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Nonparabolicity 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 nonparabolic 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 of the slab model for the confined LO-phonon modes has been considered. An expression for the scattering rates has been obtained. Our results show that, for transitions related to the emission of confined LO-phonon, the scattering rates are significantly increased in the band nonparabolicity case.

Keywords: scattering rate, band structure, nonparabolicity effect.

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1. Introduction

Recently there has been much interest in the study of electron-phonon interaction in III-V semiconductor quantum wells (QWs) and superlattices (SLs) [1-3]. This is because the phonon scattering determines the electron transport properties at room temperature and high electric fields as well as at low temperatures. For instance, the cooling of photoexcited carriers, carrier tunnelling and mobility high-speed heterostructure devices are primarily governed by the scattering of electrons by polar-optical-phonons. Some results in the Raman scattering, cyclotron-resonance and magneto-phonon-resonance measurements show the dominance of electron interaction with LO-phonons and reveal an important information about the vibration modes in the layers forming SL [4-10]. The electron-LO-phonon interaction was found to be strongly dependent on both the geometrical shape and the parameters of the constituent materials [11-12]. The polaron effect in heterostructures of confined size is, however, quite different from that in bulk materials. Several models have been proposed to describe the electron-confined LO-phonon interaction in superlattices. Dielectric continuum models [13-14], microscopic lattice dynamical models [17-19], or slab model [20-21] are well known. Already the several theoretical studies reported on calculations of the relaxation time related to scattering of carriers in semiconductor heterostructures by optical phonons treated the case of single or multiple quantum wells [22-25].

The purpose of this paper is to present a set of calculated results for scattering rates in superlattices, we have considered the carrier scattered by LO-phonon. The effect of band nonparabolicity on the calculated scattering rates has been analyzed. The organization of the present paper is as follows: Section II summarizes the theoretical framework used in the calculations, while Section III describes the discussion of numerical results presented graphically, then a brief conclusion is given.

2. Theoretical model

A. Miniband structure and envelope wave functions

Using an effective-mass Hamiltonian and the transfer-matrix method, the total energy of electron associated to the first miniband and analytically the exact normalized wave function [26] are:

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

$$\Psi_w(z) = \frac{e^{-ik\frac{1}{2}} e^{ink_z l}}{\sqrt{N}} \left\{ b_2 e^{ik(z-(n-\frac{1}{2}))} + \beta e^{-ik(z-(n-\frac{1}{2}))} \right\} -$$

$$-L + l_b < z - nl < l_b , \qquad (2)$$

$$\Psi_b(z)=\frac{e^{-ik\frac{1}{2}}e^{ink_z l}}{\sqrt{N}} \tag{3}$$
$$\times\{p\cosh[\rho(z-nl+l_b)]+q\sinh[\rho(z-nl+l_b)]\}\times$$
$$\times l_b\ \langle z-nl\langle l_b\ ,$$

$$\hbar^2k^2=2m_w{}^*E\ ,\ h^2\rho^2=2m_b^*(V_b-E)\ ,$$
$$\lambda=m_w^*/m_b^*,\ L=l_b+l_w\ . \tag{4}$$
$$x=kl_w,\quad y=\rho\, l_b\ ,$$
$$\beta^-=\sin(x)\cosh(y)-K^-\cos(x)\sinh(y)-\sin(k_z l)\ . \tag{5}$$
$$p=b_2\mathrm{e}^{(ix/2)}+\beta^-\mathrm{e}^{-(ix/2)}\ ,\ q=\frac{ik}{\lambda\rho}\left(\mathrm{e}^{(ix/2)}-\beta^-\mathrm{e}^{-(ix/2)}\right). \tag{6}$$
$$k^\pm=\frac{1}{2}\left(\frac{\lambda\rho}{k}\pm\frac{k}{\lambda\rho}\right),\ b_2=k^+\sinh(y), \tag{7}$$
$$N=A'\left(b_2^2+\left(\beta^-\right)^2\right)+B'\beta^-\ . \tag{8}$$

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

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

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

B. Scattering rates

The interaction electron-phonon Hamiltonian in low-dimensional systems depends on the specific phonon spectra of the system and differs from the Fröhlich Hamiltonian for a bulk phonon. The macroscopic dielectric continuum model [27-30] gives the functional form of the interface modes, confined and half space LO-modes. The electron-confined LO-phonon interaction Hamiltonian as derived from the Fröhlich interaction is given by [31, 32]

$$H_{e\text{-}p}=\lambda\sum_{q_\perp,n}\sum_{\alpha=\pm}\mathrm{e}^{iq_\perp r}H(z)t_{n,\alpha}(q_\perp)u_{n,\alpha}(z)\times$$
$$\times\left[a_{n,\alpha}(q_\perp)+a^+{}_{n,\alpha}(-q_\perp)\right], \tag{12}$$

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

$$\lambda^2=iC_\mu/\sqrt{V}q\ , \tag{13}$$

where V is the volume. From [33] C can be written explicitly as

$$C=\left[\frac{e^2\hbar\omega_{\mathrm{LO}}}{2\varepsilon_0}\left(\frac{1}{\varepsilon(\infty)}-\frac{1}{\varepsilon(0)}\right)\right]^{\frac{1}{2}}, \tag{14}$$

where $\hbar\omega_{\mathrm{LO}}$ is the energy of LO-phonons in the n-th miniband, $\varepsilon(\infty)$ and $\varepsilon(0)$ are the optical static dielectric constants, respectively, Ω is the volume and e is the electronic charge. For the slab model [27, 34] $u_{n,\alpha}(z)$ is defined as

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

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

$t_{n,\alpha}$ is given by

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

Finally

$$H(z)=\begin{cases}1, & \text{if } -w\le z\le w\\ 0, & \text{otherwise}\end{cases}. \tag{18}$$

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

$$w_{i\to f}(k)=\frac{2\pi}{\hbar}\sum_f\left|\langle\xi_f\ |H_{e\text{-}p}\ |\xi_i\rangle\ \right|^2. \tag{19}$$

With the Hamiltonian given by (14), we obtain

$$w_{i\to f}=\frac{\pi}{2\pi V\hbar}\int(N_{\mathrm{LO}}+\frac{1}{2}\pm\frac{1}{2})\frac{e^2\hbar\omega_{\mathrm{LO}}}{q_\pm}\left(\frac{1}{\varepsilon(\infty)}-\frac{1}{\varepsilon(0)}\right)\times$$
$$\times\delta(U^\pm)I(k_z^i,k_z^f,q_\perp)dN_f\ . \tag{20}$$

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

$$I_n(k_z^i,k_z^f,q_\perp)=\sum_{q_\perp}\sum_{n,\alpha}\left|G_{n,\alpha}^{i\to f}(k_z^i,k_z^f)\right|^2\left|t_{n,\alpha}(q_\perp)\right|^2. \tag{21}$$

A δ-function represents the energy conservation quantity

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

$\pm$ denote the absorption and emission processes. For optical phonon scattering

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

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

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

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

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

where ψ_i, ψ_f are the electron envelope miniband wave function in the initial and final states, respectively [31]. L is the period of SL: $L = L_w + L_b$. At $U^{\pm} = 0$, $k_{\perp}^f$ and $k_{\perp}^i$ terms must be equal.

C. Nonparabolicity effect

According to the Kane model [35-37], the eigenfunctions of the Hamiltonian in the direction of the superlattice (with $k_x = k_y = 0$) associated with the conduction band electron [38, 39] with an energy $0 < E < V_b$, are solutions of the Schrödinger equation [40]:

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

$$a_2 = \frac{1}{2m^*(z)} , \quad a_4 = \frac{1}{E_g} \frac{1}{2m^*} - \frac{1}{2m_0} . \tag{26}$$

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

$$a_{2,w}\psi_w' + a_{4,w}\hbar^2 \psi_w''' = = a_{2,b}\psi_b' + a_{4,b}\hbar^2 \psi_b''' . \tag{27}$$

This expression that ensures the continuity of the local current density generalizes that of Refs [41, 43] where $a_4 = 0$. In case of nonparabolicity, the wave functions corresponding to the new condition (27) generalize those where the continuity of $\frac{1}{m^*}\frac{d\Psi(z)}{dz}$ is used. As the latter Hamiltonian does not take parabolicity into account, the wave functions are given at the n-th well and barrier by Eqs (2) and (3). Due to the new conditions (27) on the derivative 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 (4) and (25), expressions of k, ρ and μ are given by:

$$\hbar^2 k^2 = 4 m_w^* E_{w,\max} \left\{ 1 - \sqrt{1 - \frac{E}{E_{w,\max}}} \right\} ;$$

$$E_{w;\max} = \left(\frac{a_2^2}{4a_4} \right)_w ; \tag{28}$$

$$\hbar^2 \rho^2 = 4 m_b^* (E_{b,\max} - V_0) \times$$

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

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

When introducing the new expressions of wave vectors k and ρ in Eqs (1), (2), and (3), we obtained the new expressions for the dispersion relation and the wave functions in the barrier and wells of SL by continuation those of the times of relaxation and mobility. If the effect of the nonparabolicity becomes negligible ($a_4 = 0$), $\mu \to \lambda = \frac{m_w^*}{m_b^*}$ as 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 the relation (4).

3. Numerical results and discussion

For numerical computation, we have chosen $GaAs\text{-}Ga_{1-x}Al_xAs$ with $x = 0.45$ as a superlattice. The parameters pertaining to the system are: $m_w^* = 0.067 m_0$, $m_b^* = 0.104 m_0$, where m_0 is the free electron mass. The dielectric constant in the wells is taken equal to that in the barrier: $\varepsilon_d = 12.8$, $\varepsilon_\infty = 10.9$, $l_w = 108$ Å, $l_b = 38$ Å, $V_b = 495$ meV, $E_{w,\max} = 2$ eV, $E_{b,\max} - V_b = E_{w,\max}$, the energy of a bulk GaAs LO-phonon $\hbar\omega_{\text{LO}} = 36.8$ meV, the static and high frequency dielectric constants for GaAs $\varepsilon_s = 12.35$ and $\varepsilon_\infty = 10.48$.

In Fig. 1, we show the calculated rates for intraminiband transitions related to interaction electron-confined LO-phonons as a function of the SL well width. Note that the scattering rate does not qualitatively differ from that to the parabolic band approximation. In that approximation, the scattering rates related to confined LO-phonons become larger. It may be due to the overlap integrals given by Eq. (24), to the nonparabolic band approximation the electron wave function becomes more confined in the direction of SL, see Fig. 2.

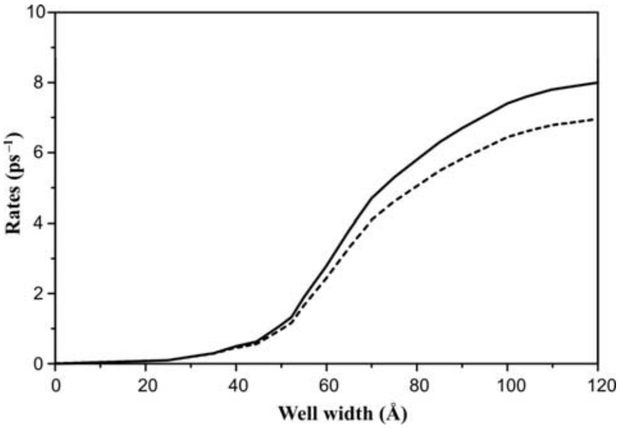

Fig. 1. Scattering rates for intraminiband transitions in GaAs-$Al_{0.45}Ga_{0.55}As$ superlattice as a function of the well width. The solid line is drawn with account of nonparabolicity, the dashed line corresponds to the parabolic approximation.

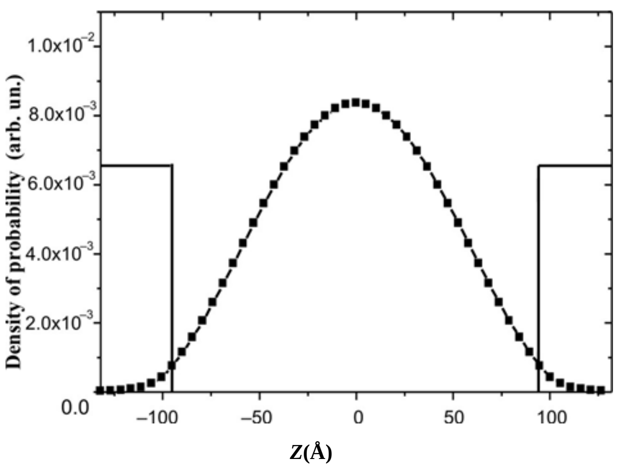

Fig. 2. Density of probability associated to an electron of the first miniband to the approximation of the binding forces. Link pace of potential is to indicate the positions of the barrier and well of superlattice.

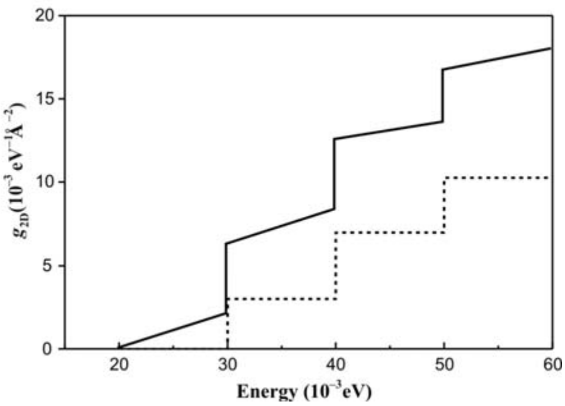

Fig. 3. Density of states calculated for superlattice GaAs-$Al_{0.45}Ga_{0.55}As$. For nonparabolic (solid line) and parabolic (dashed lines) band approximations.

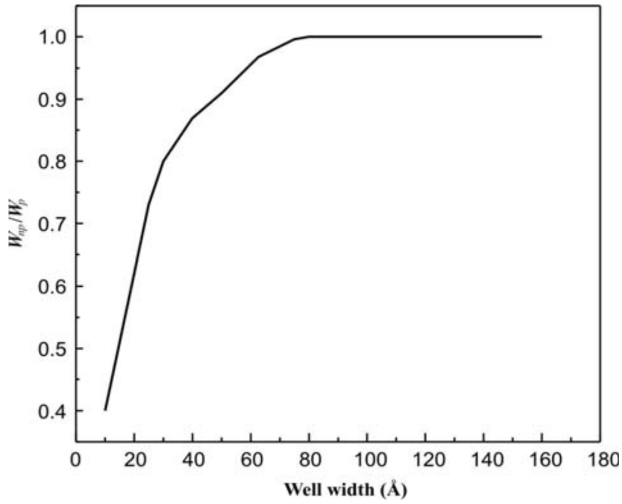

Fig. 4. Ratio of the nonparabolic and parabolic scattering rates for intraminiband as a function of the well width in superlattice.

Another element that influences the scattering rate is the density of final states. In Fig. 3, we give the density of final states to the parabolic band approximation in comparison with that to the nonparabolic band one.

We show that the density in the case of the nonparabolic band approximation is larger. In Fig. 4, we display the ratio of nonparabolic and parabolic scattering rates (w_{np}/w_p). For the intraminiband for the narrow well (the well width is as small as 45 Å) all nonparabolic scattering rates are close to those in the parabolic band approximation. For larger quantum wells, the transition rate with the band nonparabolicity is larger.

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

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