Intersubband Relaxation in Step Quantum Well Structures

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Intersubband relaxation due to electron interactions with the localized phonon modes plays an important role for population inversion in quantum well laser structures designed for intersubband lasers operating at mid-infrared to submillimeter wavelengths. In this work, intersubband relaxation rates between subbands in step quantum well structures are evaluated numerically using Fermi's golden rule, in which the localized phonon modes including the asymmetric interface modes, symmetric interface modes, and confined phonon modes and the electron–phonon interaction Hamiltonians are derived based on the macroscopic dielectric continuum model, whereas the electron wave functions are obtained by solving the Schrödinger equation for the heterostructures under investigation. The sum rule for the relationship between the form factors of the various localized phonon modes and the bulk phonon modes is examined and verified for these structures. The intersubband relaxation rates due to electron scattering by the asymmetric interface phonons, symmetric interface phonons, and confined phonons are calculated and compared with the relaxation rates calculated using the bulk phonon modes and the Fröhlich interaction Hamiltonian for step quantum well structures with subband separations of 36 meV and 50 meV, corresponding to the bulk longitudinal optical phonon energy and interface phonon energy, respectively. Our results show that for preferential electron relaxation in intersubband laser structures, the effects of the localized phonon modes, especially the interface phonon modes, must be included for optimal design of these structures.

Keywords: Localized phonons, relaxation rates, intersubband laser

1 INTRODUCTION

In recent years, novel tunneling injection lasers using structures based on semiconductor quantum wells have provided the means for achieving lasing wavelengths from the mid-infrared to the submillimeter wave region [1, 2, 3]. These lasers incorporate narrow quantum well regions that
must have thicknesses as small as 30–50 Å and have transition level separations engineered to one unit or a multiple of bulk Longitudinal-Optical (LO) phonon energy. It is now well known that the shape and energies of LO phonon modes are modified by quantum wells. Specifically, LO phonons in quantum wells may be described by the dielectric continuum model in terms of confined and interface modes that have properties different from those of bulk phonons [4, 5, 6]. In this paper, the interface and confined LO phonon modes of the continuum model [7] are used with Fermi’s golden rule to calculate relaxation rates between quasi bound states in step quantum well structures. We show that the electron relaxation rates are dominated by the interface phonon scattering, and that the symmetries of phonon modes induce inherent selection rules of transitions among well levels. In addition, the sum rule for the form factors [6] is verified numerically for the step quantum well structures.

2 INTERFACE PHONON ASSISTED TRANSITION

The well structure in this study is shown in Figure 1, denoting the innermost GaAs to be layer 1, the next Al0.25Ga0.75As layer 2 and the outermost Al0.6Ga0.4As layer 3. There are six types of phonon modes due to the double interfaces between layers 1 and 2: (1) symmetric interface modes, (2) antisymmetric interface modes, (3) confined LO modes, (4) confined TO modes, and (5) half-space LO modes. With the eigenmodes given by [6], we can obtain the electron-phonon interaction from the Fröhlich continuum model

\[ H_{e-p} = e \int d^2r \int dz \rho(r, z) \phi(r, z), \]

where \( \rho(r, z) \) is the generalized electron density operator and \( \phi(r, z) \) the electrostatic potential created by the LO phonons. Since wavefunctions of the first two levels have opposite parities, only the antisymmetric modes may contribute significantly to electron transition rates between these two levels. For the antisymmetric phonon modes,

\[ H_{A^+} = \sum_q \left[ \frac{\hbar \omega_{A^+} e^2}{2\varepsilon_0 L^2} \right] \left[ \beta_{A^+}^{-1}(\omega_{A^+}) \coth \left( \frac{1}{2} qa \right) \right] + \beta_{A^+}^{-1}(\omega_{A^+})^{-1} \times \frac{1}{\sqrt{2q}} e^{i\pi f_A(q, z)} [a_{A^+}(q) + h.c.], \]

where \( q \) is the two dimensional phonon wavevector parallel to the heterostructure interface,

\[ \beta_n(\omega) = \left[ \frac{1}{k_{\infty n}} - \frac{1}{k_0 n} \right] \frac{\omega_{Ln}^2}{\omega^2} \left[ \frac{\omega^2 - \omega_{Tn}^2}{\omega_{Ln}^2 - \omega_{Tn}^2} \right]^2, \quad n = 1, 2 \]

where \( \omega_{Tn} \) and \( \omega_{Ln} \) are the frequencies of the longitudinal optical (LO) phonon and the transverse-optical (TO) phonon, respectively. \( \omega_{A^+} \) are the antisymmetric mode frequencies and are given...
by solutions of the following equation,

\[ \varepsilon_1(\omega) \coth \left( \frac{1}{2} Qa \right) + \varepsilon_2(\omega) = 0. \]  

(4)

For long wavelengths they approach \( \omega_{L1} \) and \( \omega_{T2} \).

\( f_A \) is defined as

\[
    f_A(z) = \begin{cases} 
    -e^{q(z+\frac{1}{2}a)} & \text{if } z \leq -\frac{1}{2}a \\
    \frac{\sinh(qz)}{\sinh(\frac{1}{2}qa)}, & \text{if } -\frac{1}{2}a \leq z \leq \frac{1}{2}a \\
    e^{q(z-\frac{1}{2}a)}, & \text{if } z \geq \frac{1}{2}a
    \end{cases}
\]

(5)

The electron-phonon interaction induces electron transition between the two well levels. Using Fermi’s golden rule, the rates of transitions assisted by various modes of the interface phonon and bulk phonon are calculated as functions of electron in-plane energy. In Figure 2, numerical results of the antisymmetric and bulk phonon assisted transitions are given at a well level energy separation of \( E_2 - E_1 = 47 \) meV, which shows that the antisymmetric interface phonon assisted transition dominates at a level separation close to the antisymmetric phonon frequency. Contributions from the other phonon modes are generally negligible.

The maximum transition rates occur when the electron in-plane energy compensates the difference between the mode frequency and energy level separation. Figure 3 presents a comparison of the maximum transition rates of the bulk mode and antisymmetric mode at various values of \( E_2 - E_1 \), which are obtained by varying the quantum well width. A device structure which is engineered with an energy level separation of the antisymmetric interface mode frequency would have a relaxation rate several times larger than that with a bulk mode frequency separation, as shown in Figure 3.

For the structure under study, the upper antisymmetric mode plays the most important role in the transition between the energy level 2 and level 1. For other transitions (e.g. between level 3 and level 1) the symmetric modes may become important. The selection rule is due to well

![FIGURE 2 Transition rates of antisymmetric and bulk modes.](image)

![FIGURE 3 Resonant transition rates.](image)
3 SUM RULE OF FORM FACTORS

The form factors [6] can be defined through effective electron–electron interaction due to exchange of optical phonons. The form factors are independent of material parameters but depend on the spatial shape of the phonon modes and subband electron wavefunctions. In this double heterostructure, the form factors for a subband and different phonon modes are given by

\[ F_S(q) = \frac{1}{1 + \tanh(\frac{1}{2}qa)} \left[ \int_{-\infty}^{\infty} dz |\psi(z)|^2 f_S(qz) \right]^2, \]

\[ F_A(q) = \frac{1}{1 + \coth(\frac{1}{2}qa)} \left[ \int_{-\infty}^{\infty} dz |\psi(z)|^2 f_A(qz) \right]^2, \]

\[ F_C(q) = \int_{-\frac{1}{2}a}^{\frac{1}{2}a} dz \int_{-\frac{1}{2}a}^{\frac{1}{2}a} dz' |\psi(z)|^2 |\psi(z')|^2 \left[ e^{-q|z-z'|} - \frac{1}{1 + \tanh(\frac{1}{2}qa)} \frac{\cosh(qz)\cosh(qz')}{\cosh^2(\frac{1}{2}qa)} \right], \]

\[ F_{H+}(q) = \int_{-\frac{1}{2}a}^{0} dz \int_{-\frac{1}{2}a}^{0} dz' |\psi(z)|^2 |\psi(z')|^2 \left[ e^{-q|z-z'|} - \left[ e^{-q|z+z'-a|} \right] \right], \]

\[ F_{H-}(q) = \int_{0}^{\frac{1}{2}a} dz \int_{0}^{\frac{1}{2}a} dz' |\psi(z)|^2 |\psi(z')|^2 \left[ e^{-q|z-z'|} - \left[ e^{-q|z+z'+a|} \right] \right]. \]

(6)

where \( f_S \) is given by

\[ f_S(qz) = \begin{cases} e^{q(z+\frac{1}{2}a)}, & z \leq -\frac{1}{2}a \\ \cosh(qz)/\cosh(\frac{1}{2}qa), & -\frac{1}{2}a \leq z \leq \frac{1}{2}a \\ e^{-q(z-\frac{1}{2}a)}, & z \geq \frac{1}{2}a \end{cases} \]

(7)

These form factors always satisfy the sum rule [6]

\[ F_B(q) = F_S(q) + F_A(q) + F_C(q) + F_{H+}(q) + F_{H-}(q), \]

which is a direct consequence of the complete orthonormality of the interface eigenmodes. Verifying the sum rule provides a justification of our numerical calculations. The sum rule between the various form factors has been verified for different well levels of the step quantum well structure. As an example, in Figure 4, the calculated form factors for level 2 are plotted. The sum of form factors of the symmetric mode and half space modes is indeed equal to that of the bulk mode. The form factors for the confined LO mode and antisymmetric mode in this case are negligible compared to those for the symmetric and half space (\( H^+ \) and \( H^- \)) modes, although this is not always true for other levels.

4 CONCLUSION

By examining and comparing electron transition rates induced by bulk and interface phonon modes, our calculations for step quantum well structures designed for intersubband lasers have shown that, to facilitate preferential electron relaxation, it is important to consider the transition induced by the interface phonon modes and have electron subbands engineered with their separation close to the interface phonon energy in the device structures.

![Figure 4 Sum rule of form factors.](image-url)
References


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