Inhomogeneous broadening of intersubband transitions due to nonscreening roughness of heterointerfaces

F. T. Vasko
Institute of Semiconductor Physics, Kiev, 252650, Ukraine

J. P. Sun[a] and G. I. Haddad
Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan 48109-2122

V. V. Mitin
Department of Electrical and Computer Engineering, Wayne State University, Detroit, Michigan 48202

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The shape of the terahertz absorption peak in quantum wells with rough heterointerfaces is studied. Although the long-range variations of the ground level are screened in heavily doped structures, the intersubband in-plane energy remains nonuniform due to the second-level variations. The equation for intersubband polarization is considered in the resonant approximation, taking into account the depolarization shift. The line shape of the intersubband absorption peak is described for the case with long-range variations of heterointerfaces. © *2000 American Institute of Physics.* [S0021-8979(00)02707-9]

The resonant intersubband transitions in heterostructures with two-dimensional electron gas have been widely examined over the last decades[1,2] and the shape of the absorption peak has been studied for the case of infrared excitation. Both the Gaussian shape of the absorption peak, due to broadening under large-scale nonuniformities[3] or under large subband dispersion,[4] and the Lorentzian shape, due to spontaneous emission of optical phonons by the electrons,[5] have been discussed. In spite of recent measurements of intersubband transitions in the terahertz (THz) spectral region,[6–8] the line shape of absorption is not completely understood. Since nonparabolicity effects and phonon emission are not essential in this spectral region, the inhomogeneous broadening due to roughness of heterointerfaces contributes significantly to the width of the absorption peak. In this letter, we study the line shape of the intersubband absorption peak in a heavily doped quantum well (QW) for the case of simple long-range nonuniformities.

For the QW with heterointerface roughness being considered, the width of the QW $d_{\mathbf{x}}$, depends on the in-plane coordinate $\mathbf{x}$. The energy levels $\epsilon_{s\mathbf{x}}$ vary with $\mathbf{x}$ in the long-range case; $s=1,2,...$, is the subband index. The variations of the ground level $\epsilon_{1\mathbf{x}}$ are screened in the heavily doped samples, while the energy of the first excited level $\epsilon_{2\mathbf{x}}$ changes four times greater, so that the intersubband separation $\delta\epsilon_{\mathbf{x}}$ remains unscreened (see Fig. 1). In the simple flat-band approximation, we have

$$\epsilon_{s\mathbf{x}} \simeq \frac{(s\pi\hbar/d_{\mathbf{x}})^2}{2m} \simeq \epsilon_s\left(1-2\frac{\delta d_{\mathbf{x}}}{d}\right), \quad \delta\epsilon_{\mathbf{x}} \simeq 6\epsilon_1\frac{\delta d_{\mathbf{x}}}{d}, \quad (1)$$

where $\delta d_{\mathbf{x}}$ is the random variation of the QW width due to the interface roughness and m is the electron effective mass.

Consider first the case of a QW with very long-range nonuniformities formed by the heterointerface islands (see the inset in Fig. 2). The relative absorption ξ_ω, introduced as a ratio of the absorbed power to the Poynting vector of radiation through the structure, is given by

$$\xi_\omega = \sum_{k=0,\pm} P_k \xi(\omega-\omega_k), \quad \xi(\Delta\omega) = \frac{\xi_m \nu^2}{\Delta\omega^2+\nu^2}. \quad (2)$$

Here, ω_k are the resonant frequencies, corresponding to three types of transitions ($k=0,\pm$), ξ_m is the maximum absorption, and ν is the relaxation frequency due to scattering processes. The contributions of these transitions are determined by the probability factors $P_+=\gamma_l\gamma_r$, $P_-=(1-\gamma_l)(1-\gamma_r)$, and $\Sigma_k P_k=1$, where $\gamma_{l,r}$ are the degree of roughness for the left (l) and right (r) heterointerface, respectively, i.e., the ratio of the island area to the sample area. In Fig. 2, we use the parameters of a GaAs-based QW with $d=220$ Å and $\hbar\nu=0.6$ meV, and the characteristic intersubband energies $\hbar\omega_k$ are equal to 29.6, 30.3, and 31.0 meV. For rough heterointerfaces, as shown in Fig. 2, the Lorentzian peak is shifted to lower energies with modified shapes. If there is only one heterointerface with roughness, a flattop absorption peak is obtained; for the case with the roughness on both sides of the QW, the absorption shape is widened and the contributions from the three transitions are discernible on the absorption curve.

In the resonant approximation, the Fourier component of intersubband current is written as $(2e^2/L^2)\Sigma_{\mathbf{p}} v_{12}\delta f_{12}(\mathbf{p},\mathbf{x})$, where L^2 is the normalization area, v_{12} is the intersubband velocity between the first and second energy levels, and $\delta f_{12}(\mathbf{p},\mathbf{x})$ is the intersubband component of the density matrix in the Wigner representation. The function δf_{12} describes the contribution of electrons with in-plane momenta $\mathbf{p}$ to the intersubband polarization at point $\mathbf{x}$ induced by the

[a]Electronic mail: jpsapo@engin.umich.edu

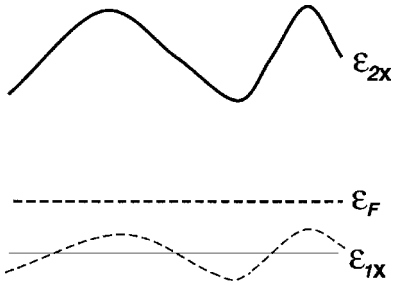

FIG. 1. Spatial variations of the energy levels $\epsilon_{1,2\mathbf{x}}$ for the heavily doped quantum wells.

electric field $E_\perp \exp(-i\omega t)$. The quantum kinetic equation for the above density matrix component is written as follows:

$$(-i\omega+\nu+\mathbf{v}\cdot\nabla_x)\,\delta f_{12}(\mathbf{p},\mathbf{x})+i\omega_{21}(\mathbf{x})\,\delta f_{12}(\mathbf{p},\mathbf{x}) + \frac{i}{\hbar}\,\delta h_{21} f_{1p}=0, \tag{3}$$

where $\mathbf{v}=\mathbf{p}/m$ is the in-plane velocity, $\omega_{21}(\mathbf{x})=(\epsilon_{21}+\delta\epsilon_{\mathbf{x}})/\hbar$ is the intersubband frequency, ϵ_{21} is the intersubband energy separation with the variation $\delta\epsilon_{\mathbf{x}}$ introduced by Eq. (1), and $f_{1p}=\theta(\epsilon_F-\epsilon_p)$ is the Fermi distribution $\epsilon_p=p^2/2m$. Neglecting the exchange contributions, we use the perturbation operator δh_{21} in the form[2]

$$\delta h_{21}=\frac{ie}{\omega}E_\perp v_{21}+\frac{4\pi e^2}{\kappa}L_s\,\delta n_{21}(\mathbf{x}), \tag{4}$$

where

$$L_s=\int_{-\infty}^{\infty}dz\,\varphi_{2z}\varphi_{1z}\int_{-\infty}^{z}dz'(z'-z)\,\varphi_{2z'}\varphi_{1z'},$$

and the second term is the self-consistent depolarization potential proportional to the induced concentration $\delta n_{21}(\mathbf{x})$ and is determined from Poisson's equation (κ is the dielectric permittivity, assumed to be constant across the structure). The characteristic length L_s is generally smaller than d because of the different coordinate dependencies of the wave functions φ_{1z} and φ_{2z} ($L_s\simeq 0.06d$ for the flatband QW). In Eq. (3), we have also neglected the fourth term contribution because $\overline{\delta\epsilon}/(mv_F l_c)$ is smaller than the linewidth, where v_F is the Fermi velocity, l_c is the in-plane correlation length, and $\overline{\delta\epsilon}$ is the variation of the intersubband energy, $\langle\delta\epsilon_{\mathbf{x}}^2\rangle \equiv \overline{\delta\epsilon}$. The relative absorption is given by

$$\xi_\omega=\frac{4\pi}{c\sqrt{\kappa}}\mathrm{Re}\frac{ie^2}{\hbar\omega}|v_{21}|^2\langle\delta n_{\mathbf{x}}\rangle, \tag{5}$$

where

$$\delta n_{21}(\mathbf{x})=\frac{2}{L^2}\sum_{\mathbf{p}}\,\delta f_{12}(\mathbf{p},\mathbf{x})\equiv\frac{ie}{\hbar\omega}E_\perp v_{21}\delta n_{\mathbf{x}},$$

and $\langle\cdots\rangle$ means the average over the two-dimensional (2D) plane.

The general solution of Eq. (3) can be obtained using the trajectory method, but the averaging is complicated enough; this problem is similar to the case of electron-spin resonance in a nonuniform alloy.[9] In this work, we only consider the long-range variations when $\delta n_{\mathbf{x}}$ can be obtained from the balance equations described below. After summation of $(2/L^2)\Sigma_{\mathbf{p}}\cdots$ of Eq. (3), we obtain

$$\{-i[\omega-\overline{\omega_{21}}(\mathbf{x})]+\nu\}\,\delta n_{\mathbf{x}}+\nabla_x\cdot\mathbf{Q}_{\mathbf{x}}=n_{2\mathrm{D}},\qquad \overline{\omega_{21}}(\mathbf{x})=\omega_{21}(\mathbf{x})-\Delta\omega_d, \tag{6}$$

where we have introduced the depolarization shift of the intersubband frequency $\Delta\omega_d=4\pi e^2L_s n_{2\mathrm{D}}/(\hbar\kappa)$, and $n_{2\mathrm{D}}$ is the 2D electron concentration. The induced in-plane flux $\mathbf{Q}_{\mathbf{x}}$ obeys the next balance equation:

$$\{-i[\omega-\omega_{21}(\mathbf{x})]+\nu\}Q_{\mathbf{x}i}+\sum_j\,\nabla_j E_{ij}(\mathbf{x})=0, \tag{7}$$

in which the induced in-plane energy tensor $E_{ij}(\mathbf{x})$ is obtained after summation of $(2/L^2)\Sigma_{\mathbf{p}}v_iv_j\cdots$ of Eq. (3). The balance equation for $E_{ij}(\mathbf{x})$ contains the derivative of the next moment of distribution, which corresponds to the summation $(2/L^2)\Sigma_{\mathbf{p}}v_iv_jv_k\cdots$. For the slow-varying nonuniformities, under the condition $v_F/(l_c\overline{\delta\omega})\ll 1$, $\overline{\delta\omega}=\overline{\delta\epsilon}/\hbar$ is the average variation of the intersubband frequency, we neglect such a contribution to obtain the energy tensor

$$E_{ij}(\mathbf{x})\simeq\delta_{ij}\delta n_{\mathbf{x}}\frac{\epsilon_F}{2m}\,\frac{\Delta\omega_d}{\nu-i[\omega-\omega_{21}(\mathbf{x})]}. \tag{8}$$

For the near-resonant spectral region the denominator in Eq. (8) is replaced by $i\Delta\omega_d$, taking into account that $\Delta\omega_d$ is larger than the linewidth. As a result, the in-plane flux is equal to $\mathbf{Q}_{\mathbf{x}}\simeq\epsilon_F\nabla\delta n_{\mathbf{x}}/(i2m\Delta\omega_d)$, and the diffusion equation for $\delta n_{\mathbf{x}}$ takes the following form:

$$D_p\nabla_x^2\delta n_{\mathbf{x}}+\{-i[\omega-\overline{\omega_{21}}(\mathbf{x})]+\nu\}\,\delta n_{\mathbf{x}}=n_{2\mathrm{D}}, \tag{9}$$

with the effective diffusion coefficient for intersubband polarization $D_p=v_F^2/(4\Delta\omega_d)$.

For the long-range case $D_p/l_c^2\ll\overline{\delta\omega}$, the diffusion term in Eq. (9) is negligible. After substitution of $\delta n_{\mathbf{x}}$ into Eq. (5)

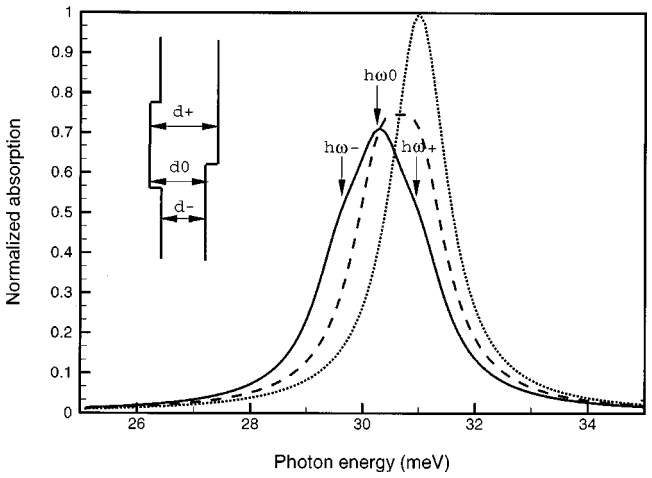

FIG. 2. Normalized absorption (ξ_ω/ξ_m) vs photon energy ($\hbar\omega$) for QWs with ideal heterointerfaces ($\gamma_{l,r}=0$, dotted line), one-side rough heterointerface ($\gamma_r=0.5$, $\gamma_l=0$, dashed lines) and rough heterointerfaces on both sides of the QW ($\gamma_l=\gamma_r=0.5$, solid line).

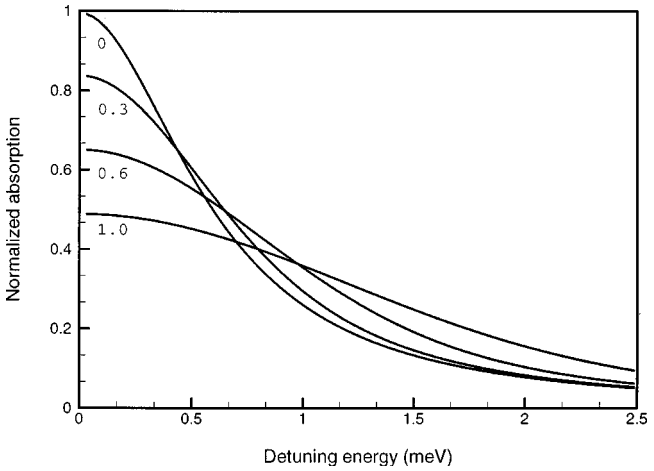

FIG. 3. Modified line shape (ξ_ω/ξ_m) vs detuning energy ($\hbar\Delta\omega$) for $\overline{\delta\omega}/\nu = 0$, 0.3, 0.6, and 1.0, and $\nu = 0.6$ meV.

and taking the average of the random variations of the intersubband energy in the exponential term, we transform the absorption ξ_ω to the final form

$$\xi_\omega = \frac{e^2}{\hbar c}\,\frac{4\pi|v_{21}|^2 n_{2D}}{\sqrt{\kappa}\omega}\,\mathrm{Re}\int_{-\infty}^{0} d\tau e^{\tau(\nu - i\Delta\omega) - (\tau\overline{\delta\omega})^2/2}, \quad (10)$$

where $\Delta\omega \equiv \omega - \epsilon_{21}/\hbar$ is the frequency detuning. This integral is expressed through the error function. The line shape of absorption is shown in Fig. 3 for the different relative contributions of the collision processes and the inhomogeneous broadening. We obtain the broadening of the absorption peak and transformation of the Lorentzian to Gaussian line shape with the increasing ratio $\overline{\delta\omega}/\nu$. This modification is significant when the ratio becomes greater than 0.5.

In conclusion, we have presented a simplified analysis which demonstrates the efficient inhomogeneous broadening of the intersubband THz transitions in QWs due to the nonscreening roughness of heterointerfaces. As noted in the Refs. 6–8, the experimental results of THz emission spectra cannot be explained using only the common mechanisms of broadening, and inhomogeneous broadening should be considered. For a direct comparison between the theory and experiment, we suggest far-infrared spectroscopic investigations of QWs with rough heterointerfaces. The modification of the absorption line shape of the structures with different levels of heterointerface imperfection would permit verifications of such a broadening mechanism. In this study we have employed the resonant approximation, which is valid for the case of small depolarization shifts. On the other hand, $\Delta\omega_d$ is assumed to be larger than the linewidth in the evaluation of the diffusion-type Eq. (9). We have also used the long-range approximation and only discussed the simplified case where the diffusion is not essential. We note that both Eqs. (2) and (10) take only into account the local contributions to the intersubband polarization, and that a more accurate solution of these equations and a self-consistent calculation of $\delta\epsilon_{\mathbf{x}}$ instead of the simple estimation in Eq. (1) are necessary for a complete consideration of the problem. In spite of the above simplifications, our results clearly demonstrate the existence and importance of the broadening mechanism due to the nonscreening roughness of heterointerfaces. This mechanism is of significance not only to describe the spectral characteristics of THz detectors and modulators, but also to the gain of THz lasers.

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