transition to the band offset (ΔE_c) energy state. The SL structure of Fig. 1(a) is the typical one in which the first excited subband state is located below ΔE_c. The absorption bands which neglect the L_w fluctuation are shown by the horizontal bars [at the top of Fig. 1(a)]. The most pronounced effects of the well thickness fluctuation can be seen in the $0\rightarrow1$ transition. Note that the $0\rightarrow1$ transition shows absorption coefficients much larger than the $0\rightarrow2$ and $0\rightarrow3$ transitions (these latter two transitions are to bands above ΔE_c). This reflects the large oscillator strength of the transition to first excited state. Through the calculation for many SL structures of this type, we found that transitions to the state n below ΔE_c follow exactly the selection rule (it is allowed only for odd n): the oscillator strength ratio for forbidden or allowed transitions is usually of the order of 10^{-4}, even if the excited state has a broad band. This is in contrast to the results shown in the following figure [Fig. 1(b)]. Our calculated results agree well with the experiments,[13] the peak height of which has been ad-

justed to the calculated value $(1.4 \times 10^4 \text{ cm}^{-1})$ since its value is not determined experimentally.

Figure 1(b) shows another example of the absorption coefficient spectrum for the same conditions as in Fig. 1(a), except for $L_w = 30$ Å. This structure is the typical one in which the first excited subband state is located above ΔE_c. The solid and dashed lines indicate the results considering and not considering, respectively, the well thickness fluctuation. The sharp absorption edge becomes rounded and the peak height is cut short by considering the fluctuation of well thickness. Figure 1(b) also shows that the transition to the states above ΔE_c does not follow the conventional selection rule described in the preceding paragraph. This is presumably because the excited states above ΔE_c are extended throughout the SL so that it deteriorates the parity of the wave function.

Figure 2 shows (a) resonance energy and (b) linewidth

and maximum absorption coefficient as a function of the well thickness at room temperature for the $0 \rightarrow 1$ transition in an $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{In}_{0.53}\text{Al}_{0.47}\text{As}$ SL with $L_b = 100$ Å and $N = 1 \times 10^{18} \text{ cm}^{-3}$. The experimental results[13,14] for the resonance energy and the linewidth are also plotted in Fig. 2. The arrow (denoted by L_w^c) indi-
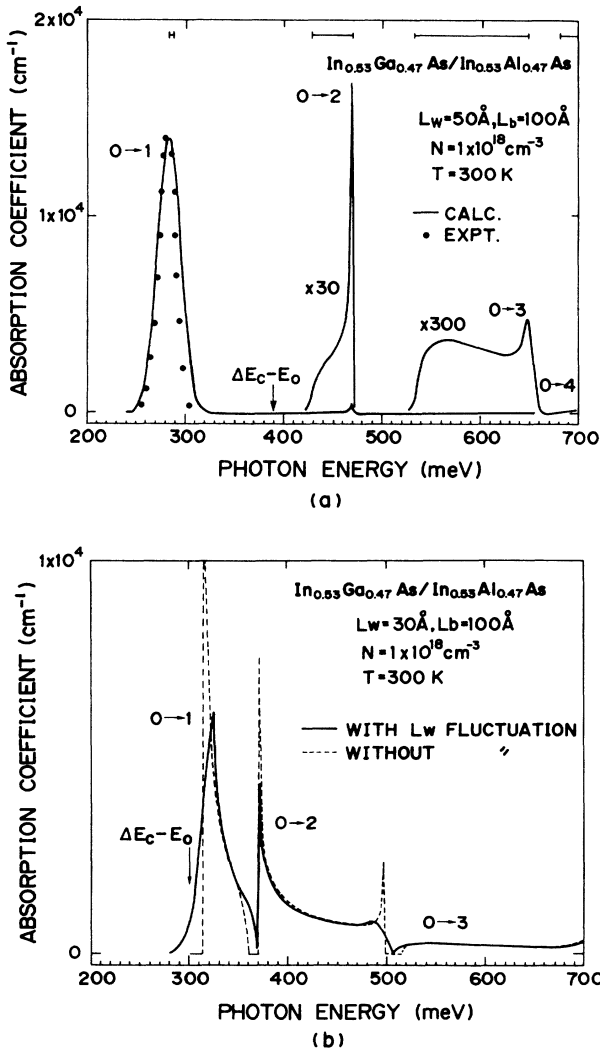

FIG. 1. Absorption coefficient spectra for $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{In}_{0.53}\text{Al}_{0.47}\text{As}$ SL at room temperature with $N = 1 \times 10^{18} \text{ cm}^{-3}$ and (L_w, L_b) of (a) (50 Å, 100 Å) and (b) (30 Å, 100 Å). The bars at the top of (a) indicate the absorption bands which do not consider L_w fluctuation. The experimental results are taken from Ref. 13.
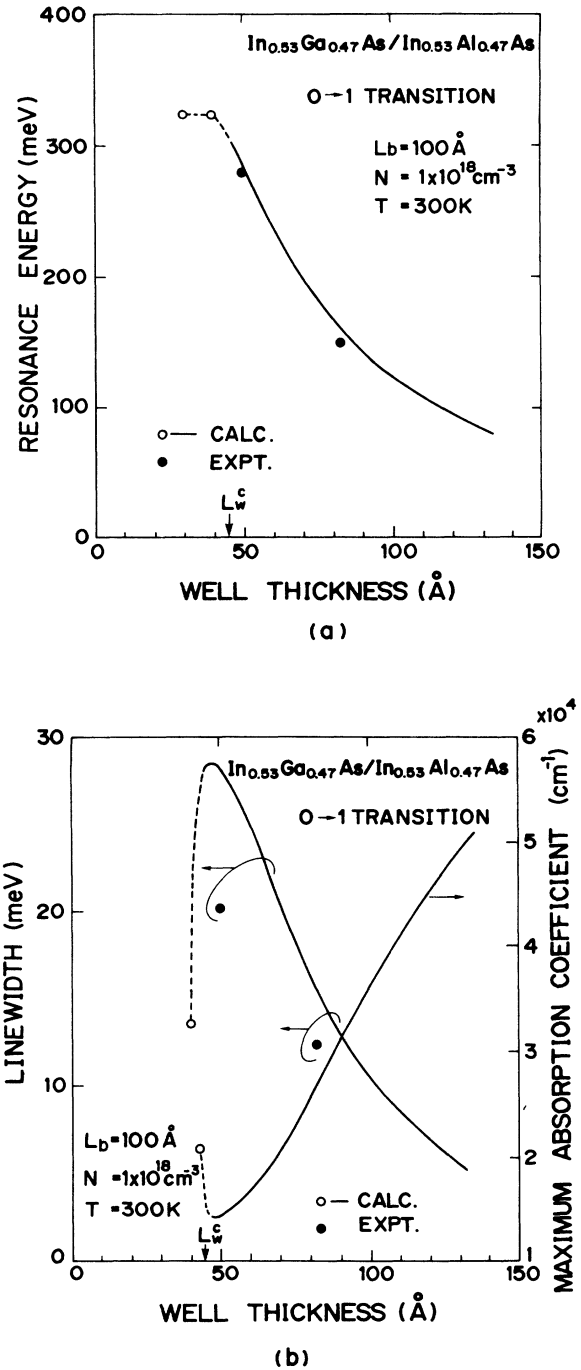
FIG. 2. (a) Resonance energy and (b) linewidth and maximum absorption coefficient as a function of L_w for $0 \rightarrow 1$ transition in $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{In}_{0.53}\text{Al}_{0.47}\text{As}$ SL of $L_b = 100$ Å and $N = 1 \times 10^{18} \text{ cm}^{-3}$. The experimental points are taken from Refs. 13 and 14.

cates the critical well thickness below which the first excited state exceeds ΔE_c. The resonance energy in Fig. 2(a) was obtained from the absorption spectrum which considers both the subband width and the line broadening effects. The calculated results show good agreement with the experiments. The resonance energy for L_w below L_w^c cannot be extrapolated from the values for L_w above L_w^c, because of the large bandwidth of the excited states above ΔE_c. The effect of the well thickness fluctuation on the absorption linewidth can be clearly seen in Fig. 2(b): the linewidth is increased with decreasing well thickness. This tendency is reasonable since small-L_w SL's are more liable than those with a large L_w to be affected by its fluctuation. The experimental points are seen to trace the above theoretical prediction for the linewidth. Below L_w^c, however, this tendency fails. This is because the excited states above ΔE_c cannot be greatly modulated by the well thickness since they are already broad without a fluctuation. In contrast to this, the maximum absorption coefficient decreases with the decrease in L_w, which is closely correlated with the variation of the linewidth.

Figure 3 shows the maximum absorption coefficient (α_p) for the $0 \rightarrow 1$ transition at room temperature for the same SL material system as in Figs. 1 and 2, as a function of electron concentration (N) for several combinations of well and barrier thicknesses (L_w, L_b). These absorption coefficient values are those obtained from the spectra which have taken the well thickness fluctuation into account. The $(50 \text{ Å}, 100 \text{ Å})$ SL corresponds to Fig. 1(a) and $(30 \text{ Å}, 100 \text{ Å})$ to Fig. 1(b). The α_p values increase with increasing N and deviate from the line at higher N values. This deviation is thought to imply the onset of occupation by electrons of the first excited state to which the transition from the ground state should occur. The critical N value for this deviation approximately coincides with the value at which the Fermi function goes into the first excited state to some extent. As shown in Fig. 3, the α_p value depends on the SL structure (L_w, L_b). Note that the α_p value has been defined in this paper by treating the SL's as a continuous medium. In actual transitions, however, the well region tends to con
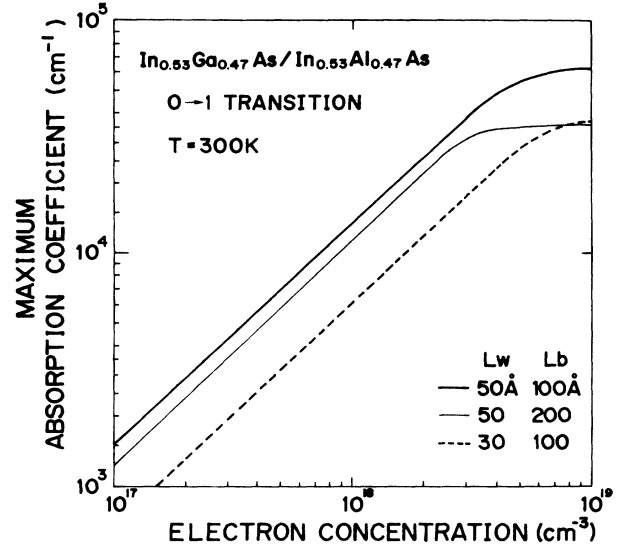

FIG. 3. Maximum absorption coefficient as a function of N, for $0 \rightarrow 1$ transition in $In_{0.53}Ga_{0.47}As/In_{0.53}Al_{0.47}As$ SL of several combinations of L_w and L_b.

tribute to the oscillator strength more than the barrier region, because the ground state is confined primarily in the well region. From this, we can predict that a large-L_w, small-L_b SL structure would yield a large absorption coefficient: this is clearly verified in Fig. 3. We would also note that the effect of accumulation has been neglected in this calculation. The effective electron concentration in the well region of an actual SL can be approximately given by $N_{eff} = N(L_b + L_w)/L_w$, when the SL is uniformly doped. Combining this effect and the preceding effect (that is, the actual transition occurring primarily in the well layer), the abscissa of Fig. 3 should be read as the effective electron concentration when these α_p values are to be compared with the experiments.

The author would like to thank M. Naganuma for his helpful suggestions and T. Sugeta for his support during this work.

[1] For example, S. Nojima, Y. Kawamura, K. Wakita, and O. Mikami, J. Appl. Phys. 64, 2795 (1988).

[2] L. C. West and S. J. Eglash, Appl. Phys. Lett. 46, 1156 (1985).

[3] A. Harwit and J. S. Harris, Jr., Appl. Phys. Lett. 50, 685 (1987).

[4] S. Y. Yuen, Appl. Phys. Lett. 43, 813 (1983).

[5] A. Seilmeier, H. J. Hubner, G. Abstreiter, G. Weiman, and W. Schlapp, Phys. Rev. Lett. 59, 1345 (1987).

[6] Perng-fei Yuh and K. L. Wang, Phys. Rev. B 37, 1328 (1988).

[7] T. Ando and S. Mori, J. Phys. Soc. Jpn. 47, 1518 (1979).

[8] D. D. Coon and R. P. G. Karunasiri, Appl. Phys. Lett. 45, 649 (1984).

[9] D. Ahn and S. L. Chuang, Phys. Rev. B 35, 4149 (1987).

[10] J. M. Luttinger and W. Kohn, Phys. Rev. 97, 869 (1955).

[11] G. Bastard, Phys. Rev. B 25, 7584 (1982).

[12] D. J. Newson and A. Kurobe, Appl. Phys. Lett. 53, 2516 (1988).

[13] B. F. Levine, A. Y. Cho, J. Walker, R. J. Malik, D. A. Kleinman, and D. L. Sivco, Appl. Phys. Lett. 52, 1418 (1988).

[14] H. Lobentanzer, W. Konig, W. Stoltz, K. Ploog, T. Elsaesser, and R. J. Bäuerle, Appl. Phys. Lett. 53, 571 (1988).

[15] S. Nojima and K. Wakita, Appl. Phys. Lett. 53, 1958 (1988); S. Nojima, ibid. 55, 1868 (1989).

[16] S. Nojima and H. Asahi, J. Appl. Phys. 63, 479 (1987).