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Single-valued estimation of the interface profile from intersubband absorption linewidth data

We study the ratio between different linewidths of the intersubband absorption in a quantum well. For roughness-related absorption, this ratio turns out to be independent of the roughness amplitude, so being a function of the correlation length only. Therefore, in contrast to the earlier belief, we may propose an efficient method for individual single-valued estimation of the two sizes of an interface profile from optical data. Instead of the simultaneous fitting of both sizes to the functional dependence of the linewidth at many experimental points, we perform a two-step fitting of (i) correlation length to the linewidth ratio at one point and then (ii) roughness amplitude to a linewidth at one point. This method is useful for experimental study of the interface morphology.

Roughness-related scatterings are usually the key scattering mechanisms in heterostructures (HSs), especially, thin quantum wells (QWs). These determine a great deal of their properties, viz., lateral transport,<sup>1</sup> intersubband optical transition,<sup>2-8</sup> and excitonic lineshape.<sup>9</sup> Roughness is shown to give rise to strong scattering sources in HSs: surface (interface) roughness scattering,<sup>1</sup> misfit deformation potential,<sup>10,11</sup> and misfit piezoelectric field in strained HSs,<sup>11</sup> as well as polarization surface roughness scattering in polar HSs.<sup>12</sup> Thus, interface profile is critical in study of the HS properties.

Ước lượng đơn trị biên dạng bề mặt phân cách từ dữ liệu độ rộng vạch phổ hấp thụ giữa các vùng con **checked**

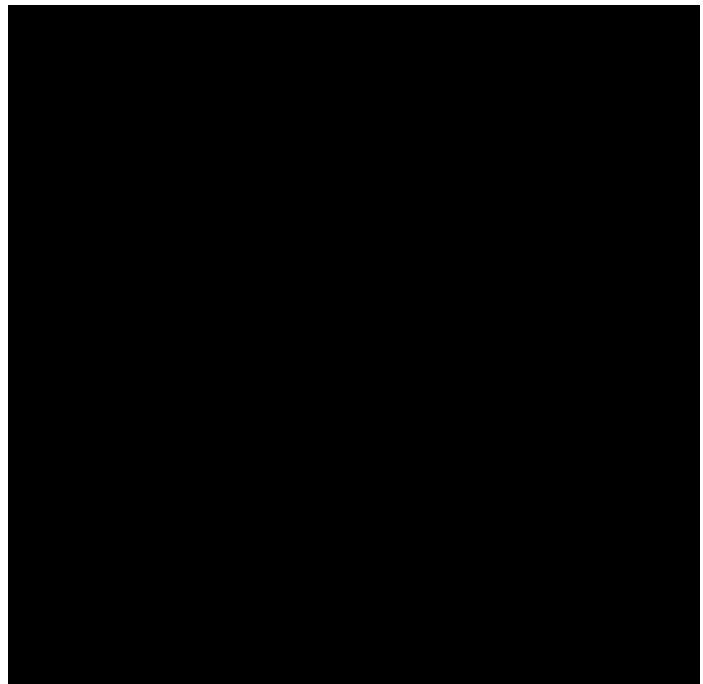
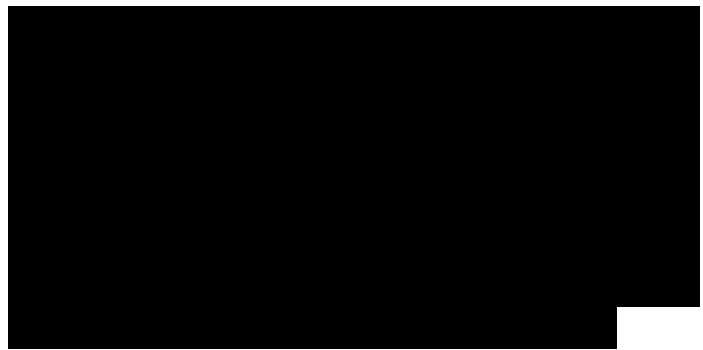
Chúng tôi nghiên cứu tỷ số giữa độ rộng vạch phổ hấp thụ giữa các vùng con khác nhau trong một giếng lượng tử. Đối với quá trình hấp thụ liên quan đến roughness (độ nhấp nhô, gồ ghề), hóa ra tỷ số này không phụ thuộc vào biên độ roughness, vì vậy nó chỉ là một hàm theo chiều dài tương quan. Do đó, trái ngược với quan niệm trước đây, chúng tôi đề xuất một phương pháp hiệu quả để ước tính đơn trị hai kích thước biên dạng bề mặt phân cách từ dữ liệu quang học. Thay vì khớp đồng thời cả hai kích thước với sự phụ thuộc hàm của độ rộng vạch phổ ở nhiều điểm thực nghiệm, chúng tôi thực hiện khớp hai bước của (i) chiều dài tương quan với tỷ số độ rộng vạch phổ tại một điểm và sau đó (ii) biên độ roughness với độ rộng vạch phổ tại một điểm. Phương pháp này rất có ích trong các nghiên cứu thực nghiệm về hình thái học bề mặt phân cách.



The interface profile is described by some roughness distribution in the in-plane. This is quantified by two size parameters: a roughness amplitude ( $A$ ) and a correlation length  $\lambda^2(A)$ . The former is the average height of roughness in the quantization direction (vertical size). The latter is the size of an in-plane region, where roughness at different spatial points are correlated (lateral size). Within the phenomenological model, the interface profile in two-dimensional (2D) wave vector space is given by

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where  $F^A(q)$  is a form factor that depends on  $A$  only and is specified by some interface morphology: Gaussian,<sup>1</sup> power-law,<sup>10</sup> or exponential.<sup>13</sup>  $A$  is simply a scaling factor, so fixing the scattering strength, while  $\lambda$  appears not only in the combination  $\lambda A$  but also in  $F^A(q)$ , so fixing both the strength and angular distribution of scattering.

For any theoretical study of the roughness-related effects,<sup>13-13</sup> one must assume some interface profile with  $(A, \lambda)$  as input parameters. It is critical to have  $A$  and  $\lambda$  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 employed the following methods: (a) direct measurement by atomic force microscopy and (b) 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 useful 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 of them to optical data; however, so far no attempt has been able to separately evaluate  $A$  and  $A$ .

With the simultaneous fitting of  $(A, A)$  to data on the traditional features of the lineshape (linewidth and peak height), one obtained generally not a single roughness profile, but a set of profiles with various  $(A, A)$ . It was believed<sup>6</sup> that in principle one is unable to uniquely deduce the interface profile from optical data alone; thus, one must invoke data on other properties, e.g., mobility.

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 linewidth.

In Sec. II, the basic equations are formulated for calculating the lineshape of intersubband absorption in QWs. In Sec. III, our method for deducing the roughness profile from experimental data on the linewidth ratio is applied, as an example, to the GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As QW. A summary is given with the merits of the method

in Sec. IV.

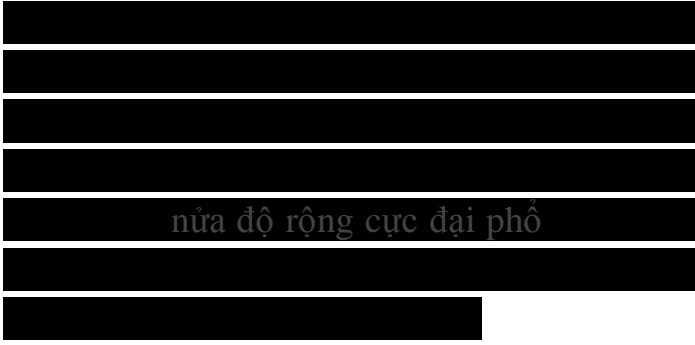
For illustration, we consider the case when only the ground subband is occupied by electrons, and the light energy is close to the energy separation between the two lowest subbands  $T_{10} \sim E_{10} - E_{00}$ . The absorption of light polarized in the growth (z) direction is proportional to the real part of the dynamical 2D conductivity. That was derived by a microscopic theory due to Ando,<sup>14,15</sup> and for single particle excitation reads as follows:

Here,  $m^*$  and  $m_z$  are the in-plane and out-of-plane effective masses of the electron,  $f$  is the oscillator strength for the transition  $0 \rightarrow E$ .  $f(E)$  is the Fermi distribution function.  $2T(E)$  means the full width at half maximum (FWHM) of the Lorentzian lineshape with energy  $E$ , i.e., its energy broadening, given by

where the first term arises from intrasubband processes, and the second from intersubband ones.

It is worth mentioning that the absorption lineshape described by Eq. (2) may be interpreted<sup>15,16</sup> as superposition of Lorentzian lineshapes with different energies distributed following the Fermi function. Therefore, its linewidth  $\gamma$  may be defined in a good approximation by the average of their FWHMs with the weight  $f(E)$ <sup>15</sup>

The electrons in intersubband transition are generally subject to various scattering sources:<sup>2-8</sup> surface roughness (SR), polar-optical (LO) phonons, deformation-



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potential acoustic (LA) phonons, alloy disorder (AD), and ionized impurities (II). The energy broadening  $T(E)$  is regarded as some measure of the scattering rate, so being additive. According to Eq. (4), the observed absorption linewidth is a sum of the partial line widths<sup>5-7</sup>

As for SR scattering, the interface profile is often assumingly Gaussian. The contribution from SR scattering to the energy broadenings is then supplied by<sup>5-7</sup>

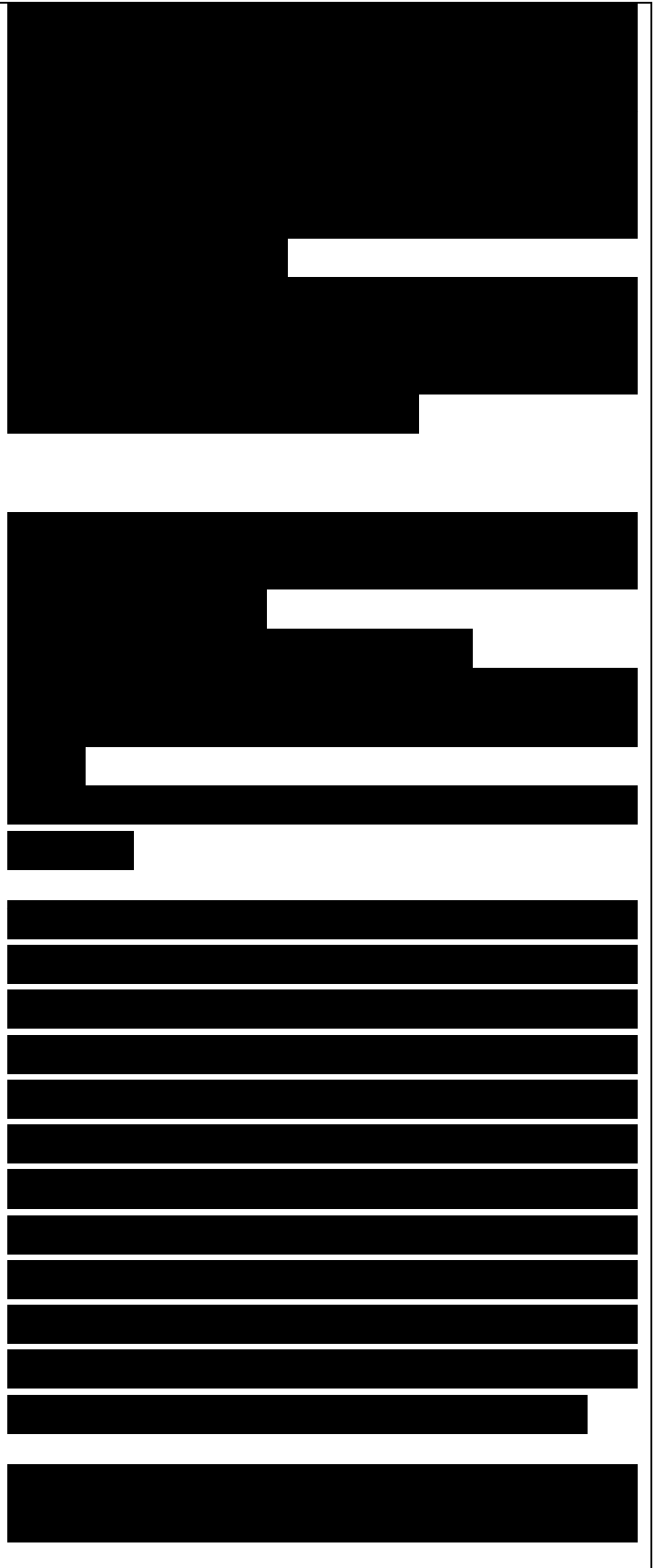
Here,  $q$  and  $q'$  are the 2D scattering vectors, defined as follows for the intrasubband processes:

and the intersubband ones:

$F_{nm}$  are the scattering form factors, defined by the local value of the wave function at the barrier  $z = -L/2$  with  $L$  being the well width, and  $V_f$  the barrier height.

It was found<sup>2-7</sup> that in thin QWs, especially at low temperatures, intersubband transition is often limited by SR scattering. The electron distribution is determined by the Fermi energy:  $E_p = \hbar^2 k_f^2 / 2m^*$  and  $k_f = \sqrt{2m^* n_s} / \hbar$  with  $n_s$  as a sheet electron density. According to Eq. (4), the roughness-limited linewidth depends on the parameters of the QW (well width  $L$  and sheet electron density) as well as of the interface profile ( $A$ ,  $A$ , roughness amplitude and correlation length):  $\Gamma_{sr} = T_{sr}(L, n_s, A, A)$ .

In order to evaluate the two roughness sizes ( $A$ ,  $A$ ), one usually employed data about the  $L$ - and  $n_s$ -dependences of  $\Gamma_{sr}$  the

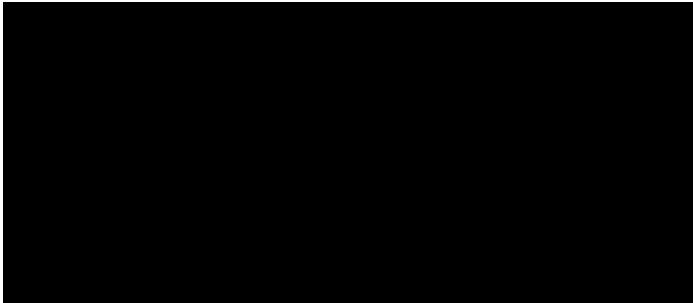
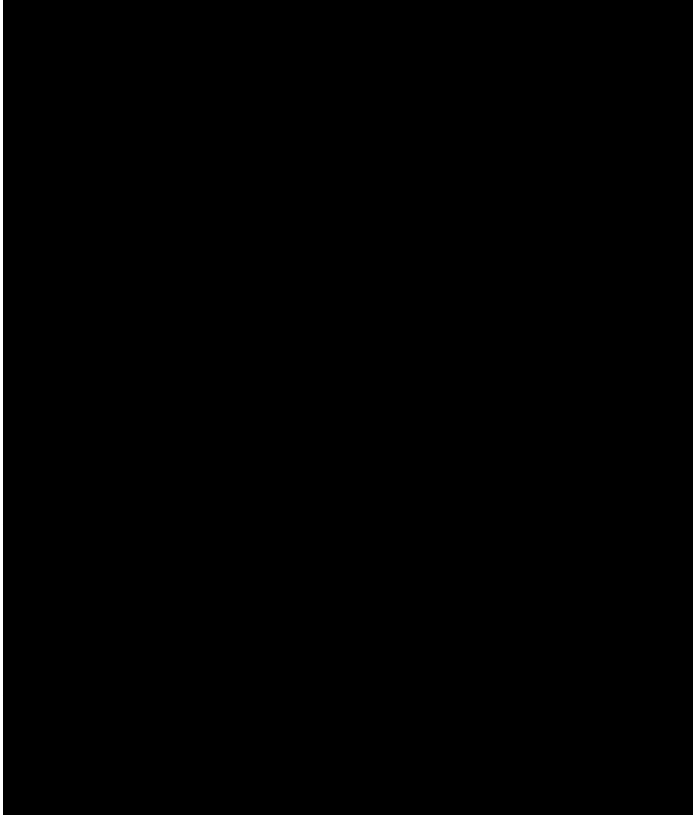


linewidth  $\gamma_{SR}(L, \omega; A, A)$ . However, it is difficult to ascertain either of them from a comparison between the model and the data because they appear in the product  $AA$ , but  $A$  also in the scattering integrals in Eqs. (6) and (7). Hence, one must adjust simultaneously both  $A$  and  $A$  until a good match between the calculated and the observed linewidths is achieved. Then, as in the case of mobility,<sup>17,18</sup> it turns out that one obtained not a single interface profile, but a set of profiles with various  $(A, A)$ .<sup>5,6</sup> Thus, it was believed<sup>6</sup> that up to date there has been no method for individual singlevalued estimation of two roughness sizes from optical data alone, one must invoke data on other properties, e.g., mobility.

Therefore, we need to introduce such lineshape characteristics that depend on a single roughness parameter, say, correlation length  $A$ . A typical example is the ratio between two different roughness-limited linewidths. Following Eqs. (6) and (7),  $A$  is a scaling factor, it must drop out of the ratio, so this is a function of  $A$  only

where  $L, \omega, L', \omega'$  as parameters with  $(L, \omega) \sim (L', \omega')$ .

It is worth mentioning that in the literature, one studied the traditional lineshape features (linewidth and peak height) and view them as measured functions of the controllable variables (well width and carrier density). In this paper, we examine the linewidth ratio and view it from a new



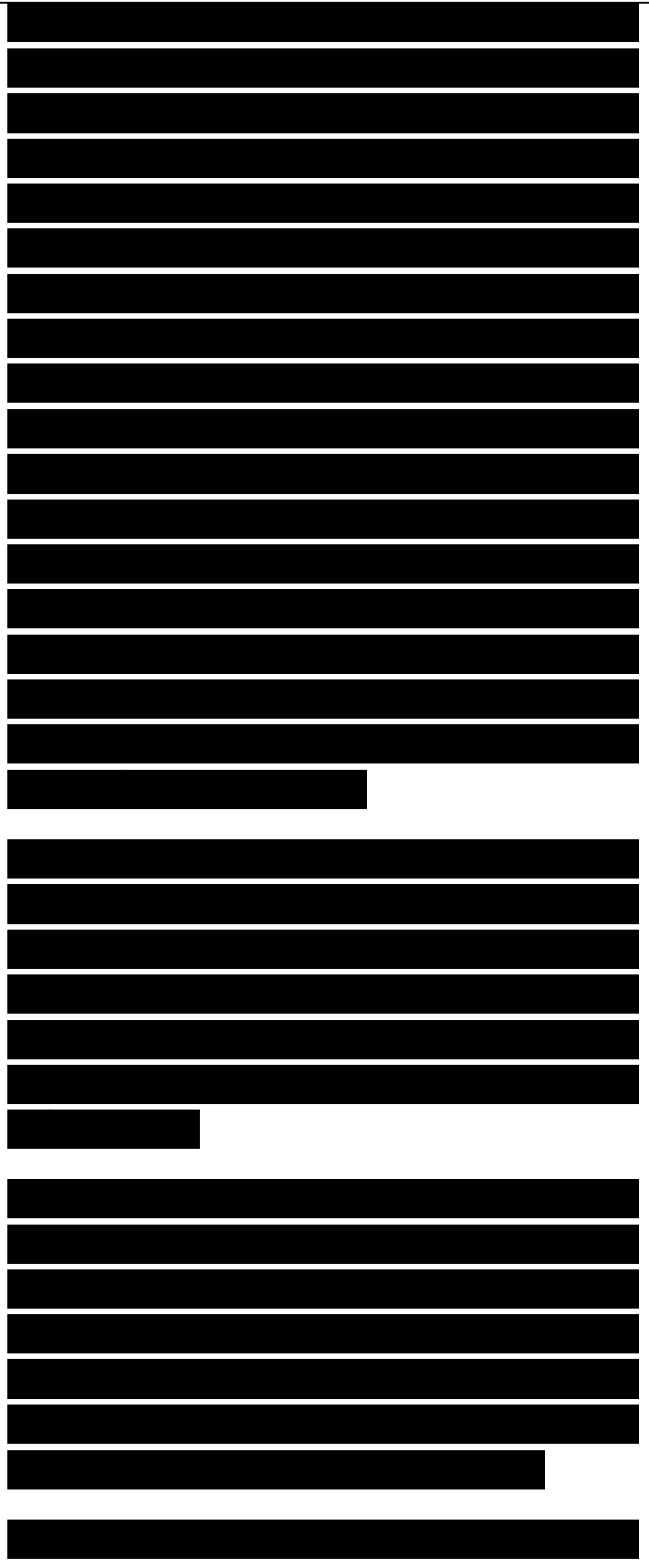
aspect as a function of correlation length. Since  $A$  is non-controllable, one cannot measure the function  $Ry(A)$ .

This is calculated following Eq. (11) from data about the linewidth as measured functions of well width and carrier density. With the function  $Ry(A)$  thus obtained, we can singly estimate  $A$ . With a fixed  $A$ , we can singly estimate  $A$  by a subsequent fit to some linewidth  $ySR(A)$ . In other words, we obtain a single interface profile. So, with two-step fitting we archive an individual single-valued evaluation of both roughness sizes, basing on one observed property (optical absorption).

To illustrate the method, we deduce the interface profile from intersubband absorption linewidths observed<sup>2</sup> in the GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As QW with material parameters listed in Ref. 6. The transition is mainly limited by SR and LO

FIG. 1. (Color online) Ratio of roughness-limited linewidths,  $Ry(A) = Ry\{L, n\&.L',A\}$ , in the Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs QW as a function of correlation length  $A$  with the fixed QW parameters (well width in  $\text{\AA}$ , sheet electron density in  $10^{10} \text{ cm}^{-2}$ ):  $L = 85$ ,  $n_s = 6.7$ ;  $L' = 95$ ,  $n_l = 5.7$ .

FIG. 2. (Color online) Roughness-limited





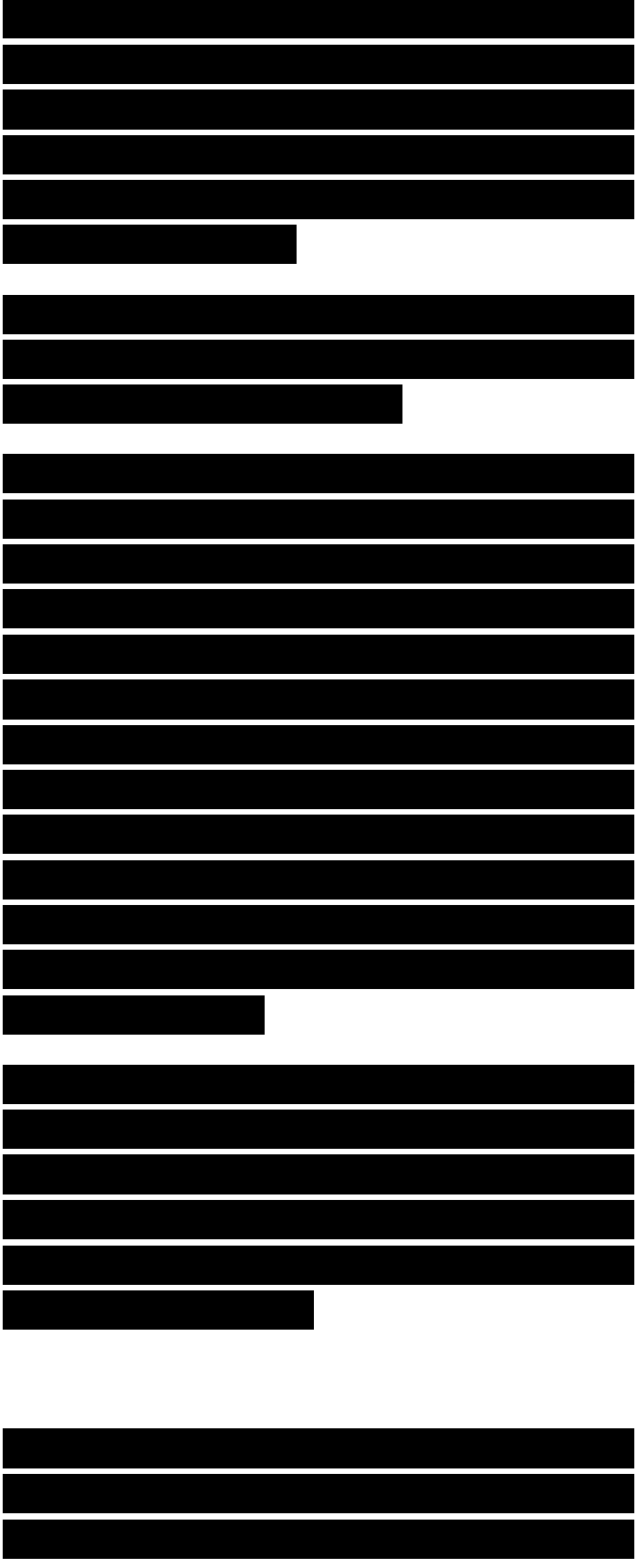
linewidth,  $\gamma_{SR}(A) = \gamma_{SR}(L, w_s; A, A)$ , in the  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  QW as a function of roughness amplitude  $A$  with the fixed QW parameters:  $L = 85 \text{ \AA}$ ,  $n_s = 6.7 \times 10^{11} \text{ cm}^{-2}$ , and the correlation length taken from Fig. 1:  $A = 84 \text{ \AA}$ .

scattering,  $\gamma_{SR} = \gamma_{tot} - \gamma_{LO}$ , with  $\gamma_{LO}$ , i.e.,  $\gamma_{exp}$ , and  $\gamma_{LO}$  given in Refs. 2 and 6, respectively.

The ratio of roughness-limited linewidths  $R_y(A) = R_y(L, w_s, Z/w; A)$  is plotted following Eq. (11), in Fig. 1, versus correlation length  $A$  with the fixed QW parameters. The wave functions are solved for a symmetric QW of finite barrier.<sup>19</sup> The QW parameters are taken from the 4.2 K experiment<sup>2</sup> (well width in  $\text{\AA}$ , sheet electron density in  $10^{11} \text{ cm}^{-2}$ , linewidth in meV):  $L = 85$ ,  $n_s = 6.7$ ,  $\gamma_{tot} = 3.6$ ,  $\gamma_{LO} = 0.76$ ,  $\gamma_{SR} = 2.84$ ;  $L_f = 95$ ,  $n_s = 5.7$ ,  $\gamma_{tot} = 3.1$ ,  $\gamma_{LO} = 0.93$ ,  $\gamma_{SR} = 2.17$ . Then, with  $R_y(A) = 1.31$ , we get  $A = 84 \text{ \AA}$ .

In Fig. 2, the roughness-limited linewidth  $\gamma_{sr}(A) = \gamma_{SR}(L, w_s; A, A)$  is plotted versus roughness amplitude  $A$  with the fixed QW parameters:  $L = 85$ ,  $n_s = 6.7$ , and the correlation length taken from Fig. 1:  $A = 84 \text{ \AA}$ . With  $\gamma_{sr}(A) = 2.84 \text{ meV}$ , we get  $A = 2.5 \text{ \AA}$ .

Thus, the interface profile ( $2.5 \text{ \AA}$ ,  $84 \text{ \AA}$ ), obtained by two-step fitting based on optical data is nearly equal to ( $3 \text{ \AA}$ ,  $85 \text{ \AA}$ ) obtained by simultaneous fitting based on



optical and mobility data.<sup>6</sup> The slight divergence may be due to the fact that the variation detected<sup>2</sup> in the sheet electron density for various well widths is included in the present calculation, while omitted in the previous one.<sup>0</sup>

In summary, 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 (i)  $A$  to the linewidth ratio at one point, and then (ii)  $A$  to the linewidth at one point.

The merit of our method is to provide a single-valued estimation of the interface profile. This is useful for experimental study of the interface morphology. Our method is economical since we need two experimental points rather than the whole dependence at many points.

In case that intersubband transition is limited singly by SR scattering, instead of the linewidth ratio one may employ the peak-height ratio, which also is a function of correlation length only.

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Trong trường hợp dịch chuyển nội vùng chỉ do cơ chế tán xạ chi phối, thay vì tỷ số độ rộng vạch phổ, chúng ta có thể dùng tỷ số chiều cao peak, đó cũng là một hàm theo chiều dài tương quan.