Low-temperature exciton linewidth in short-period superlattices

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The expressions for absorption and luminescence linewidths of Wannier excitons in short-period superlattices are derived for several scattering mechanisms. The wave function of the 1*s* excitons is assumed to be a product of (i) a variational function describing relative motion of electrons and holes, and (ii) the envelope functions for the electrons and holes obtained from the Kronig-Penney model. The scattering rates are calculated by using Fermi's golden rule for deformation potential, interface roughness, and alloy-disorder scattering. The linewidth due to interface-roughness scattering is also expressed by employing the self-consistent Born approximation. Numerical values presented for $GaAs/Al_{0.3}Ga_{0.7}As$ superlattices indicate that the deformation-potential scattering is weak and that the alloy-disorder scattering is significant for lower values of the superlattice period. The most significant contribution to the linewidth comes from the interface-roughness scattering; the golden rule yields quite large values, whereas reasonable values are obtained from the self-consistent Born approximation.

I. INTRODUCTION

Excitonic absorption and luminescence in semiconductor heterostructures like quantum wells (QW's) and superlattices (SL's) have intrigued a large number of researchers around the world over the past decade because of a number of physical phenomena and technological applications in a new generation of optoelectronic and photonic devices.[1,2] It is also recognized that the study of the luminescence line shape may provide otherwise inaccessible information regarding chemical and structural properties of heterointerfaces in QW's and SL's.[3,4] In the past, emphasis was given mainly to the study of excitonic process in QW's (Refs. 5–11) from both the theoretical and the experimental points of view, because of the technological nonviability of growing high-purity interfaces with an accurate *in situ* monitoring of the periodic structure of the SL. It is only recently that similar studies are being extended to SL's, owing to the immense development achieved in the techniques of crystal growth as well as that of the post-growth analysis of the material properties. Study of the excitonic features in the luminescence from SL's is, therefore, an important field to be explored. Theories of excitons in SL's developed so far concern mainly the calculation of the oscillator strength and the excitonic binding energy. To our knowledge, absorption and photoluminescence (PL) line shapes of excitons in SL's have so far remained fairly unexplored from the theoretical point of view.

It is well known that the absorption (emission) peaks due to formation (recombination) of excitons are broadened by several intrinsic and extrinsic mechanisms.[8–10] In the present paper a theory for the excitonic linewidth (LW) is developed, taking into account the scatterings by deformation-potential (DP) acoustic phonons, interface roughness (IFR), and alloy disorder (AL). We have not considered polar-optic phonon scattering since its contribution at low temperatures is negligible.[12] At higher temperatures this scattering contributes significantly to the LW; however, the calculations become quite involved since the contribution from both the bound excitonic states and the continuum states must be taken into consideration. The theory is presented in Sec. II. In Sec. III results obtained for a $GaAs/Al_{0.3}Ga_{0.7}As$ SL are presented and discussed. A comparison is also made between the values obtained by using envelope functions derived from the Kronig-Penney (KP) model[13,14] and from the tight-binding (TB) approximation.[15]

II. THEORY

A. Envelope function

The two-particle Schrödinger equation in the present case is written as[16,17]

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z_e}\left[\frac{1}{m_e}\frac{\partial}{\partial z_e}\right]-\frac{\hbar^2}{2}\frac{\partial}{\partial z_h}\left[\frac{1}{m_h}\frac{\partial}{\partial z_h}\right]-\frac{\hbar^2}{2M_{\parallel}}\nabla_{\mathbf{R}}^2-\frac{\hbar^2}{2\mu_{\parallel}}\nabla_{\mathbf{r}}^2+V_e(z_e)+V_h(z_h)-\frac{e^2}{\{r^2+(z_e-z_h)^2\}^{1/2}}-E\right]\psi(\mathbf{R},\mathbf{r},z_e,z_h)=0\ , \quad (1)$$

where $V_e(z_h)$ and $V_h(z_h)$ are, respectively, the periodic potentials seen by the electron and the hole. In the above equation the center of mass and the relative coordinates, **R** and **r**, respectively, are used to describe the in-plane motion only, as has been done in the case of single QW's. $M_{\parallel}$ and $\mu_{\parallel}$ are, respectively, the total and the reduced

masses in the layer plane, m_i and z_i are the mass and the coordinate in the z direction for the ith particle ($i=e,h$). The wave function for the exciton in the QW's is expressed as a product of (i) $\exp(i\mathbf{K}_\parallel \mathbf{R})$, describing free center-of-mass motion in the x-y plane, (ii) a function for bound excitonic state, and (iii) envelope functions for the confined electron and hole. In the present case, electron and hole wave functions are not confined but extended along the z direction also. We now assume that

$$z_i=\hat{z}_i+n_iL, \quad i=e,h \ , \tag{2}$$

where L is the period of the SL, and $n_{e(h)}$ represents the supercell in which the electron (hole) is present, and $|\hat{z}_i|\le L/2$. In Eq. (1) we may neglect $|\hat{z}_e-\hat{z}_h|$ since it is much smaller than the excitonic Bohr radius and may write the Coulomb potential term as $-e^2/(r^2+n^2L^2)^{1/2}$, with $n=n_e-n_h$. This leads to the following wave function for the exciton in a SL

$$\begin{aligned}\psi_{1s}=&(L/V)^{1/2}N_{1s}\exp(i\mathbf{K}_\parallel\cdot\mathbf{R})\\&\times\exp\{i(n_ek_{ze}+n_hk_{zh})L\}f_e(\hat{z}_e)f_h(\hat{z}_h)\\&\times\exp\left\{-\frac{\beta}{2}(r^2+n^2L^2)^{1/2}\right\},\end{aligned} \tag{3}$$

where V is the volume of the SL, $\mathbf{K}_\parallel$ and $\mathbf{R}$ are the wave vector and the position vector of the excitonic center of mass in the layer planes, r is the corresponding spatial separation of the electron and the hole, and $k_{ze(h)}$ is the z component of the electron (hole) wave vector. $f_e(\hat{z}_e)$ and $f_h(\hat{z}_h)$ are the normalized SL periodic envelope functions for electron and hole, respectively, with $\hat{z}_{e(h)}$ ranging over a single period. The parameter β is the variational parameter obtained by minimizing the binding energy, and the constant N_{1s} is calculated from the normalization condition that the total probability of finding an exciton in the entire volume of the SL is unity. N_{1s} may, therefore, be expressed as

$$N_{1s}=[\beta^2/2\pi]^{1/2}\frac{1-\exp(-\beta L)}{\{1-(1-\beta L)\exp(-\beta L)\}^{1/2}} \ . \tag{4}$$

It should be noted that in the absence of the periodic potential the problem reduces to that for a QW and the wave function contains the terms $f_i(\hat{z}_i)$ instead of $f_i(\hat{z}_i)\exp(in_ik_{zi}L)$. Thus Eqs. (1)–(4) describe the excitonic envelope function in short-period SL's, with which one can proceed to derive expressions for excitonic linewidths (LW's) due to various scattering mechanisms.

B. Deformation-potential acoustic-phonon scattering

The squared matrix element for the transition from a state of wave vector $\mathbf{K}$ to another state of wave vector $\mathbf{K}'$, without any change in the internal state due to DP acoustic-phonon scattering, may be expressed as[6,12]

$$\begin{aligned}&|M^{\pm}_{\rm DP}(\mathbf{K},\mathbf{K}')|^2\\&=|H_c^{\rm DP}(-\alpha_h\mathbf{Q}_\parallel,Q_z)-H_v^{\rm DP}(\alpha_e\mathbf{Q}_\parallel,Q_z)|^2\\&\quad\times(N_{\rm Q}+\tfrac{1}{2}\pm\tfrac{1}{2})\times\delta_{\pm\mathbf{Q}_\parallel,\mathbf{K}_\parallel-\mathbf{K}'_\parallel}\delta_{\pm Q_z,K_z-K'_z} \ ,\end{aligned} \tag{5}$$

where K_z is defined as $K_z=k_{ze}+k_{zh}$, $\alpha_{e(h)}=m_{e(h)}/M$, $M_\parallel=m_{\parallel e}+m_{\parallel h}N_{\rm Q}$ is the occupation number of the three-dimensional (3D) phonons of wave vector $(\mathbf{Q}_\parallel,Q_z)$, and + (−) refers to the emission (absorption) process. $H^{\rm DP}_{c(v)}$ represents the contribution from the interaction of electron (hole) with DP acoustic phonons, and can be expressed as

$$H^{\rm DP}_{c(v)}(\alpha\mathbf{Q}_\parallel,Q_z)=N_{1s}^2I_{e(h)}(Q_z)\sum_n\xi_{n,e(h)}(\mathbf{Q}_\parallel) \ . \tag{6}$$

In Eq. (6)

$$I_{e(h)}(Q_z)=\int d\hat{z}_{e(h)}\exp(iQ_z\hat{z}_{e(h)})E^{\rm DP}_{c(v)}|f_{e(h)}(\hat{z}_{e(h)})|^2 \tag{7}$$

and

$$\xi_{n,e(h)}(\mathbf{Q}_\parallel)=\int d^2r\exp\{i\alpha\mathbf{Q}_\parallel\cdot\mathbf{r}-\beta(r^2+n^2L^2)^{1/2}\} \ , \tag{8a}$$

where

$$\begin{aligned}\alpha&=-\alpha_h \quad \text{for } \xi_{n,e}\\&=\alpha_e \quad \text{for } \xi_{n,h} \ .\end{aligned} \tag{8b}$$

$E^{\rm DP}_{c(v)}$ is defined as[12,18]

$$E^{\rm DP}_{c(v)}=\left[\frac{\hbar|\mathbf{Q}|}{2\rho uV}\right]^{1/2}D_{c(v)} \ . \tag{9}$$

In Eq. (9) $D_{c(v)}$ is the DP constant for the conduction (valence) band, $\hbar$ is the reduced Planck's constant, ρ is the mass density of the crystal material, and u is the velocity of the acoustic wave in the crystal. The interaction potential is assumed to be unscreened. Working out the integration in Eq. (8a) and performing the summation involved in Eq. (6), we get.

$$\begin{aligned}&|M^{\pm}_{\rm DP}(\mathbf{K},\mathbf{K}')|^2\\&=\left[\frac{\beta^3[1-\exp(-\beta L)]^2}{1-(1-\beta L)\exp(-\beta L)}\right]^2(N_{\rm Q}+\tfrac{1}{2}\pm\tfrac{1}{2})\\&\quad\times\left|\frac{I_e(Q_z)\Theta_e(\mathbf{Q}_\parallel)}{\eta_e^3\chi_e^2(\mathbf{Q}_\parallel)}-\frac{I_h(Q_z)\Theta_h(\mathbf{Q}_\parallel)}{\eta_h^3\chi_h^2(\mathbf{Q}_\parallel)}\right|^2,\end{aligned} \tag{10}$$

where $I_{e(h)}(Q_z)$ is as defined in Eq. (7), and

$$\Theta_{e(h)}(\mathbf{Q}_\parallel)=1-(1-\eta_{e(h)}L)\exp(-\eta_{e(h)}L) \ , \tag{11a}$$

$$\chi_{e(h)}(\mathbf{Q}_\parallel)=1-\exp(-\eta_{e(h)}L) \ , \tag{11b}$$

$$\eta_{e(h)}(\mathbf{Q}_\parallel)=[\beta^2+\alpha^2_{h(e)}Q^2_\parallel]^{1/2} \ .$$

The transition rate may now be written as

$$W^{\pm}_{\rm DP}(\mathbf{K})=\frac{2\pi}{\hbar}\sum_{\mathbf{K}'}|M^{\pm}_{\rm DP}(\mathbf{K},\mathbf{K}')|^2\delta(E_{\mathbf{K}'}-E_{\mathbf{K}}\pm\hbar\omega_{\mathbf{Q}}) \ , \tag{12}$$

where $\omega_{\mathbf{Q}}$ is the angular frequency of phonons defined as $\omega_{\mathbf{Q}}=u|\mathbf{Q}|$. The summation in Eq. (12) is converted into an integral over $\mathbf{K}'$ by the following conversion rule:[19]

$$\sum_{\mathbf{K}'}\rightarrow\frac{V}{8\pi^3}\int dK'_z\int d^2K'_\parallel \ . \tag{13}$$

The integration over $\mathbf{K}'$ is performed following the

method developed by Palmier and Chomette[19] using the δ function in Eq. (12). The transition rate is finally expressed as follows:

$$W^{\pm}_{\mathrm{DP}}(\mathbf{K})=\left[\frac{MV}{4\pi^2\hbar^3}\right]\int_{-\pi/L}^{\pi/L}dK_z'\int_0^{2\pi}d\vartheta_K|M^{\pm}_{\mathrm{DP}}(\mathbf{K},\mathbf{K}')|^2\ , \tag{14}$$

with the condition $|\mathbf{K}_{\parallel}'|=|\mathbf{K}_{\parallel}|$, ϑ_K being the angle between $\mathbf{K}_{\parallel}$ and $\mathbf{K}_{\parallel}'$. We can, therefore, express the in-plane component of the phonon wave vector, $\mathbf{Q}_{\parallel}$, as

$$Q_{\parallel}^2=4K^2\sin^2(\vartheta_K/2)\ . \tag{15}$$

The half-width at half maximum (HWHM) of the exciton line, Γ, is related to the transition rate by the following relation:[8–10]

$$\Gamma=\hbar W^{-}(0)/2\ . \tag{16}$$

In the above equation the emission process is not considered since at the zone center it is only the absorption of phonons that can take place. We can finally express the HWHM of the excitonic PL spectra due to the DP acoustic phonon scattering by the following expression:

$$\Gamma_{\mathrm{DP}}=\left[\frac{k_BTM_{\parallel}}{4\hbar^2\rho u^2}\right]\int d\hat{z}[D_c(\hat{z})|f_e(\hat{z})|^2-D_v(\hat{z})|f_h(\hat{z})|^2]^2\ , \tag{17}$$

where k_B is the Boltzmann constant, T is the lattice temperature, and $\hat{z}$ ranges over a single period.

C. Interface-roughness scattering

Following Dharssi and Butcher,[15] one can express the scattering potential associated with the interface roughness (IFR) as

$$H^j_{i\mathrm{IFR}}=\begin{cases}-V_0, & jL+b+\Omega_i<z<jL+b, \quad \Omega_i<0\\ V_0, & jL+b<z<jL+b+\Omega_i, \quad \Omega_i>0\\ 0 \ \text{otherwise}\ ,\end{cases} \tag{18}$$

TABLE I. Values of parameters used in the calculations. All data are from Ref. 20. $\lambda_1=200$ Å and $\lambda_0=35$ Å (Ref. 14). $\Delta E_e=0.6$ eV and $\Delta E_h=0.21$ eV (Ref. 20).

Parameters	GaAs	$Al_{0.3}Ga_{0.7}As$
m_e	$0.0665\times m_0$	$0.0885\times m_0$
m_h	$0.377\times m_0$	$0.453\times m_0$
u (m/s)	4.81×10^3	4.825×10^3
ρ (kg/m^3)	5.36×10^3	4.88×10^3
D_c (eV)	6.7	6.34
D_v (eV)	2.7	2.67

where Ω_i's represent the undulations in the interfaces of the order of monolayers; $i=1$ for the interfaces when $Al_x\,Ga_{1-x}\,As$ is grown on GaAs, and $i=2$ when GaAs is grown on $Al_x\,Ga_{1-x}\,As$. In Eq. (18) b is half the barrier width and V_0 is the barrier height. The total scattering potential, that includes contributions from all the interfaces, may be expressed as

$$H_{\mathrm{IFR}}=\sum_{i=1}^{2}\sum_j H^j_{i\mathrm{IFR}}\ . \tag{19}$$

It has been accepted that IFR obeys a Gaussian correlation written as

$$\langle\Omega_i^j(x,y)\Omega_{i'}^{j'}(x',y')\rangle=\delta_{jj'}\delta_{ii'}\Omega_i^2\exp[-\lambda_i^{-2}|\mathbf{r}-\mathbf{r}'|^2]\ , \tag{20}$$

where λ_i is the correlation length. The correlation lengths are found to be different for the two different interfaces discussed above.[15] The values of λ_1 and λ_2 for the materials we have considered may be found in Table I. The Fourier transform coefficient of this potential may be expressed as[15]

$$|V_i(\mathbf{Q}_{\parallel})|^2=\pi V_0^2\Omega_i^2\lambda_i^2\exp(-\lambda_i^2Q_{\parallel}^2/4)\ . \tag{21}$$

The matrix element for scattering from the potential mentioned above is given by

$$|M_{\mathrm{IFR}}(\mathbf{K},\mathbf{K}')|^2=[\pi L/V]N_{1s}^4\sum_{j=1}^{2}\sum_n[V_{0e}|f_e(b)|^2\xi_{n,e}(\mathbf{Q}_{\parallel})-V_{0h}|f_h(b)|^2\xi_{n,h}(\mathbf{Q}_{\parallel})]^2\Omega_j^2\lambda_j^2\exp(-\lambda_j^2Q_{\parallel}^2/4)\ , \tag{22}$$

where $\xi_{n,e,(h)}(\mathbf{Q})$ is as defined by Eqs. (8a) and (8b), and $V_{0e(h)}$ is the conduction- (valence-) band offset. Equation (22) can be further simplified to

$$\begin{aligned}|M_{\mathrm{IFR}}(\mathbf{K},\mathbf{K}')|^2&=\sum_{j=1}^{2}[\pi L/V]\left[\frac{\beta^3\{1-\exp(-\beta L)\}^2}{1-(1-\beta L)\exp(-\beta L)}\right]^2\\&\times[V_{0e}|f_e(b)|^2\xi_e-V_{0h}|f_h(b)|^2\xi_h]^2\\&\times\Omega_j^2\lambda_j^2\exp(-\lambda_j^2Q_{\parallel}^2/4)\ ,\end{aligned} \tag{23}$$

where

$$\xi_{e(h)}=\frac{1-(1-\eta_{e(h)}L)\exp(-\eta_{e(h)}L)}{\eta_{e(h)}^3\{1-\exp(-\eta_{e(h)}L)\}^2} \tag{24}$$

and $|\mathbf{Q}_{\parallel}|$ is given by Eq. (15).

The expression of the HWHM, obtained by using Fermi's golden rule (GR), may be written as

$$\Gamma_{\mathrm{IFR}}=\left[\frac{\pi M}{2\hbar^2}\right]\sum_{j=1}^{2}[V_{0e}|f_e(b)|^2-V_{0h}|f_h(b)|^2]^2\Omega_j^2\lambda_j^2\ . \tag{25}$$

It has been shown earlier[21] for single QW's that in the GR calculation the broadening of states is underestimat-

ed and the results calculated under a strong scattering limit based on the self-consistent Born approximation (SCBA) yield reasonable values of LW. It is of interest to compare the results under these two limiting conditions in the case of SL's, also. In the strong scattering limit SCBA express the HWHM as

$$\Gamma^2_{\mathrm{SCBA}}=\sum_{\mathbf{K}'}|M(\mathbf{K},\mathbf{K}')|^2 . \tag{26}$$

As has been done in the case of DP phonon scattering, the summation over $\mathbf{K}'$ in Eq. (26) is converted into an integration, and after performing the integration the final expression becomes

$$\Gamma^2_{\mathrm{IFR,SCBA}}=\sum_j \Gamma_j^2 , \tag{27}$$

where

$$\Gamma_j=\left[\frac{\beta^3\{1-\exp(-\beta L)\}^2}{1-(1-\beta L)\exp(-\beta L)}\right]^2 \Omega_j I_{j,\mathrm{IFR}} , \tag{28}$$

with

$$I^2_{j,\mathrm{IFR}}=\int_0^\infty dx_j \exp(-x_j)[\zeta_e(x_j)-\zeta_h(x_j)]^2 . \tag{29}$$

In Eq. (29), $\zeta_{e(h)}(x_j)$ is given by Eq. (24), $X_j=\lambda_j^2 Q_\parallel^2/4$, and

$$\eta_{e(h)}=\beta\{1+(2\alpha_{h(e)}/\lambda_j\beta)^2 x_j\}^{1/2} .$$

Rudin, Reinecke, and Segall[11] considered weak coupling versus strong coupling in the exciton-phonon interaction. We have assumed, following their argument, a zero bandwidth for the exciton in-plane motion, in deriving Eq. (26) of the present paper. Including the vertex correction diagrams, one obtains the following series for the exciton Green's function:[11,22,23]

$$\begin{aligned}G(E)=&(E-E_0+i\varepsilon)^{-1}+\Gamma^2(E-E_0+i\varepsilon)^{-3}\\&+3\Gamma^4(E-E_0+i\varepsilon)^{-5}\\&+15\Gamma^6(E-E_0+i\varepsilon)^{-7}+\cdots ,\end{aligned} \tag{30}$$

where E is the energy, E_0 is the ground-state energy, ε is the positive infinitesimal, and Γ is defined in Eq. (26). It may be noted that

$$\int_X^\infty \exp(X^2-t^2)dt=\frac{1}{2X}-\frac{1}{2^2X^3}+\frac{1\times3}{2^3X^5}-\frac{1\times3\times5}{2^4X^7}\cdots .$$

Using this the Green's function can be written as

$$\begin{aligned}G(E)&=-\frac{i}{2\pi}\frac{\sqrt{2}}{\Gamma}\int_T^\infty \exp(T^2-t^2)dt\\&=-i\frac{\sqrt{2}}{2\pi\Gamma}\exp(T^2)\frac{\sqrt{\pi}}{2}\operatorname{erfc}(iz) ,\end{aligned} \tag{31}$$

where

$$T=-\frac{1}{\Gamma\sqrt{2}}(E-E_0+i\varepsilon) \quad\text{and}\quad z=-\frac{E-E_0+i\varepsilon}{\Gamma\sqrt{2}} ,$$

and erfc (iz) is the complementary error function.[24]

The expression has been obtained along the same lines as in the exciton-phonon case.[11,22] Through analytical continuation one obtains

$$\operatorname{Re}\operatorname{erfc}(iz)\xrightarrow[\varepsilon\to0]{}1,$$

and so

$$\operatorname{Im}G(E)=-\frac{\sqrt{2\pi}}{2\Gamma}\exp\{-(E-E_0)^2/2\Gamma^2\} . \tag{32}$$

The above expression once again establishes the fact that in the strong scattering limit the line shape changes from Lorentzian to Gaussian with a half-width given by Eq. (26).

The criteria to distinguish between strong scattering and weak scattering has been discussed in terms of the respective half-widths by several authors.[11,25]

D. Alloy-disorder scattering

Our theory is based on the virtual crystal approximation (VCA). We also consider the inner-potential model,[26,27] in which the alloy-scattering potential is taken to be a spherically symmetric square well of height ΔE and radius r_0. The Fourier series expansion of such a potential is written as[28]

$$\Delta V_j=\sum_{Q_\parallel}(2\pi\rho_j\Delta E)\frac{J_1(\rho_j Q_\parallel)}{Q_\parallel}\exp(-i\mathbf{Q}_\parallel\cdot\boldsymbol{\rho}_j) , \tag{33}$$

where

$$|\boldsymbol{\rho}_j|=\{r_0^2-(z-z_j)^2\}^{1/2} , \tag{34}$$

z_j being the z coordinate of the jth cation site, and $\mathbf{Q}_\parallel$ the Fourier conjugate of ρ, and J_1 the first-order Bessel function of the first kind.

Following the procedure for deriving the matrix element for electrons in a SL, as described in Ref. 23, we may express the same for excitons by the equation given below:

$$|M_{\mathrm{AL}}(\mathbf{K},\mathbf{K}')|^2=[\tfrac{4}{3}\pi r_0^3]^2(L/V)N_0x(1-x)\phi(\mathbf{Q}_\parallel) . \tag{35}$$

In Eq. (32) N_0 is the number of alloy sites per unit volume, x is the mole fraction of Al in $\mathrm{Al}_x\,\mathrm{Ga}_{1-x}\,\mathrm{As}$, and

$$\phi(\mathbf{Q}_\parallel)=\sum_j\left[N_{1s}^2\sum_n\{\Delta E_e|f_e(\hat{z}_j)|^2\xi_{n,e}-\Delta E_h|f_h(\hat{z}_j)|^2\xi_{n,h}\}\right]^2 , \tag{36}$$

where $\Delta E_{e(h)}$ is the alloy-scattering potential for electron (hole), and $\xi_{n,e(h)}$ is as defined in Eq. (8a). Replacing the summation over the alloy sites by an integration over $\hat{z}$ one may write

$$\phi(\mathbf{Q}_\parallel)=\int d\hat{z}\left[\frac{\beta^3\{1-\exp(-\beta L)\}^2}{1-(1-\beta L)\exp(-\beta L)}\right]^2\times[\Delta E_e|f_e(\hat{z})|^2\zeta_e-\Delta E_h|f_h(\hat{z})|^2\zeta_h]^2 , \tag{37}$$

where $\zeta_{e(h)}$ is as defined in Eq. (24).

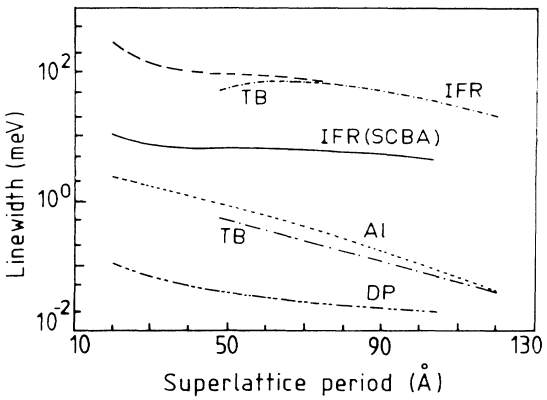

FIG. 1. Linewidths of Wannier excitons as a function of superlattice period at 300 K for scattering due to the deformation-potential (DP) acoustic phonons, the alloy disorder (AL), and the interface roughness (IFR) by using Kronig-Penney envelope functions; TB represents the corresponding results from tight-binding calculations. The plot marked IFR (SCBA) shows the results for IFR scattering under the self-consistent Born approximation.

The expression for HWHM in this case, obtained from Eqs. (32), (34), and (16), is given by

$$\Gamma_{\mathrm{AL}}=\left[\frac{8\pi^2}{9\hbar^2}r_0^6 N_0 M_{\|} x(1-x)\right] \times \int d\hat{z}\{\Delta E_e |f_e(\hat{z})|^2-\Delta E_h |f_h(\hat{z})|^2\}^2 . \quad (38)$$

III. RESULTS AND DISCUSSIONS

The values of the physical parameters used in our calculations are given in Table I. Figure 1 shows the plot of the LW values against the SL period for a $GaAs/Al_{0.3}Ga_{0.7}As$ SL at 300 K, due to DP, AL, and IFR scattering. The envelope functions $f_e(\hat{z}_e)$ and $f_h(\hat{z}_h)$ are calculated by using both the KP and TB models. In the KP calculations the widths of the wells and the barriers are taken to be equal. The results indicate that the contributions from DP scattering to the LW is insignificant. We have not shown the results obtained by using the TB envelope functions, as the values are not much different from those calculated using the KP envelope functions. As one compares the values obtained with KP and TB envelope functions for IFR and AL scatterings, one notices that the two methods give almost the same values for large SL periods. When the period is large, the barrier widths are also large and hence the carriers are confined within the wells. Thus the envelope functions and the values of Γ obtained from the two models are identical. On the other hand, for small periods ($L < 6$ nm) the TB model gives LW values smaller than what is obtained from the KP model. This is due to the fact that in the TB model coupling between the wells is underestimated. For smaller periods our calculations reveal that the leakage of the particle wave function into the barriers becomes too large, so that the TB model becomes invalid. It is worthwhile to note as well that LW's in the TB model vary with well widths (SL period) in the same fashion as the LW's in the MQW's, i.e., the values increase with increasing well widths, show a peak, and then decrease.[1]

We now examine the values of LW for IFR scattering obtained by using Fermi's golden rule and under SCBA. As may be seen from the curves in Fig. 1, the values using the golden rule are considerably larger than the experimental values for a multiple-quantum-well (MQW) structure. Although experimental data for SL's are not available, we believe that the values will not be much different from the values for MQW's. The SCBA calculation, on the other hand, gives reasonable values for LW for IFR scattering. Similar results have already been found for single QW's.[21]

It is now appropriate to give a rigorous justification for the use of strong-coupling theory for IFR scattering by using the arguments of previous works[11,25] and the numerical results obtained in the present one. It was pointed out that the weak-scattering theory is applicable and the line shape is Lorentzian if the ratio $\Gamma_{\mathrm{GR}}/\Gamma_{\mathrm{SCBA}} \ll 1$. On the other hand, if this ratio is $\gg 1$ then the strong-coupling theory would be valid. Comparing the results given in Fig. 1 it may be concluded that for IFR scattering the strong-coupling limit is appropriate and the line shape should be Gaussian. For phonon and alloy-disorder scatterings, however, the usual weak scattering limit is valid in SL's also, as has been concluded by Rudin, Reinecke, and Segall.[11]

IV. CONCLUSIONS

In conclusion, we have derived the expressions for the linewidths of excitons in a superlattice, considering acoustic phonon, alloy-disorder, and interface roughness scattering. The numerical values obtained by using Kronig-Penney and tight-binding envelope functions agree for large superlattice periods, but are different for short-period superlattices. For IFR scattering it is found that the broadening of states plays a vital role and Fermi's golden rule breaks down, so that the self-consistent Born approximation calculation proves to be a better approach.

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