

NON-PARABOLICITY EFFECTS ON ELECTRON-CONFINED LO-PHONON SCATTERING RATES IN GaAs - Al_{0.45}Ga_{0.55}As SUPERLATTICE

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Abstract

We investigate theoretically the effect of non-parabolic band structure on the electron-confined LO-phonon scattering rate in GaAs-Al_{0.45}Ga_{0.55}As superlattice using the quantum treatment, the new wave function of electron miniband conduction of superlattice and a reformulation slab model for the confined LO-phonon modes. An expression for the scattering rates is obtained. Our results show that for transitions due to the emission of confined LO-phonon the scattering rates significantly increase for non-parabolicity case.

Keywords: Confined LO-phonon, miniband, non-parabolicity, scattering rate, superlattice.

INTRODUCTION

Recently there has been much interest in the study of electron-phonon interaction in III-V semiconductor quantum wells (QWs) and superlattice (SLs) [Klein 1986, Cardona 1989, Thatan *et al.* 1989]. This is because the phonon scattering determines the electron transport properties at room temperature and high electric fields also at low temperature. For instance, the cooling of photoexcited carriers, carrier tunnelling and mobility high-speed heterostructure devices are primarily governed by the scattering of electron by polar-optical-phonons. Some results in Raman scattering, cyclotron-resonance and magnetophonon-resonance measurements show the dominance of electron interaction with LO-phonons and reveal important information about the vibration modes in the layers forming (SL) [Jusserand and Cardona, Priester *et al.* 1983, Jusserand *et al.* 1984, Klein 1986, Seilmcier *et al.* 1987, Huang and Fen 1988, Guntherodt 1989]. The electron-LO-phonon interaction where found to be strongly dependent on both the geometrical shape and the parameters of the constituent materials [Fomin and Pokatilov 1985, Pokatilov *et al.* 1993]. The polaron effect in heterostructures of size is, however, quite different from that in bulk materials. Several models have been proposed to describe the electron-confined LO-phonon interaction in superlattice. Dielectric continuum models [Rudin and Reinecke 1990, Weker *et al.* 1991, Weber 1993, Shi and Pan 1995],

microscopic lattice dynamical models [Wu and Woot 1971, Rücker *et al.* 1992, Bhatt *et al.* 1993], or slab model [Fuch and Kliewer 1965, Licari and Evrard 1997]. The already several theoretical studies reported on calculations of relaxation time due to scattering of carriers semiconductor hetero-structure by optical-phonon, treated the case single or multiple quantum wells [Lassmig 1984, Ferrira and Bastard 1989, Liang 1992, Duan *et al.* 1993].

The purpose of this paper is to present a set of calculated results of scattering rates in superlattice, we have considered the carrier scattering by LO-phonon. The effect of band nonparabolicity on scattering rates calculated is analyzed. First section summarizes the theoretical framework used in the calculations, while next section presents the discussion of numerical results presented graphically and lastly brief conclusion is given.

THEORETICAL MODEL

MINIBAND STRUCTURE AND ENVELOPE WAVEFUNCTIONS

Using an effective-mass Hamiltonian and the transfer-matrix method the total energy of electron associated to the first miniband and the analytically the exact normalized wave function [Osted *et al.* 2003] are:

$$\varepsilon_{\xi} = \frac{\hbar^2 k_{\perp}^2}{2m_w^*} + E_1^* - \frac{\Delta_1}{2} \cos(k_z l) \quad (1)$$

$$\Psi_w(z) = \frac{e^{-ik_z \frac{l}{2}} e^{ink_z l}}{\sqrt{N}} \left\{ b_2 e^{ik(z-n-\frac{l}{2})} + \beta e^{-ik(z-n-\frac{l}{2})} \right\} \quad \mathbf{-L+1}_b \langle z-nl \rangle \mathbf{1}_b, \quad (2)$$

$$\Psi_b(z) = \frac{e^{-ik_z \frac{l}{2}} e^{ink_z l}}{\sqrt{N}} \left\{ p \cosh[\rho(z-nl+1_b)] + q \sinh[\rho(z-nl+1_b)] \right\} \quad \mathbf{-1}_b \langle z-nl \rangle \mathbf{1}_b, \quad (3)$$

$$\hbar^2 k^2 = 2m_w^* E, \quad h^2 \rho^2 = 2m_b^* (V_b - E), \quad \lambda = m_w^* / m_b^*, \quad \mathbf{L} = \mathbf{1}_b + \mathbf{1}_w. \quad (4)$$

$$\mathbf{x} = \mathbf{k} \mathbf{l}_w, \quad \mathbf{y} = \rho \mathbf{1}_b, \quad \beta^{\pm} = \sin(x) \cosh(y) - K^{\pm} \cos(x) \sinh(y) - \sin(k_z l). \quad (5)$$

$$p = b_2 e^{(ix/2)} + \beta^{-} e^{-(ix/2)}, \quad q = \frac{ik}{\lambda \rho} \left(e^{(ix/2)} - \beta^{-} e^{-(ix/2)} \right). \quad (6)$$

$$k^{\pm} = \frac{1}{2} \left(\frac{\lambda \rho}{k} \pm \frac{k}{\lambda \rho} \right), \quad b_2 = k^+ \sinh(y), \quad N = A' \left(b_2^2 + (\beta^{-})^2 \right) + B' \beta^{-}. \quad (7)$$

$$\Pi^{\mp} = \left(\frac{2k}{\lambda \rho} \right) K^{\pm}, \quad (8)$$

$$A' = 1_w + \left(1_b \left[\frac{\Pi^-}{2} + \Pi^- \frac{\sinh(2y)}{4y} \right] \cos(x) + \left[\frac{1}{k} - \frac{k}{\lambda \rho} \frac{\cosh(2y) - 1}{2\rho} \right] \sin(x) \right), \quad (10)$$

$$B' = 2b_2 \left\{ L_b \left[\Pi^+ / 2 + \Pi^- (\sinh(2L_b \rho) / 4L_b \rho) \right] \cos(kL_w) + \right. \\ \left. [(1 - \cosh(2L_b \rho) / 2\lambda \rho^2)k + 1/k] \sin(kL_w) \right\} \quad (11)$$

SCATTERING RATES

The interaction electron-phonon Hamiltonian in low dimensional systems depends on the specific phonon spectra in the system and is different from the Fröhlich Hamiltonian for bulk phonon. The macroscopic dielectric continuum model [Lucas *et al.* 1970, Licari and Evrard 1977, Pokatilov and Beril 1983, Wendler 1985] gives the functional form of the interface modes, confined and half space LO modes. The electron-confined LO-phonon interaction Hamiltonian as derived from Fröhlich interaction is given by [Saitoh 1972, Khuang and Zhu 1988]

$$H_{e-p} = \lambda \sum_{q_{\perp}, n\alpha=\pm} e^{iq_{\perp} \cdot r} H(z) t_{n\alpha}(q_{\perp}) u_{n\alpha}(z) \times [a_{n\alpha}(q_{\perp}) + a_{n\alpha}^{\dagger}(-q_{\perp})] \quad (12)$$

where $a(q)$ and $a^{\dagger}(q)$ are the creation and annihilation operators for a bulk phonon phonons in the mode q , the even (-) and odd (+) confined phonon modes and n is the miniband index, while the coupling

$$\lambda^2 = iC_{\mu} / \sqrt{V} q \quad (13)$$

where V is the volume. C can written explicitly [Weber 1992] as

$$C = \left[\frac{e^2 \hbar \omega_{LO}}{2\epsilon_0} \left(\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)} \right) \right]^{\frac{1}{2}} \quad (14)$$

where $\hbar \omega_{LO}$ is the optic of the n th miniband, $\epsilon(\infty)$ and $\epsilon(0)$ are the optical static dielectric constants respectively, Ω is the volume and e the electronic charge. For the slab model [Kane 1957, Lucas *et al.* 1970] $u_{n\alpha}(z)$ are defined as

$$u_{n+}(z) = \cos(n \pi z / L_w) \quad n=1,3,5,\dots \quad (15)$$

$$u_{n-}(z) = \sin(n \pi z / L_w) \quad n=2,4,6,\dots \quad (16)$$

$t_{n\alpha}$ is given by

$$t_{n\alpha} = \frac{1}{[q_{\perp}^2 + (n \pi / L_w)^2]^{1/2}} \quad n=1,2,3,\dots \quad (17)$$

Finally

$$H(z) = \begin{cases} 1 & \text{if } -w \leq z \leq w \\ 0 & \text{otherwise} \end{cases} \quad (18)$$

The scattering rate $w_{i \rightarrow f}$ appearing is obtained from the Fermi Golden Rule

$$W_{i \rightarrow f}(\mathbf{k}) = \frac{2\pi}{\hbar} \sum_f \left| \langle \xi_f | H_{e-p} | \xi_i \rangle \right|^2 \quad (19)$$

with the Hamiltonian given by Eq. (14) we obtain

$$W_{i \rightarrow f} = \frac{\pi}{2\pi V \hbar} \int (N_{LO} + \frac{1}{2} \pm \frac{1}{2}) \frac{e^2 \hbar \omega_{LO}}{q_{\pm}} \left(\frac{1}{\varepsilon(\infty)} - \frac{1}{\varepsilon(0)} \right) \delta(U^{\pm}) I(k_z^i, k_z^f, q_{\pm}) dN_f \quad (20)$$

In this expression the integration is over the number of final states N_f , where

$$I_n(k_z^i, k_z^f, q_{\pm}) = \sum_{q_{\pm}} \sum_{n, \alpha} |G_{n, \alpha}^{i \rightarrow f}(k_z^i, k_z^f)|^2 |t_{n, \alpha}(q_{\pm})|^2 \quad (21)$$

A δ - function represents the energy conservation quantity

$$\delta(U_{\pm}) = \delta \left(\frac{\hbar^2}{2m^*} (k_{\perp}^i{}^2 - k_{\perp}^f{}^2) + E_{k_z^f} - E_{k_z^i} \pm \hbar \omega_{LO}(q_{\pm}) \right)$$

\pm absorption and emission process. For optical phonon scattering

$$q_{\pm}^2 = k_{\perp}^i{}^2 - k_{\perp}^f{}^2 - 2k_{\perp}^i k_{\perp}^f \cos(\theta) + (k_z^i - k_z^f \mp G)^2 = \text{cte} \quad (22)$$

G is the reciprocal lattice vector of the SL. N_{LO} is the LO phonon occupation number defined:

$$N_{LO} = (\exp \frac{\hbar \omega_{LO}}{k_B T} - 1)^{-1} \quad (23)$$

$G_{n, \alpha}^{i \rightarrow f}(k_z^i, k_z^f)$ is the overlap integral of the electron wave function and the z -dependent of the electron – confined – phonon Hamiltonian

$$G_{n, \alpha}^{i \rightarrow f}(k_z^i, k_z^f) = \int_{-l/2}^{l/2} \psi_f^*(z) u_{n, \alpha} \psi_i(z) dz \quad (24)$$

where ψ_i , ψ_f are the electron envelope miniband wave function in the initial and final states respectively [Khuang and Zhu 1988]. L is the period SL; $L = L_w + L_b$. At $U^{\pm} = 0$, k_{\perp}^f and k_{\perp}^i terms must equal.

NON-PARABOLICITY EFFECT

According to the model of Kane [Ando 1982, Ekenberg 1988, Person and Cohen 1988] two model, the eigenfunctions of the Hamiltonian in the direction of the superlattice (with $k_x = k_y = 0$) associated to a conduction band electron [Ando 1982, Vasilopoulos and Ait-el-Habti 1989] with an energy $0 < E < V_b$, are solutions the Schrödinger equation [Bastard 1981]:

$$\left(\hbar^2 a_2 \frac{\partial^2}{\partial z^2} + \hbar^4 a_4 \frac{\partial^4}{\partial z^4} \right) y(z) + (E - V(z)) y(z) = 0 \quad (25)$$

$$a_2 = \frac{1}{2m^*(z)} \quad ; \quad a_4 = \frac{1}{Eg} \left(\frac{1}{2m^*} - \frac{1}{2m_0} \right) \quad (26)$$

The corrective term reflects the nonparabolicity effect (via a_4). The integration of Eq. (25) through an interface of small arbitrary thickness provides the new boundary conditions:

$$a_{2,w}\psi_w + a_{4,w}\hbar^2\psi_w'' = a_{2,b}\psi_b + a_{4,b}\hbar^2\psi_b'' \quad (27)$$

This expression which ensures the continuity of the local current density generalizes that of [Bastard and 1986, Ait-el-Habti 1990] where $a_4=0$. In case of non-parabolicity, the wave functions corresponding to the new condition Eq. (27)

generalize those where the continuity of $\frac{1}{m^*} \frac{d\Psi(z)}{dz}$ is used. As the last

Hamiltonian without parabolicity, the wave functions are given in the n^{th} well and barrier by expressions (2) and (3); Due to the new conditions Eq. (27) on the derivation of the wave function, the analysis of the preceding sections can be used with λ replaced by μ which we define as follows. From Eqs. (25) and (4), expressions of k, ρ and μ are given by:

$$\hbar^2 k^2 = 4m_w^* E_{w,\max} \left\{ 1 - \sqrt{1 - \frac{E}{E_{w,\max}}} \right\}; \quad E_{w,\max} = \left(\frac{a_2^2}{4a_4} \right)_w \quad (28)$$

$$\hbar^2 \rho^2 = 4m_b^* (E_{b,\max} - V_0) \left\{ -1 + \sqrt{1 + \frac{V_0 - E}{E_{b,\max} - V_0}} \right\}; \quad E_{b,\max} = \left(\frac{a_2^2}{4a_4} \right)_b \quad (29)$$

$$\mu = \frac{a_{2,b} + \hbar^2 \rho^2 a_{4,b}}{a_{2,w} - \hbar^2 k^2 a_{4,w}} \quad (30)$$

When introducing the new expressions of wave vectors k and ρ in Eqs. (1), (2) and (3), we obtained the new expressions for dispersion relation and the waves functions in the barrier and the wells of SL, by continuation those of the times relaxations and mobility. If the effect of the nonparabolicity becomes negligible ($a_4 = 0$), $\mu \rightarrow \lambda = \frac{m_w^*}{m_b^*}$, defined in the parabolic case. Expressions (28), (29)

allow an explicit relationship of ρ in relation with k . For $E_{\max}^b - V_b = E_{\max}^w$ (i.e. $k_0^2 = \lambda \rho_0^2$) insignificant values of ρ and k , we find the parabolic case given by relation (4).

NUMERICAL RESULTS AND DISCUSSION

For numerical computation, we have chosen the GaAs-Ga_{1-x}Al_xAs with $x=0.45$ as a superlattice. The parameters pertaining to the system are:

$m_w^* = 0.067m_0$, $m_b^* = 0.104m_0$, where m_0 the free electron mass. The dielectric constant in wells is taken equal to the one in barrier: $\varepsilon_d = 12.8$, $\varepsilon_\infty = 10.9$, $I_w = 108 \text{ \AA}^0$, $I_b = 38 \text{ \AA}^0$, $V_b = 495 \text{ meV}$, $E_{w,\max} = 2 \text{ eV}$, $E_{b,\max} - V_b = E_{w,\max}$,

the energy of a bulk GaAs LO-phonon $\hbar \omega_{LO} = 36.8$ meV, the static and high frequency dielectric constant for GaAs: $\epsilon_s = 12.35$ and $\epsilon_\infty = 10.48$.

In Fig. 1 calculated rates for intra-miniband transitions due to interaction electron-confined LO-phonon as function of well width of superlattice are shown. Note that the scattering rate is not qualitatively different from those in the parabolic - band approximation. In the non- parabolic band approximation, scattering rates due to confined LO-phonon become larger. It is can be due to the overlap integrals given by Eq. (24), in band-non-parabolic electron wave function become more confined in the direction of superlattice (Fig. 2).

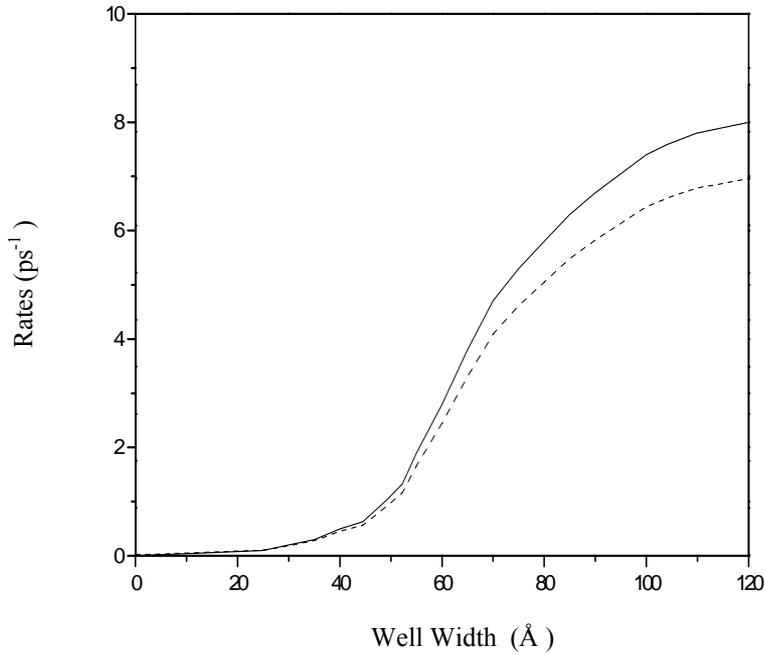


Fig. 1: Scattering rates for intra-miniband transitions in GaAs-Al_{0.45}Ga_{0.55}As superlattice as a function of well width. Solid line contains non-parabolicity and dashed line is parabolic approximation.

Another element which influences the scattering rates the densities of final states. In Fig. 3 we give the density of final states in the parabolic band-approximation compares it with the density of final states in the non-parabolic band-approximation.

It is shown that density in the non-parabolic band approximation is larger. In Fig. 4, the ratios of non-parabolic and parabolic scattering rate (W_{np}/W_p) has been displayed. For intra-miniband of narrow well (width well inferior to 45 Å) all non-parabolic scattering rates are close to those in the parabolic-band approximation. For quantum wells the transition rates with band non-parabolicity are larger.

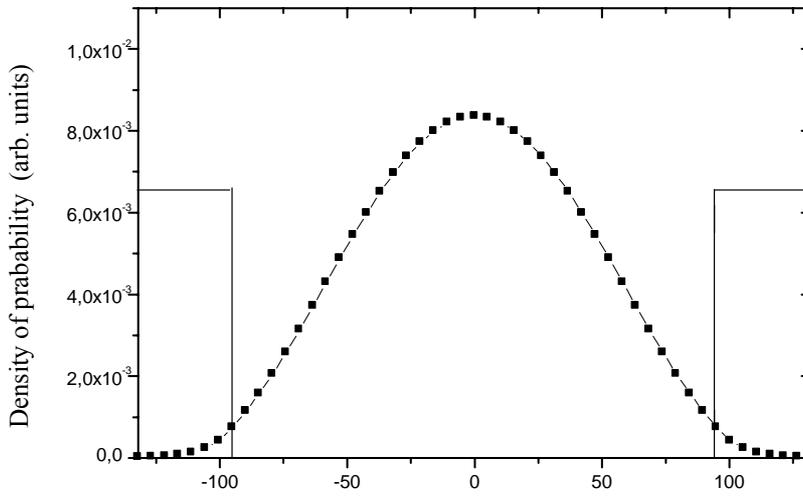


Fig. 2: Density of probability associated to an electron of the first miniband in the approximation of the liaisons fortes. Links pace of potential is to indicate the positions of the barrier and well of superlattice.

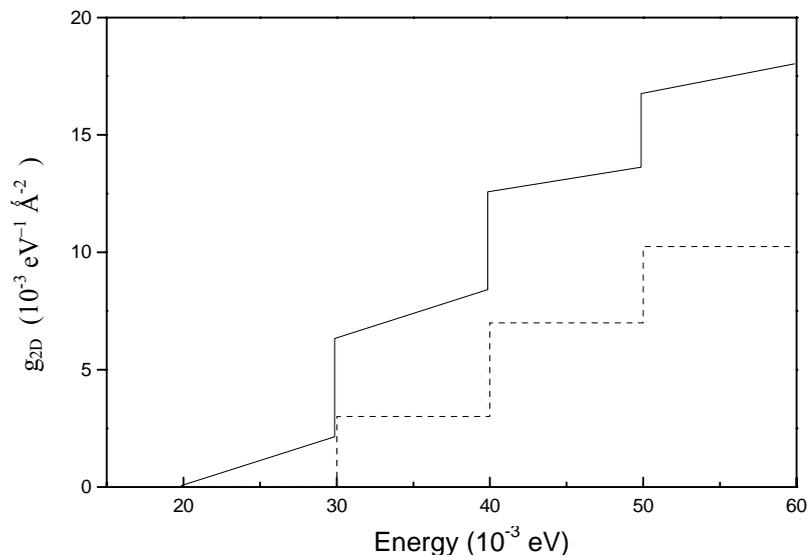


Fig. 3: Density of states calculated for a GaAs- $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$ superlattice: For non-parabolic (solid line) and parabolic (dashed lines).

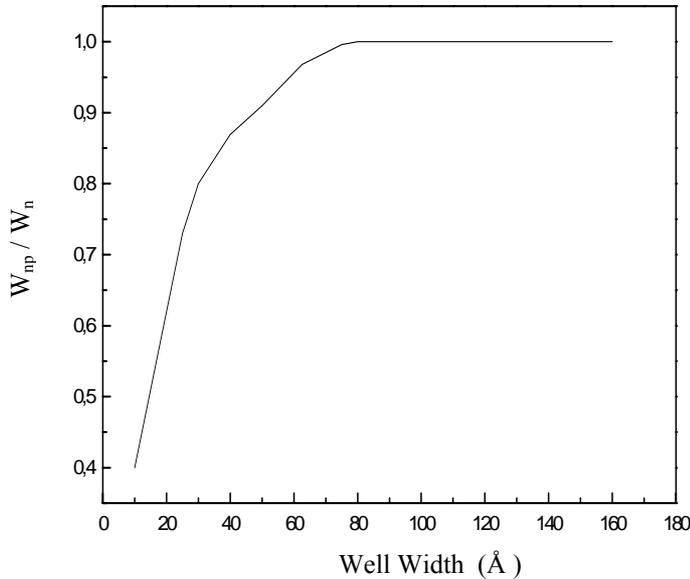


Fig. 4: Ratio of non-parabolic and parabolic scattering rates for intra-miniband as a function of the well width of superlattice.

In conclusion with the new analytic wave function associated to electron in conduction minibands. We have evaluated the expressions relaxation time due to electron-confined LO-phonon, including band non-parabolicity. It is found that for transitions from higher energy states the band non-parabolicity affects the scattering rate. The enhancement of the scattering rates with the inclusion of band non-parabolicity results from a larger electron-phonon overlap as well as from a larger density of final electrons states.

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