INDIVIDUAL DEDUCTION OF TWO ROUGHNESS PARAMETERS FOR QUANTUM WELLS FROM INTERSUBBAND ABSORPTION PEAK DATA

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Abstract. For roughness-dominated intersubband absorption in quantum wells (QWs), the optical characteristics depend on roughness parameters of the heterointerface (roughness amplitude and correlation length). Following the earlier belief in the literature, a single-valued estimation of them from measurement of these characteristics is impossible. On the contrary, in our report we present an attempt at providing a possibility for single-valued deduction of the roughness parameters from optical data. For this purpose, we introduce the lineshape characteristics that are independent of roughness amplitude, so being a function of correlation length only. As a typical example, we examine the ratio between two different absorption-peak heights. Thus, we may propose an efficient method for individual estimation of the roughness parameters from optical data. Instead of the normal simultaneous fitting of both parameters to the functional dependence of the absorption-peak height (APH) at many experimental points, we perform a two-step fitting at one point.

I. INTRODUCTION

Roughness-related scatterings are usually key scattering mechanisms in heterostructures (HSs), especially, thin quantum wells. These determine a great deal of their various properties, viz., lateral transport [1], intersubband optical transition [2], and excitonic lineshape [3]. Roughness is shown to give rise to strong HS scattering sources, viz., misfit deformation potential, misfit piezoelectric field in strained HSs [4], and polarization surface roughness scattering in all polar HSs [5]. Thus, interface profile is critical in study of the HS properties. Within the phenomenological model, the interface profile in two-dimensional wave vector space is written as follows

$$\langle |\Delta_{\mathbf{q}}|^2 \rangle = \pi (\Delta \Lambda)^2 F_{\mathrm{R}}(q\Lambda), \tag{1}$$

where the form factor $F_{\rm R}(q\Lambda)$ depends on Λ only and is specified by some interface morphology, e.g., Gaussian, [1] power-law, [6] or exponential [7]. Δ is simply a scaling factor, so fixing the scattering strength, while Λ appears not only in the combination $\Delta\Lambda$ but also in $F_{\rm R}(q\Lambda)$, so fixing both the strength and angular distribution of scattering.

For any theoretical study of the roughness-related effects, [1, 8] one must adopt some interface profile with Δ and Λ as input parameters. It is critical to have Δ and Λ individually in order to test the validity of the interface model and the key scattering mechanisms adopted in the theory. It is worth mentioning that for finding two roughness sizes in the literature one adopted the following methods: i) direct measurement by atomic force microscopy and ii) indirect deduction from some measured properties. The former is useful for surfaces that are open on the side of vacuum or air, while the latter for interfaces that are buried between two material layers. There were a number of attempts to get information on two roughness sizes by simultaneously fitting both sizes to optical data, however, so far none of them has been able to separately evaluate Δ and Λ . With a simultaneous fitting of Δ and Λ to data on conventional features (peak height or linewidth) of the absorption lineshape, one obtained generally not a single roughness profile, but a set of different profiles with various Δ and Λ . It was believed [9] that in principle one is unable to uniquely deduce the interface profile from optical data alone.

On the contrary, in this paper we present an attempt to provide a possibility of individual single-valued estimation of two roughness sizes, merely basing on optical data. For this purpose, we introduce such characteristics of the absorption lineshape that are independent of roughness amplitude, so being a function of correlation length only. As a representative, we examine the ratio between two different values of the absorption-peak height.

II. INTERSUBBAND OPTICAL ABSORPTION IN QUANTUM WELL

II.1. Basic equations

To illustrate our method, we consider the case when only the ground subband in QWs occupied by electrons and the light energy is close to the energy separation between the two lowest subbands $\hbar\omega \sim E_{10} = E_1 - E_0$ (\hbar is the induced Planck constant). For a symmetric square QW (centered at z = 0) of well width L and potential barrier height $V_{\rm b}$, the wave functions are given as follows [10], for the ground state:

$$\zeta_0(z) = C_0 \begin{cases} e^{\kappa_0(z+L/2)} \cos(k_0 L/2), & \text{if } z < -L/2\\ \cos(k_0 z), & \text{if } |z| \le L/2\\ e^{-\kappa_0(z-L/2)} \cos(k_0 L/2), & \text{if } z > L/2 \end{cases}$$
(2)

$$C_0 = \frac{1}{\sqrt{L/2 + (V_{\rm b}/\kappa_0 E_0)\cos^2(k_0 L/2)}}$$
(3)

with

$$\cos(k_0 L/2) - \frac{m_z^{\rm o} k_0}{m_z^{\rm c} \kappa_0} \sin(k_0 L/2) = 0, \tag{4}$$

and for the first excited state:

$$\zeta_1(z) = C_1 \begin{cases} -e^{\kappa_1(z+L/2)} \sin(k_1L/2), & \text{if } z < -L/2\\ \sin(k_1z), & \text{if } |z| \le L/2\\ e^{-\kappa_1(z-L/2)} \sin(k_1L/2), & \text{if } z > L/2 \end{cases}$$
(5)

$$C_1 = \frac{1}{\sqrt{L/2 + (V_{\rm b}/\kappa_1 E_1)\sin^2(k_1 L/2)}} \tag{6}$$

with

$$\cos(k_1 L/2) + \frac{m_z^c \kappa_1}{m_z^b k_1} \sin(k_1 L/2) = 0, \tag{7}$$

where $m_z^{c/b}$ is the out of-plane effective masses of the electron in the channel and barrier, respectively. The wave number in the channel is $k_{0,1} = \sqrt{2m_z^c E_{0,1}}/\hbar$, and in the barrier $\kappa_{0,1} = \sqrt{2m_z^b (V_b - E_{0,1})}/\hbar$. The absorption quantum efficiency of beam polarized through one well is directly proportional to the oscillator strength, and is given by [10]

$$\eta \sim \frac{e^2 h}{4\varepsilon\varepsilon_0 mc} n_s \frac{1}{\pi\gamma} \left(\frac{f_{0-1}}{1 + [(E_1 - E_0) - \hbar\omega)/\gamma]^2} \right),\tag{8}$$

here, e is the electron charge, h is the Planck constant, ε is the dielectric constant of the well material, m is the effective mass of electrons, c is the velocity of light in vacuum, n_s is the two-dimensional carrier density in the well, γ is the linewidth and f_{0-1} is the oscillator strength for the E_0 to E_1 transition give by

$$f_{0-1} = \frac{8\hbar C_0^2 V_b^2}{m\omega (E_1 - E_0)^2} \cos^2(k_0 \frac{L}{2}) \frac{E_1 \kappa_1 \sin^2(k_1 \frac{L}{2})}{E_1 \kappa_1 \frac{L}{2} + V_b \sin^2(k_1 \frac{L}{2})}$$
(9)

II.2. Surface roughness scattering

The electrons involved in intersubband transition are, in general, subject to various scattering sources: [2, 8, 9] surface roughness (SR), LO and LA phonons, alloy disorder (AD), and ionized impurities (II). The energy broadening is to be regarded as a measure of the scattering rate. Thus, the observed linewidth is a sum of the partial linewidths (fig 1):

$$\gamma_{\rm tot} = \gamma_{\rm SR} + \gamma_{\rm LO} + \gamma_{\rm LA} + \gamma_{\rm AD} + \gamma_{\rm II}.$$
(10)

Here, $\gamma = 2\Gamma(E)$ means the full width at half maximum (FWHM) of the Lorentzian



Fig. 1. The energy broadening: linewidth

lineshape with energy E, i.e., the energy broadening, given by

$$\Gamma(E) = \frac{1}{2} [\Gamma_{\text{intra}}(E) + \Gamma_{\text{inter}}(E)], \qquad (11)$$

where the first term arises from intrasubband processes, and second one from intersubband process. As for SR scattering, the interface profile is often assumingly Gaussian. The

contribution from SR scattering to the energy broadenings is supplied by [9]

$$\Gamma_{\rm intra}^{\rm SR}(E) = \frac{m^* (\Delta \Lambda)^2}{\hbar^2} (F_{00} - F_{11})^2 \int_0^\pi d\theta \ e^{-q^2 \Lambda^2/4}$$
(12)

and

$$\Gamma_{\rm inter}^{\rm SR}(E) = \frac{m^* (\Delta \Lambda)^2}{\hbar^2} F_{01}^2 \int_0^{\pi} d\theta \ e^{-\tilde{q}^2 \Lambda^2/4},\tag{13}$$

where the in-plane scattering 2D vectors are defined as follows for the intrasubband processes:

$$q^2 = \frac{4m^*}{\hbar^2} E(1 - \cos\theta) \tag{14}$$

and the intersubband one:

$$\tilde{q}^2 = \frac{4m^*}{\hbar^2} \Big[E + \frac{1}{2} E_{10} - \sqrt{E(E + E_{10})} \cos\theta \Big].$$
(15)

The scattering form factors are fixed by the local value of the wave function at the barrier, it holds:

$$F_{mn} = V_{\rm b} \zeta_m (-L/2) \zeta_n (-L/2), \quad (m, n = 0, 1).$$
(16)

III. ESTIMATION OF INTERFACE PROFILE FROM THE ABSORPTION-PEAK HEIGHT DATA

III.1. The absorption-peak height ratio

It was found [2, 9, 11] that in thin QWs, especially at low temperatures, intersubband transition is often dominated by SR scatterings. The electron distribution is determined by the Fermi Energy: $E_{\rm F} = \hbar^2 k_{\rm F}^2 / 2m^*$ with $k_{\rm F} = \sqrt{2\pi n_{\rm s}}$. It is clear that the roughness-induced APH from Eq. (8, 9, 12, and 13) depend on the parameters of QW (well width and sheet electron density) as well as of interface profile (roughness amplitude and correlation length).

We introduce such lineshape characteristics that depend on a single roughness parameter only, say, correlation length Λ . A typical example is the ratio between two different values of the absorption-peak height. Following Eqs. (12) and (13), Δ appears as a scaling factor, it must drops out of the ratio, so this depends on Λ only:

$$R(L, n_{\rm s}, L', n'_{\rm s}; \Lambda) = \frac{peak_{\eta}(L, n_{s}; \Delta; \Lambda)}{peak_{\eta}(L', n'_{s}; \Delta; \Lambda)},\tag{17}$$

where the variables of the involved functions are shown explicitly, and $(L, n_s) \neq (L', n'_s)$.

It is worth mentioning that in the literature, one defined the lineshape features and view these as functions of well width and carrier density, which are controllable quantities. Here, we examine the APH ratio and view this from a new aspect, namely, as a function of correlation length, which is a non-controllable quantity. This ratio is inferred from data about the APH as a function of well width and carrier density. So, one can get a singlevalued estimation of Λ . With a fixed Λ , one can completely estimate Δ by a subsequent fit to some APH value. In other word, one can single-valued estimate the interface profile. Thus, with the two-step fitting one archives an individual single-valued evaluation of the two roughness parameters that employs data on one observed property only: intersubband absorption alone or lateral mobility alone [12].

III.2. Numerical results

In order to illustrate the above method, we deduce the interface profile from intersubband APH in the QW made of GaAs/Al_{0.3}Ga_{0.7}As [2, 9] with barrier height: $V_{\rm b} = 210$ meV and effective mass: $m_{\rm c}^*/m_0 = 0.0665$, $m_{\rm b}^*/m_0 = 0.09155$.



Fig. 2. The absorption-peak height ratio in Eq. (17), $\mathcal{R}(\Lambda) = \mathcal{R}(L, n_{s}, L', n'_{s}; \Lambda)$ is plotted versus correlation length Λ for the GaAs/Al_{0.3}Ga_{0.7}As QW.

In Fig. 2, the APH ratio in Eq. (17), $\mathcal{R}(\Lambda) = \mathcal{R}(L, n_{\rm s}, L', n'_{\rm s}; \Lambda)$ is plotted versus correlation length Λ for the GaAs/Al_{0.3}Ga_{0.7}As QW. The transition is assumed to be dominated by the SR scattering mechanism [2, 9] (marked by solid lines). The QW parameters are given in Refs. [2, 9] and taken from Fig. 4 of Ref. [13] (well width in Å and sheet electron density in 10¹¹ cm⁻²) as follows: a) $L = 90, n_{\rm s} = 13.5; L' = 70, n'_{\rm s} = 10.5$ and $\mathcal{R}_{exp} = 2.34$.

b) $L = 100, n_s = 15; L' = 80, n'_s = 12 \text{ and } \mathcal{R}_{exp} = 2.54.$

c) $L = 100, n_s = 15; L' = 70, n'_s = 10.5$ and $\mathcal{R}_{exp} = 3.74.$

d) $L = 90, n_s = 13.5; L' = 60, n'_s = 9$ and $\mathcal{R}_{exp} = 2.41$.

In Fig. 3, the absorption-peak height $peak_{\eta}(\Delta) = peak_{\eta}(L, n_s; \Delta; \Lambda)$ is plotted versus roughness amplitude Δ with the correlation length deduced from Fig. 2: $\bar{\Lambda} = 71$ Å and QW parameters: a) L = 100 Å, $n_s = 15 \times 10^{11}$ cm⁻² and $peak_{\eta} = 34.7\%$. b) L = 90Å, $n_s = 13.5 \times 10^{11}$ cm⁻² and $peak_{\eta} = 30.6\%$ and c) L = 80 Å, $n_s = 12 \times 10^{11}$ cm⁻² and $peak_{\eta} = 26.6\%$. From here, we deduce the value of the roughness amplitude is $\bar{\Delta} = 1.9$ Å.

IV. CONCLUSION

In contrast to the earlier belief, we have proposed an efficient method for individual estimation of two sizes of the interface profile, based on the processing of optical data by a two-step fitting of



Fig. 3. The absorption-peak height $peak_{\eta}(\Delta) = peak_{\eta}(L, n_s; \Delta; \Lambda)$ is plotted versus roughness amplitude Δ with the correlation length deduced from Fig. 2.

(i) to the absorption-peak heights ratio at one point, and then

(ii) to the absorption-peak height at one point.

The merit of our method is to provide a single-valued estimation of the interface profile. This is also economical since one needs two experimental points rather than the whole functional dependence at many points.

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