# Nonparabolicity Effects on Transition Rates Due to Confined Phonons in Quantum Wells

Augusto M. Alcalde and Gerald Weber

*Instituto de Física, Universidade Estadual de Campinas,*
*Caixa Postal 6165, 13083-970 Campinas SP, Brazil*

Received July 21, 1995

We calculate the electron-LO-confined-phonon scattering rates in GaAs- AlGaAs quantum wells considering the influence of nonparabolicity on the energy bands. A reformulated slab model is employed to describe the confined phonon and a simple model is assumed to take these nonparabolicity effects into account. An expression for the intra and intersubband scattering rates in the extreme quantum limit is obtained. We find that the nonparabolicity increasses significantly the scattering rates in all transitions. Some scattering rates for interface modes are also reported in order to evaluate the nonparabolicity effect on the total scattering rates.

The subject of electron-phonon interaction in polar semiconductor quantum wells has recently attracted a great deal of interest. This is because electronic properties such as the cooling of photoexcited carriers, carrier tunneling and the mobility of high-speed heterostructure devices are primarily governed by the scattering of electrons by polar-optical phonons. Particular interest has been directed at the possibility that LO-phonon confinement may affect significantly the scattering rates. The electron confined LO phonon interaction has been studied using either dielectric continuum models[1,2] or microscopic lattice dynamical models[3]. The macroscopic continuum models are commonly employed in literature, and calculations of electron-intra and intersubband scattering rates in GaAs- AlGaAs quantum wells and superlattices due to the confined phonons compare successfully with experimental results[4,5]. On the other hand, is known that the influence of nonparabolicity of the energy bands on the several electronic properties cannot be considered negligible[6–8]. The energy of the bottom of an electron subband in a quantum well can often be determined to a reasonable accuracy by a simple parabolic $E-\mathbf{k}$ relation. For subbands fairly far from the bulk conduction band edge, corrections due to the nonparabolicity can be important. The determination of electron-phonon scattering rates in a realistic analysis has a great practical importance, particulary in carrier capture processes with large kinetic energy. For these processes, which implies large momenta, the parabolic-band approximation becomes less justified even for GaAs-AlGaAs structures where nonparabolicity effects can be safely neglected.

In this work, we have investigated the influence of subband nonparabolicity on the electron-LO-confined phonon intra and intersubband scattering rates in GaAs-AlGaAs quantum wells. We show also results of scattering rates in the parabolic approximation in order to make comparisons and show that important quantitative differences occur, in this way we are able to determine for which situations the subband nonparabolicity can be neglected or not.

Several schemes have been proposed to take these nonparabolicity effects into account[9–11]. The more important difference between those models is the form of the nonparabolic energy dispersion relation and the definition of the appropiate boundary conditions and effective masses. For the description of band nonparabolicity we follow the model proposed by Nag and Mukhopadhyay[11] which is thought to adequately represent the subband nonparabolicity of GaAs-AlGaAs quantum wells, the nonparabolic $E-\mathbf{k}$ relation is given by

$$E - V_i = \frac{\hbar^2 k^2}{2m_i^*}(1 - \gamma_i k^2) \quad (1)$$

where $E$ is the total electron energy, $m_i^*$ is the band edge mass and $\gamma_i$ the nonparabolicity parameter. The subscript $i$ indicates the well layer ($i = W$) and the barrier layer ($i = B$) and $V_i$ is the bulk conduction band offset taken as $V_w = 0$ and $V_B = V_0$.

The electron-LO-confined phonon scattering rates are obtained from the Fermi golden rule and with the well known electron-confined-phonon interaction Hamiltonian[12,13], we obtain the following expression for the intra and intersubband nonparabolic scattering rates

$$W_{np}^{(i)} = \frac{m_i^* \lambda^2 L}{\hbar^3} \sum_n |G_n|^2 (N_{LO} + 1) \frac{1}{\alpha_i} \left\{ \frac{a_n L^2}{2\gamma} [(1 - 2\gamma k_z^2) - \alpha_i] + b_n \right\}^{-1} , \quad (2)$$

with

$$\alpha_i = [(2\gamma k_z^2 - 1)^2 + 4\gamma Q_i^2]^{1/2} , \quad (3)$$

where $k_z$ is the $z$-component of the initial (final) electron wave vector for intrasubband (intersubband) transitions, and $G_n$ is the electron-phonon overlap integral. For phonon emission we define

$$Q_i^2 = \pm \frac{2m_i^*}{\hbar^2} (E_{\text{initial}} - E_{\text{final}} - \hbar\omega_{LO}) , \quad (4)$$

where the upper sign corresponds to intrasubband transitions, while the lower sign corresponds to intersubband transitions. Further parameters in Eq. (2) are defined in previous works[2,14].

An elementary application of L'Hopital rule shows that in the limit $\gamma \to 0$ the Eq. (2) becomes the parabolic scattering rates expressions reported in the literature[1,2]

$$W_p^{(i)} = \frac{m_i^* \lambda^2 L}{\hbar^3} \sum_n |G_n|^2 (N_{LO} + 1)[b_n - a_n L^2 Q_i^2]^{-1} \quad (5)$$

The $a_n$ and $b_n$ constants are obtained from the normalization of the phonon displacement and depends on the description of the confined phonon modes. For the description of the confined phonon modes we used the corrected slab model[15] which gives scattering rates very close to the phenomenological Huang and Zhu model[16] and compares successfully with experimental results[4,5]. However, any confined phonon model can be used for the scattering rates given in Eq. (2), by using the appropriate expressions for the coefficients $a_n$ and $b_n$ and the electron-phonon overlap integral $G_n$ [2,14]. The expression for the scattering rates given by Eq. (2) is consequence exclusively from the nonparabolic energy dispersion relation given by Eq. (1), no aditional assumptions about the model which calculates the energy eingenvalues and eigenstates was so far.

In order to obtain the electron energy levels and wave functions we use the model proposed by Nag and Mukhopadhyay[11], this model has the advantage that the overlap functions have the same analytic form of the parabolic case, thus it allows a straightforward inclusion of the nonparabolicity effects into existing parabolic-band calculations[1,2].

We express our results as an average scattering rate $W = p_W W^{(W)} + p_B W^{(B)}$, where $p_W(p_B)$ is the probability of finding the electron initially in the well (barrier) subband. This procedure is necessary because the effective masses as well as the nonparabolicity parameters in the well are different from those of the barrier.

For the calculations of scattering rates due to emission of confined longitudinal optical phonons we assume a GaAs-$Al_xGa_{1-x}As$ quantum well with finite barriers of 224 meV corresponding to $x = 0.3$. The material parameters used in our calculations are: for GaAs, the effective mass $m^* = 0.0665m_0$, the dielectric constants

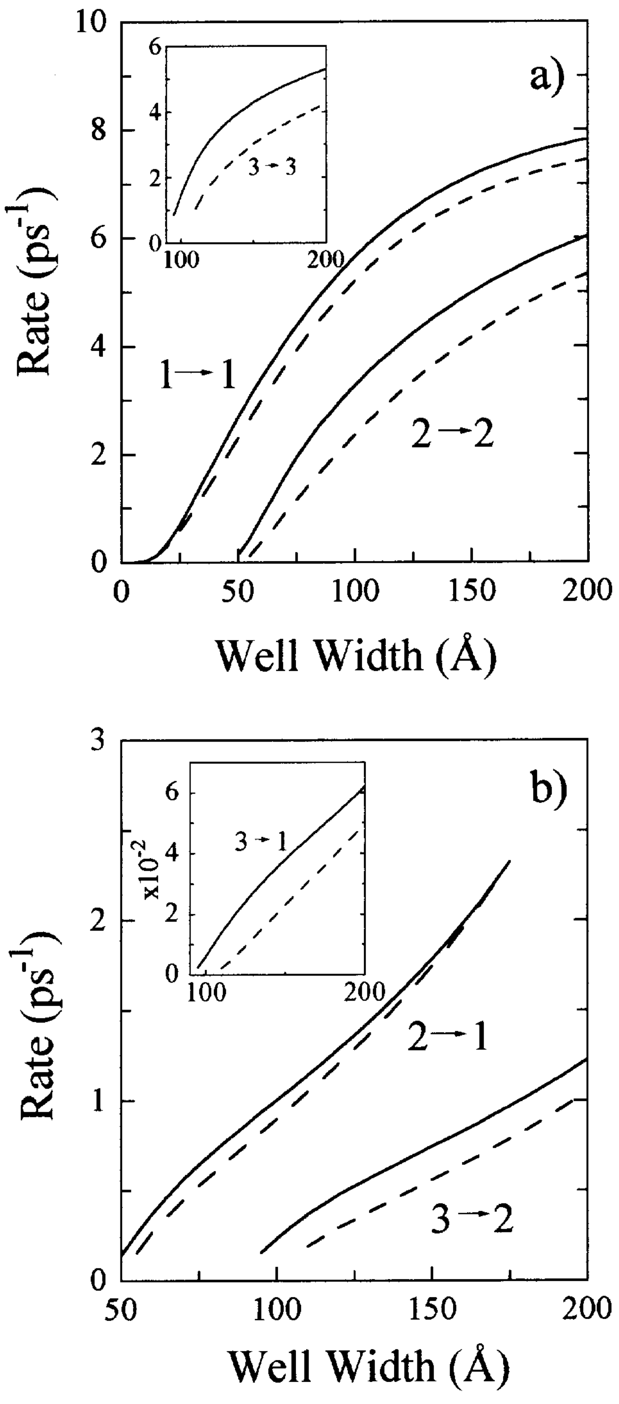


Figure 1. Scattering rates for (a) intrasubband and (b) intersubband transitions in a GaAs-Al$_x$Ga$_{1-x}$As quantum wells as a function of a well width. Solid lines contains nonparabolicity dashed lines is parabolic calculation.

$\epsilon_0 = 12.35$ and $\epsilon_\infty = 10.48$, the bulk phonon energies $\hbar\omega_{LO} = 36.8$ meV and $\hbar\omega_{TO} = 33.29$ meV, the nonparabolicity parameter is taken as $\gamma = 4.9 \times 10^{-19}$ m$^2$; for GaAlAs, the effective mass $m^* = 0.0901 m_0$, the dielectric constants $\epsilon_0 = 14^{-12}$ and $\epsilon_\infty = 10.07$, the phonon energies $\hbar\omega_{LO} = 46.97$ meV and $\hbar\omega_{TO} = 44.77$ meV, the nonparabolicity parameter $\gamma = 2.67 \times 10^{-19}$ m$^2$. The phonon occupation number is assumed $N_{LO} \sim 0$. In Fig. 1(a) we show the calculated scattering rates for intrasubband transitions due to LO-phonon as a function of the well width. The solid lines represent the scattering rates with the inclusion of subband nonparabolicity an the dashed lines are for the parabolic-band approximation. Note that the scattering rates are significantly increased in all intrasubband transitions due to effects of nonparabolicity, especially for transitions in higher subbands, but the scattering rates are otherwise not qualitatively different from those in the parabolic- band approximation. Intersubband scattering rates are shown in Fig. 1(b), where we find a similiar behaviour, but the scattering rates are less affected than intrasubband transitions when the well thickness increases. For large quantum wells where the subband separation becomes close to the LO-phonon energy, the phonon in-plane wave vector becomes zero and thus the effect of nonparabolicity should be small. The intersubband $2 \rightarrow 1$ transition shows this behaviour.

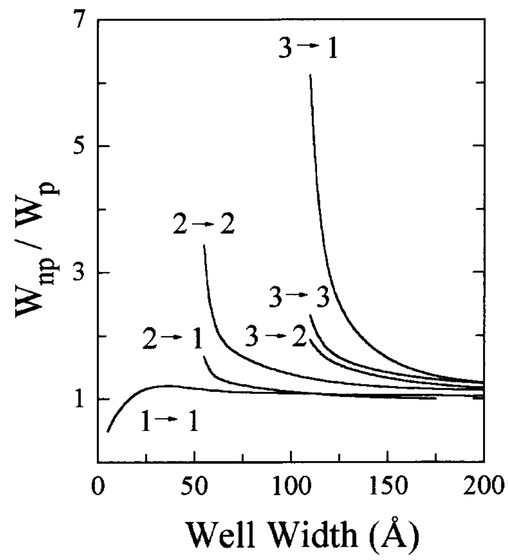


Figure 2. Ratio of the nonparabolic and parabolic scattering rates, for the intra and intersubband transitions shown in Figs. 1(a) and 1(b) as a function of the well width.

The effect of the subband nonparabolicity is better illustrated in Fig. 2 where we display the ratio of the nonparabolic and parabolic scattering rates $[W_{np}/W_p]$. Except for $1 \rightarrow 1$ transitions for narrow wells (less than 15 Å) all nonparabolic scattering rates are higher. For quantum wells larger than 150 Å the transition rates with subband nonparabolicity are very close to those in the parabolic-band approximation. In general, for transitions from higher energy states the subband nonparabolicity affects the scattering rates more strongly. The enhancement of the scattering rates with the inclusion of subband nonparabolicity results mainly from a larger electron-phonon overlap as well as from a larger density of final electron states. This enhancement occurs despite of the fact that the emitted confined phonons have a larger wave vector, due to the nonparabolicity of the electron subband, which implies in a smaller electron-phonon (Fröhlich) coupling factor. For large quantum wells (> 150 Å) the nonparabolicity effects are practically negligible. In this case as the electronic confinement is greatly reduced the subband nonparabolicity has a smaller effect on the overlap integral In order to evaluate the effects the nonparabolicity on the total scattering rates we have also calculated the scattering rates for intrasubband ad intersubband transitions due to electron- interface-phonons interaction considering the nonparabolicity of the energy subbands. In Fig. 3 we show the total scattering rates for (a) $1 \rightarrow 1$ and (b) $2 \rightarrow 1$ transitions and the individual contributions of confined and interface phonons for GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells. In general the transition rates due to interface modes are lowered by the subband nonparabolicity, in contrast to the increase by confined modes. However, the decrease of nonparabolic scattering rates due to interface phonons is not compensated by the increase due to confined phonons except in few special situations. Thus, the total scattering rates also suffers considerable changes induced by the inclusion of subband nonparabolicity. The general decrease of the interface-phonon scattering rates is due to the decrease of the electron-phonon overlap integral as the electron wave function moves away from the interfaces.

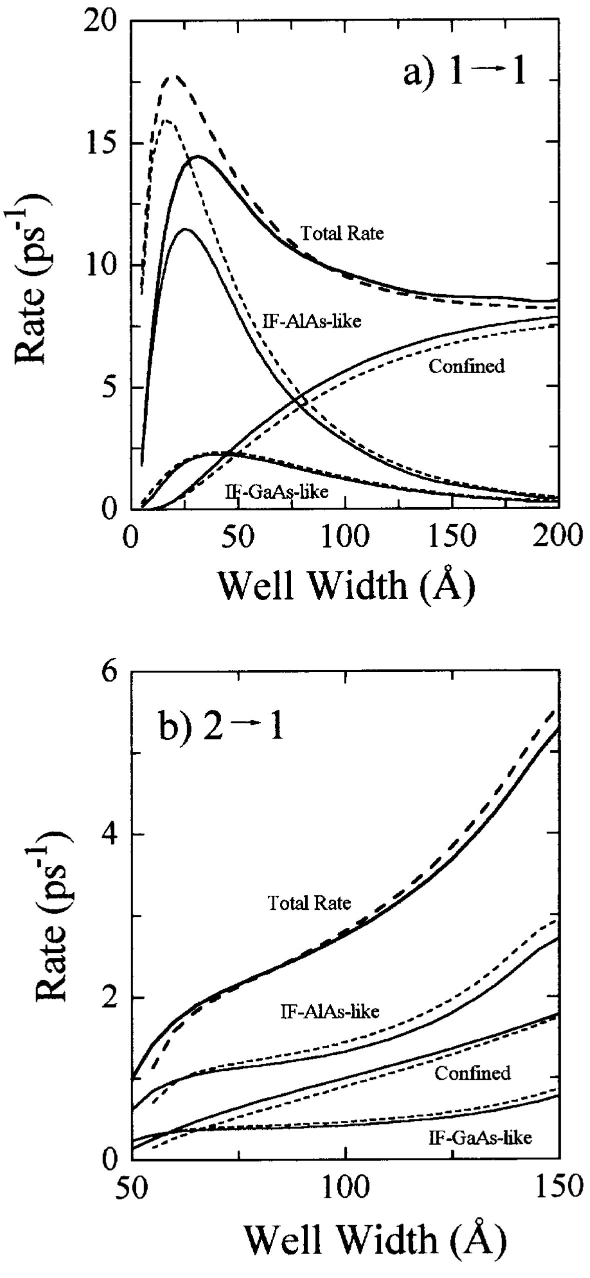


Figure 3. Total scattering rates for (a) intrasubband $1 \rightarrow 1$ transition and (b) intersubband $2 \rightarrow 1$ transition as a functions of the well width. Transition rates for confined and interface phonons are also showed. Solid lines are transitions rates with subband nonparabolicity and dashed lines are for parabolic bands.

In conclusion, we have calculated the scattering rates for intrasubband and intersubband transitions due to electron-confined and interface-phonon interaction in quantum wells, including band nonparabolicity. It is found that for intra and intersubband transitions due to emission of confined phonons the scattering rates are significantly increased, while that for interface phonons the scattering rates are decreased. The total scattering rates is considerable affected by the subbband nonparabolicity. In particular for higher subbands the nonparabolicity effects becomes more important.

We are grateful to A. M. de Paula for helpful discussions. Financial support by CNPq and CNPq/RHAE is also acknowledged.

**References**

1. S. Rudin and T. L. Reinecke, Phys. Rev. **B 41**, 7713 (1990).
2. G. Weber, A. M. de Paula, and J. F. Ryan, Semicond. Sci. Technol. **6**, 397 (1991).
3. H. Rücker, E. Molinari, and P. Lugli, Phys. Rev. **B 45**, 6747 (1992).
4. G. Weber and A. M. de Paula, Appl. Phys. Lett. **63**, 3026 (1993).
5. A. M. de Paula and G. Weber, Appl. Phys. Lett. **65**, 1281 (1994).
6. K. H. Yoo, L. R. Ram-Moham, and D. F. Nelson, Phys. Rev. **B 39**, 12808 (1989).
7. B. W. Kim and E. M. Charlson, J. Appl. Phys. **76**, 1334 (1994).
8. P. Banerji and C. K. Sarkar, Solid State Commun. **90**, 325 (1994).
9. D. F. Nelson, R. C. Miller, and D. A. Kleinman, Phys. Rev. **B 35**, 7770 (1987).
10. U. Ekenberg, Phys. Rev. **B 36**, 6152 (1987).
11. B. R. Nag and S. Mukhopadhyay, Phys. Stat. Sol. (b) **175**, 103 (1993).
12. J. J. Licari and R. Evrard, Phys. Rev. **B 15**, 2254 (1977).
13. N. Mori and T. Ando, Phys. Rev. **B 40**, 6175 (1989).
14. G. Weber and J. F. Ryan, Phys. Rev. **B 45**, 11202 (1992).
15. G. Weber, Phys. Rev. **B 46**, 16171 (1992).
16. K. Huang and B. Zhu, Phys. Rev. **B 38**, 13377 (1988).