

Intersubband absorption due to scattering on ionized impurities and acoustic phonons in parabolic quantum well

A H Gevorgyan, E M Kazaryan and A A Kostanyan

Institute of Mathematics and High Technologies, Russian-Armenian University, 123 Hovsep Emin Street, 0051 Yerevan, Armenia

Email: artavazd.kostanyan@gmail.com

Abstract. Intersubband absorption linewidth in GaAs quantum well due to scattering by LA phonons and ionized impurities is calculated. The method which used for calculations is similar to a well-known method for calculating transport mobility. The linewidth dependence on temperature, as well as on well width is presented. The estimation for absorption coefficient is proposed, based on two-dimensional dynamical conductivity expression. The coefficient is calculated for different well widths, as well as for different temperatures.

1. Introduction

Intersubband transitions (ISBT) in quantum wells (QW) are of great interest due to its unique characteristics: ultrafast relaxation, great ability to customize the wavelength of transitions, many-body effects, etc. [1-5]. This is important not only in terms of fundamental physics, but also the development of new technological applications. Many devices are developed based on ISBT in semiconductor quantum wells, such as intersubband laser [6], infrared photodetectors [7-9], ultrafast optical modulators [10], optical switches [11]. Moreover, these transitions play key role for improving the performance of quantum cascade lasers [12].

In this connection, it is important to have detailed understanding of processes behind ISBT. The performance of devices based on IBST depends on its properties, such as the transition line shape broadening. The mechanisms of the broadening depend on various scattering processes. Previously reported lack of correlation between transport broadening and intersubband linewidth brings to the necessity of detailed consideration of different scattering mechanisms input into intersubband absorption linewidth.

The linewidths have been measured for various temperatures [13], well widths [14], alloy compositions [14], and doping positions [15] in different QWs. These results show that absorption linewidth has a weak dependence on temperature and alloy composition and apparently has little correlation with mobility. However, its strong well-width dependence suggests that the main contribution is from interface roughness scattering.

In a paper [16], authors discussed the effect of interface roughness scattering on linewidth by comparing calculations based on a theory by Ando [17] and experimental data for modulation-doped GaAs/AlAs QWs with a well width of 80 Å. The results show that linewidth is much more sensitive to interface roughness scattering than transport mobility is, because the contribution from the intrasubband scattering in the first excited subband is much larger than that in the ground subband [16]. Even in wide GaAs QWs, where interface roughness scattering should be less effective, recent



reports [18, 19] showed that interface roughness scattering has a larger effect on linewidth than either electron-electron scattering or bulk impurity scattering.

However, owing to further development of heterostructures growing techniques it is quite natural to expect, that the contribution of interface roughness scattering mechanism should decrease. Hence, the detailed discussion of other scattering mechanisms, especially phonon scattering mechanism, are still actual and need more detailed investigation. Furthermore, quantitative estimation of intersubband absorption coefficient in QWs is still actual.

In the presented paper, we apply the method described in [20], which, in its turn based on Ando's theory [17], to calculate broadening due to scattering by LA phonons and ionized impurities (ION), in order to compare their respective contributions to intersubband absorption linewidth. Moreover, we offered a way to estimate absorption coefficient based on a formula for the two-dimensional (2D) dynamical conductivity.

On the other hand, there is a need to consider a more realistic model of the confining potential, which takes into account both the physical and chemical properties of the structure and its geometry. The first form height and shape of the potential at the interface, and the geometry determines the symmetry of the Hamiltonian (in the absence of external fields). For these purposes, different models were applied for confinement potentials in low-dimensional systems [21-25]. In the first approximation, the confinement potential can be approximated by a parabolic one. Let us mention, that the ideal parabolic approximation works well for comparably low levels. Thus, we will suppose, that QW confinement potential looks like

$$V_{conf}(z) = \frac{m^* \omega_0^2 z^2}{2}, \quad (1)$$

where m^* is the effective mass of electron, ω_0 is the frequency of QW confinement potential, defined with the help of virial theorem according to the relation $\omega_0 \sim \frac{\hbar}{m^* L^2}$. Furthermore for exact equality we will represent ω_0 over L dependence as

$$\omega_0 = \frac{\gamma \hbar}{m^* L^2}, \quad (2)$$

where γ is some fitting parameter, which provides the exact equality in equation (2).

2. Theory

A theory for absorption linewidth due to ISBT in 2D systems was formulated by Ando [10, 17] for elastic scatterers in case of single-particle excitation. Absorption lineshape for transitions between the lowest subbands is described as real part of 2D dynamical conductivity

$$\text{Re} \sigma_{zz}(\omega) = \frac{e^2 f_{10}}{2m^*} \int \frac{m^*}{\pi \hbar^2} dE f(E) \frac{\hbar \Gamma_{op}(E)}{(\hbar \omega - E_{10})^2 + \Gamma_{op}(E)^2}, \quad (3)$$

It is suggested, that all electrons are initially in the ground subband.

Here,

$$\Gamma_{op}(E) = \frac{1}{2} [\Gamma_{intra}(E) + \Gamma_{inter}(E)] \quad (4)$$

$$\Gamma_{intra}(E) = 2\pi \sum_{\vec{k}'} \left\langle \left| (0\vec{k}' | H_1 | 0\vec{k}) - (1\vec{k}' | H_1 | 1\vec{k}) \right|^2 \right\rangle \delta(\varepsilon(\vec{k}) - \varepsilon(\vec{k}')) \Big|_{E=\varepsilon(\vec{k})} \quad (5)$$

$$\Gamma_{inter}(E) = 2\pi \sum_{\vec{k}'} \left\langle \left| (0\vec{k}' | H_1 | 1\vec{k}) \right|^2 \right\rangle \delta(\varepsilon(\vec{k}) - \varepsilon(\vec{k}') + E_{10}) \Big|_{E=\varepsilon(\vec{k})} \quad (6)$$

e is the elementary charge, \hbar is the reduced Planck constant, m^* – the electron effective mass, f_{10} is the oscillator strength, $E_{10} = (E_1 - E_0)$ is the intersubband energy difference between lowest

subbands, $f(E)$ is the Fermi distribution function at temperature T , $|n\vec{k}\rangle$ is the state vector of the electron with subband index n and wave vector \vec{k} , and $\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}$, H_1 is the scattering potential, and the $\langle \dots \rangle$ denotes the average over distribution of scatterers.

Expression (5) originates from the difference in effective potentials of scatterers for the two subbands and vanishes if the effective potential is the same. The term (6) describes relaxation process connected with intersubband scatterings. A parabolic conduction band is assumed, or a constant effective mass for different subbands. As in [20] the full width at half maximum of the spectrum given by equation (4) as $2\Gamma_{\text{op}}$.

As noted above, in current paper considerations are performed within frame of single-particle model. But for full consideration of intersubband absorption problem many-body effects should be taken into account. There are two relevant many-body effects: static and dynamic screening. The former screens the potentials of elastic scatterers while the latter induces collective charge-density excitation because of the incident optoelectric field. The static screening effect can be included by replacing the scattering matrix element $\langle n\vec{k}' | H_1 | n\vec{k} \rangle$ with a new expression [20]. So the screening correction only results in dividing $\langle 0\vec{k}' | H_1 | 0\vec{k} \rangle$ in equation (4) by the factor

$$S(q, T) = \left[\frac{1}{\kappa(q, T)} - \left(\frac{1}{\kappa(q, T)} - 1 \right) \frac{F_{(00)(11)}(q)}{F_{(00)(00)}(q)} \right]^{-1} \quad (7)$$

where $\kappa(q, T)$ is the static dielectric function [26], [27], and $F_{(kl)(mn)}(q)$ is a form factor defined by [17]

$$F_{(kl)(mn)}(q) = \int dz \int dz' \xi_k(z) \xi_l(z) \xi_m(z') \xi_n(z') e^{-q|z-z'|} \quad (8)$$

In our paper we discuss parabolic infinitely high QW, so there is no screening factor in equation (5). $S(q, T)$ hardly affects absorption linewidth because it is ~ 1 .

A depolarization field is considered as the major contributor for dynamic screening effect. It brings to a new expression for absorption lineshape of collective excitation - $\text{Re} \tilde{\sigma}_{zz}(\omega)$. The resonance energy \tilde{E}_{10} of $\text{Re} \tilde{\sigma}_{zz}(\omega)$ is blue-shifted from the original resonance energy E_{10} of $\text{Re} \sigma_{zz}(\omega)$, and $\tilde{E}_{10} = \sqrt{E_{10}^2 + (\hbar\omega_p)^2}$, where ω_p is the plasma frequency. The blue-shift $\tilde{E}_{10} - E_{10} \approx (\hbar\omega_p)^2 / 2E_{10}$ is called the depolarization shift. The linewidth of $\text{Re} \tilde{\sigma}_{zz}(\omega)$ is the same as $\text{Re} \sigma_{zz}(\omega)$ if $2\Gamma_{\text{op}}$ is independent of energy [1], but they are different in general. When the depolarization shift is sufficiently small, or $\tilde{E}_{10} - E_{10} < 2\Gamma_{\text{op}}(0)$, $\text{Re} \tilde{\sigma}_{zz}(\omega)$ is approximately equal to $\text{Re} \sigma_{zz}(\omega)$.

Assuming above discussion, in most cases of GaAs QWs examined later in this paper, the depolarization shift $\tilde{E}_{10} - E_{10}$ are small compared with $2\Gamma_{\text{op}}(0)$, so the absorption linewidth is estimated directly from $\text{Re} \sigma_{zz}(\omega)$ in equation (2).

The total scattering rate can be obtained as the sum of rates for different scattering mechanisms, such as scattering by interface roughness (IFR), LO phonons, LA phonons, alloy disorder (AD), and ionized impurities (ION):

$$\Gamma_{\text{op}}(E) = \Gamma_{\text{op}}^{(\text{IFR})}(E) + \Gamma_{\text{op}}^{(\text{LO})}(E) + \Gamma_{\text{op}}^{(\text{LA})}(E) + \Gamma_{\text{op}}^{(\text{AD})}(E) + \Gamma_{\text{op}}^{(\text{ION})}(E) + \dots \quad (9)$$

We perform numerical calculations for a single QW with a parabolic confinement potential. The origin of the z axis is set at the center of the QW. Material constants are taken for a GaAs QW.

2.1. Scattering on ionized ions

When dopant impurities are ionized (donors) electrons in QW are scattered on quasi-2D Coulomb potential of donors

$$V_C = \frac{Ze^2}{\epsilon \sqrt{\rho^2 + (z - z_i)^2}}. \quad (10)$$

The scattering matrix element due to an ionized impurity is obtained by

$$M_{\text{ION}} = \left\langle |(0\vec{k}'|V_C|1\vec{k})|^2 \right\rangle = \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty \varphi_0^* V_C \varphi_1 \rho d\rho dz \quad (11)$$

where

$$\varphi_{n,\vec{k}_i}(\vec{\rho}, z) = \sqrt{\frac{1}{S}} \frac{1}{\sqrt{2^n n!}} \left(\frac{\gamma}{\pi L^2} \right)^{1/4} e^{i\vec{k}_i \cdot \vec{\rho}} e^{-\frac{\gamma z^2}{2L^2}} H_n \left(\frac{\sqrt{\gamma} z}{L} \right), \quad (12)$$

The final expression for matrix element is

$$M_{\text{ION}} = \sqrt{\frac{2}{\gamma}} \frac{\pi L}{S \epsilon} (Ze^2) \exp\left(\frac{L^2 k^2}{4\gamma}\right) \quad (13)$$

As we mentioned above the broadening term connected with intrasubband relaxation (see equation (5)) vanishes if effective potential is the same for the two subbands [17]. So here we consider only the term (6). Also, we proposed the central location of impurities ($z_i = 0$), so impurities distribution is pure 2D. Therefore, for linewidth we have

$$\begin{aligned} \Gamma_{\text{inter}}^{(\text{ION})}(E) &= 2\pi N_i \frac{S^2}{(2\pi)^2} \int d^2 \vec{k}_m (M_{\text{ION}})^2 \delta(\epsilon(\vec{k}) - \epsilon(\vec{k}') + E_{10}) = \\ &= \frac{10.92\pi^2 N_i m^* L^2 (Ze^2)^2}{\gamma \hbar^2 \epsilon^2} \exp\left(\frac{L^2 k_i^2}{\gamma}\right) I_0\left(\frac{L^2 k_i}{\gamma} \sqrt{\frac{2m}{\hbar^2} \hbar \omega_0 + k_i^2}\right) \\ \Gamma_{\text{intra}}^{(\text{ION})}(E) &\equiv 0 \end{aligned} \quad (14)$$

$$\begin{aligned} \Gamma^{(\text{ION})}(E) &= \frac{1}{2} (\Gamma_{\text{intra}}^{(\text{ION})}(E) + \Gamma_{\text{inter}}^{(\text{ION})}(E)) = \\ &= \frac{5.46\pi^2 N_i m^* L^2 (Ze^2)^2}{\gamma \hbar^2 \epsilon^2} \exp\left(\frac{L^2 k_i^2}{\gamma}\right) I_0\left(\frac{L^2 k_i}{\gamma} \sqrt{\frac{2m}{\hbar^2} \hbar \omega_0 + k_i^2}\right) \end{aligned}$$

where

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m^*}; \quad E_1 = \frac{3\hbar \omega_{\text{osc}}}{2}; \quad \epsilon(k') = \frac{\hbar^2 k'^2}{2m^*}; \quad E_0 = \frac{\hbar \omega_{\text{osc}}}{2} \quad (15)$$

We consider only intersubband scattering mechanism here.

2.2. Scattering on LA phonon

Acoustic phonon scattering via deformation potential coupling, or simply LA phonon scattering, is virtually elastic. The 3D scattering matrix element is given by [28]

$$\left\langle |M_{\text{3D}}|^2 \right\rangle = \frac{k_B T D^2}{2c_l} \quad (16)$$

for both LA phonon emission and absorption processes, where D is the deformation potential constant and c_l is the longitudinal elastic constant. Note that equation (16) is independent of the scattering vector as a result of the linear dispersion relation of LA phonons. Therefore, for intersubband scattering only we have

$$\begin{aligned}\Gamma_{\text{inter}}^{(\text{LA})}(E) &= \frac{m^* k_B T D^2}{2c_l} \int_0^\pi d\theta \int_0^\infty dz [\xi_0(z) \xi_1(z)]^2 = \frac{1}{2} \sqrt{\frac{\gamma}{2\pi}} \frac{m^* k_B T D^2}{L \hbar^2 c_l} \\ \Gamma_{\text{intra}}^{(\text{LA})}(E) &= \frac{m^* k_B T D^2}{\pi \hbar^2 c_l} \int_0^\pi d\theta \int_0^\infty dz [\xi_0(z)^2 - \xi_1(z)^2]^2 = \frac{3}{4} \sqrt{\frac{\gamma}{2\pi}} \frac{m^* k_B T D^2}{L \hbar^2 c_l}\end{aligned}\quad (17)$$

The final expression for LA scattering linewidth is

$$\Gamma^{(\text{LA})}(E) = \frac{1}{2} (\Gamma_{\text{intra}}^{(\text{LA})}(E) + \Gamma_{\text{inter}}^{(\text{LA})}(E)) = \frac{5}{8} \sqrt{\frac{\gamma}{2\pi}} \frac{m^* k_B T D^2}{L \hbar^2 c_l} \quad (18)$$

As it seen from figure 1, the linewidth due to scattering on ionized impurities increases with the growth of temperature. The increase is greater, as the temperature decreases.

On figure 2 the linewidth dependence on QW width is presented. As one can see the linewidth is also increases with the width of QW. This result is opposite to the case of scattering on interface roughness [20], which is the most significant scattering mechanism and makes a major contribution to the linewidth [20].

3. Absorption coefficient

The absorption coefficient for transitions between the two lowest subbands can be expressed as

$$\alpha(\omega) = \frac{\text{Re} \sigma_{zz}(\omega)}{L}, \quad (19)$$

where L is the QW thickness. Taking into account the expression (3) for 2D dynamical conductivity, we got

$$\alpha(\omega) = \frac{n_i e^2}{\tilde{n} c \hbar^2 L^2} \left(\frac{2\pi \hbar^2}{m^* k_B T} \right)^{3/2} \int_0^\infty e^{-\frac{E_i}{k_B T}} \frac{\hbar \Gamma_{\text{op}}(E_i)}{(\hbar \omega_0 - \hbar \omega)^2 + \Gamma_{\text{op}}(E_i)^2} dE_i \quad (20)$$

where linewidth includes both LA and ION scattering mechanisms

$$\Gamma_{\text{op}}(E) = \Gamma_{\text{op}}^{(\text{LA})}(E) + \Gamma_{\text{op}}^{(\text{ION})}(E). \quad (21)$$

The final integral expression for absorption coefficient is

$$\alpha(\omega) = C \int_0^\infty e^{-\frac{\hbar^2 y}{2m L^2 k_B T}} \frac{\left[\frac{A}{\hbar \omega_0} \left(e^{y/\gamma} I_0 \left(\frac{1}{\gamma} \sqrt{y(2\gamma + y)} \right) \right) + \frac{B}{\hbar \omega_0} \right]}{(1-x)^2 + \left[\frac{A}{\hbar \omega_0} \left(e^{y/\gamma} I_0 \left(\frac{1}{\gamma} \sqrt{y(2\gamma + y)} \right) \right) + \frac{B}{\hbar \omega_0} \right]^2} dy \quad (22)$$

where the following notations were done

$$\begin{aligned}C &= \frac{\pi}{137\gamma\tilde{n}} \frac{n_i}{2L^2} \left(\frac{2\pi\hbar^2}{m^* k_B T} \right)^{3/2} \exp\left(-\frac{\hbar\omega_0}{2k_B T}\right) \\ A &= \frac{5.46\pi^2 N_i (Ze^2)^2}{\hbar\omega_0 \epsilon^2} \\ B &= \frac{5}{8} \sqrt{\frac{\gamma}{2\pi}} \frac{m^* k_B T D^2}{L \hbar^2 c_l} \\ x &= \frac{\hbar\omega}{\hbar\omega_0} \\ y &= L^2 k_i^2.\end{aligned}\quad (23)$$

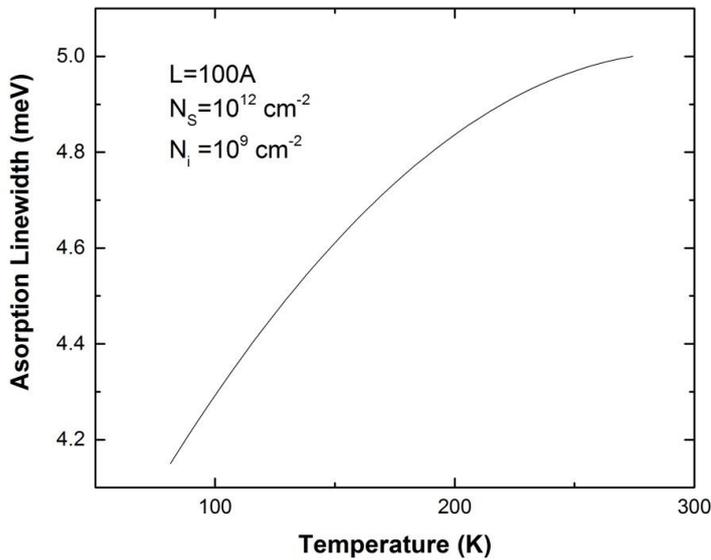


Figure 1. The dependence of $2\Gamma_{op}(E)$ due to ionized impurity and acoustic phonon scattering on temperature.

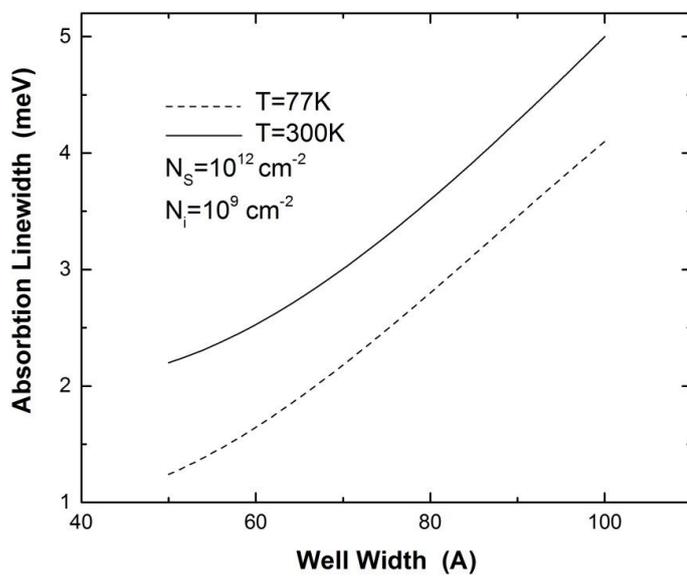


Figure 2. The dependence of $2\Gamma_{op}(E)$ on QW width.

4. Results

We obtained absorption lineshape for different temperatures, impurity concentrations and QW width. The results are in good agreement with the results of previous authors as well as with experimental data.

In figures 3, 4 absorption lineshape for different temperatures are presented. As it can be seen from Figs absorption peak is blueshifted with the decrease of QW width. Also the picture changes with the increase of temperature.

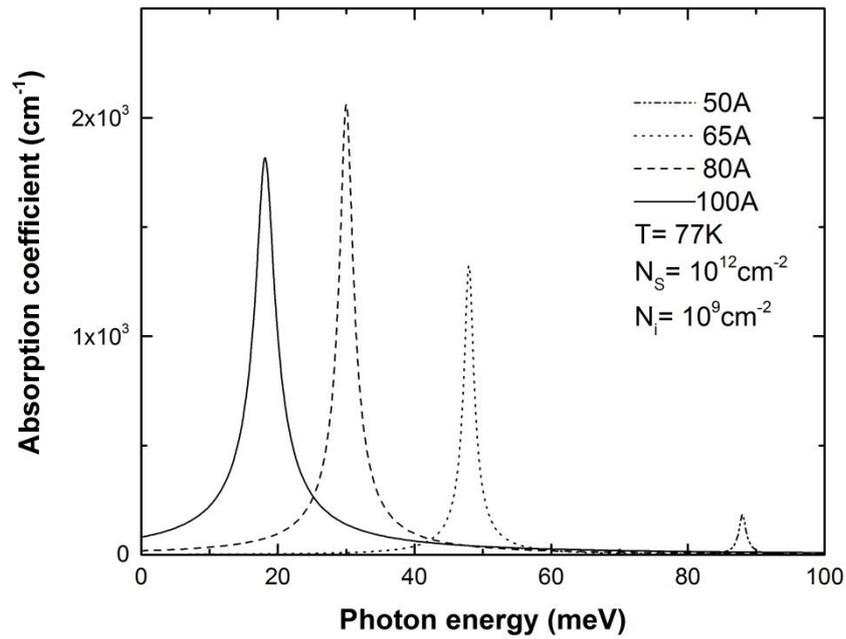


Figure 3. The dependence of absorption coefficient on QW width (for $T=77\text{K}$).

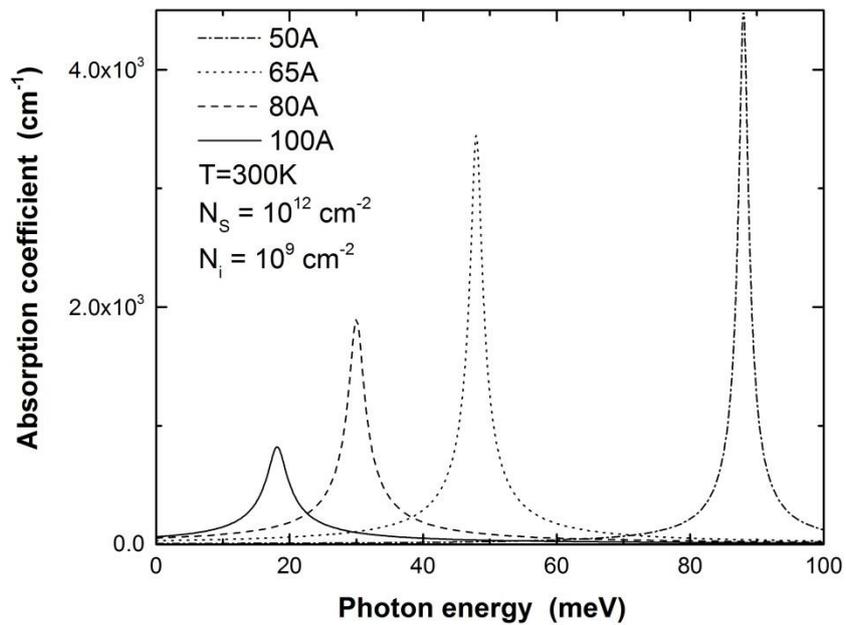


Figure 4. The dependence of absorption coefficient QW width (for $T=300\text{K}$).

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