# Inelastic scattering of electrons traversing semiconductor heterojunctions

J. F. Müller,[a] S. Schmitt-Rink, and A. F. J. Levi
*AT&T Bell Laboratories, Murray Hill, New Jersey 07974*

(Received 21 September 1987; accepted for publication 14 November 1987)

We calculate the contribution of polar optic phonons to the inelastic scattering rate for an electron traversing semiconductor heterojunctions. In typical geometries, a dramatic reduction in scattering rate compared to the bulk value is found for a limited range of electron energies. This effect is related to spatial separation of initial and final electron wave functions either side of the heterojunction caused by quantum mechanical reflection at the interface. The influence of this phenomenon on the performance of devices, such as unipolar hot-electron transistors, is discussed.

Little information exists about the dynamics of electron transport across abrupt changes in potential in semiconductor heterojunctions. However, knowledge of electron scattering processes in such structures is of fundamental interest and has technological significance. For example, it might explain the limited current gain of recently developed double heterojunction unipolar hot-electron transistors.[1]

It is well known that polar optic phonon scattering dominates nonequilibrium electron dynamics in typical intrinsic III-V compound semiconductors.[2] Therefore, as a reasonable starting point, we calculate longitudinal optic phonon scattering rates for perpendicular electron transport in prototype heterojunction geometries. The simplest case is that of a single potential step of energy $U_1$ in region 1 and $U_2 = 0$ in region 2 shown schematically in Fig. 1(a). For the purpose of discussion, we include a schematic sketch of the probability densities $|\psi|^2$ for three types of wave functions. Wave function $\psi_1$ has energy $E < U_1$ and therefore has essentially zero amplitude in region 1. Wave function $\psi_2$ is obtained for $E > U_1$. The amplitude of the wave function is larger in region 1 because an electron has lower velocity in region 1 than in region 2.[3] However, by applying the impedance matching condition for the effective masses $m_1^*$ and $m_2^*$ (see Ref. 1 and text below) the velocities on either side of the barrier become equal and the corresponding wave function, $\psi_3$, has the same amplitude in both regions.

For our problem, the normalization of the wave functions is conveniently achieved by placing infinite potential barriers on either side of the structure. The wave functions are then obtained by solving for the zeros of a function which depends on the transverse electron wave vectors in each region.[4] We consider an electron of initial energy $E_i$, with all its momentum in the $z$ direction, so that the wave vector parallel to the plane of the potential step is $k_{i,\parallel} = 0$. The zero temperature optic phonon scattering rate, $1/\tau_{\rm ph}$, is calculated by integrating over all final electron states, $\psi_f$, consistent with energy and momentum conservation:

$$\frac{1}{\tau_{\rm ph}}\bigg|_{k_{i,\parallel}=0} = \frac{2\pi}{\hbar}\sum_f \sum_{k_\parallel,k_z} \frac{2\pi e^2\hbar\omega_{\rm LO}}{V\epsilon^*(k_\parallel^2 + k_z^2)}|M_{if}(k_z)|^2 \times\delta(E_i - E_f - \hbar\omega_{\rm LO}), \quad (1)$$

where $E_i = \hbar^2 k_{i,2}^2/2m_2^*$ and $E_f = (\hbar^2 k_{f,2}^2 + \hbar^2 k_\parallel^2)/2m_2^*$. In these expressions $k_2$ is the transverse momentum in region 2, $V$ is the volume of the system, and $1/\epsilon^* = (1/\epsilon_\infty - 1/\epsilon_0)$, where $\epsilon_\infty$ and $\epsilon_0$ are the high- and low-frequency dielectric constants, respectively. The matrix element $M$ is

$$M_{if}(k_z) = \int_{-z_1}^{z_2+z_3} dz\, \phi_i^*(z) e^{ik_z z}\, \phi_f(z), \quad (2)$$

where $\phi$ is the transverse part of the wave function, i.e., $\psi(\mathbf{r}_\parallel, z) \propto e^{i(\mathbf{k}_\parallel \mathbf{r}_\parallel)}\phi(z)$.

The results of calculating $1/\tau_{\rm ph}$ as a function of initial energy $E_i$ for electrons with initial $k_{i,\parallel} = 0$ are shown in Fig. 1(b) [for comparison, the smooth curve in Fig. 1(b) is the bulk phonon scattering rate]. We note that energy conservation requires that an electron of energy $E_i < \hbar\omega_{\rm LO}$ cannot emit an optic phonon, consequently $1/\tau_{\rm ph} = 0$ for $E_i < \hbar\omega_{\rm LO}$. For energies above this threshold the scattering rate behaves similarly to that expected for phonon emission in the bulk semiconductor until $E_i$ is the same as the energy of the potential step, $U_1$. Small, peaked deviations, which occur with increasing energy, are due to the increasing separation of energy levels. However, at $E_i = U_1$ the scattering rate changes abruptly from a finite value to approximately zero. With increasing electron energy, $1/\tau_{\rm ph}$ shows some rapid oscillatory behavior until $E_i > (U_1 + \hbar\omega_{\rm LO})$, above

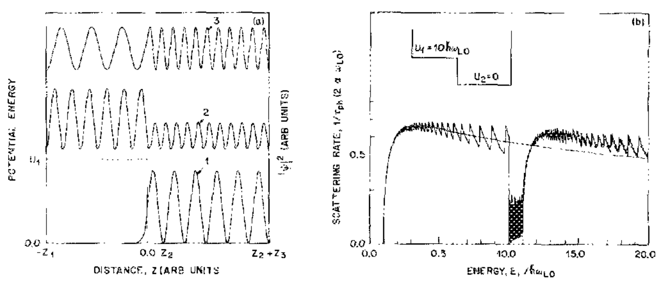


FIG. 1. (a) Schematic potential energy diagram of an abrupt heterojunction. The potential energy in region 1 is $U_1$ and that in region 2 is $U_2 = 0$. Also shown are the probability densities of three types of wave functions. (b) Inelastic optic phonon scattering rate, $1/\tau_{\rm ph}$, as a function of initial electron energy, $E_i$. $1/\tau_{\rm ph}$ is in units of $2\alpha\omega_{\rm LO}$, where $\alpha = (e^2/\hbar\epsilon^*)(m_2^*/2\hbar\omega_{\rm LO})^{1/2}$ is the polaron coupling constant. The smooth curve is the bulk phonon scattering rate. The parameters used in the calculation were $U_1 = 10\hbar\omega_{\rm LO}$, $U_2 = 0$, $m_1^* = 0.021 m_0$, where $m_0$ is the free-electron mass, $z_2 = 463$ Å, and $z_1 = z_3 = 24\,510$ Å.

[a] Permanent address: Institut für Theoretische Physik, Universität Frankfurt, Robert-Mayer-Strasse 8, 6000 Frankfurt/Main 1, West Germany.

  

which $1/\tau_{ph}$ again takes on the bulk value but shifted in energy by $U_1$. The rapid oscillations in $1/\tau_{ph}$ for $U_1 < E_i < (U_1 + \hbar\omega_{LO})$ are due to coherent interference effects arising from the presence of the infinite potential barriers used in the electron wave function normalization procedure. Of course, in a real solid, electron scattering ensures that coherent interference effects of this type cannot occur over length scales greater than a characteristic mean free path. So, at an abrupt heterojunction, in the absence of such coherence effects, the phonon scattering rate is given by a smooth curve close to the lower bound of the oscillatory curve in Fig. 1(b).

The change in scattering rate when $E_i = U_1$ is most easily explained by considering the electron wave functions shown schematically in Fig. 1(a). An electron of energy $U_1 < E_i < (U_1 + \hbar\omega_{LO})$ with initial wave function $\psi_i$ can only lose energy by making a transition to an electronic state $\psi_f$ which is essentially localized in region 2 in Fig. 1(a) where the potential $U_2 = 0$. The matrix element $M$ [Eq. (2)] is therefore small. Additionally, because of the mismatch in electron velocity across the step potential, there is a low transmission probability[5] for an electron of energy $E_i \sim U_1$ [see Fig. 1(a)] and the electron spends most of the time in region 1 where the potential has a value $U_1$. It is this spatial separation of initial and final electron states which gives rise to the decrease in $1/\tau_{ph}$ in the range $U_1 < E_i < (U_1 + \hbar\omega_{LO})$.

We now calculate nonequilibrium electron scattering rates for typical double heterojunction unipolar transistor structures.[1] The inset in Fig. 2(a) shows the potential energy diagram for one type of unipolar hot-electron transistor. The emitter barrier has energy $U_1$, the collector barrier has energy $U_3$, and the width of the quantum well forming the transistor base region is $z_2$. The result of calculating $1/\tau_{ph}$ for this asymmetric quantum well structure is shown in Fig. 2(a). In Fig. 2(b) the result of calculating $1/\tau_{ph}$ for a symmetric quantum well structure with $U_1 = U_3$ is given. The scattering rate of the electronic states confined to the quantum well of width $z_2$ is indicated with $\times$'s. For both structures, as with the case of a single potential step, there is a dramatic reduction in $1/\tau_{ph}$ at electron energies $E_i = U_1$ and $E_i = U_3$.

Relating $1/\tau_{ph}$ to the transport properties of nonequilibrium electron transistor structures is a difficult task involving, in principle, a solution of the quantum kinetic equation for the Wigner distribution function. Rather than persuing this involved procedure, we comment on the physical significance of our determination of $1/\tau_{ph}$. Naively, one might expect that the decrease in $1/\tau_{ph}$ for electrons with energy in the range $U_1 < E_i < (U_1 + \hbar\omega_{LO})$ leads to a dramatic reduction in scattering in the transistor base and hence a strong increase in current gain. In fact, this is not so. It is intuitively clear that for those nonequilibrium electrons injected into the base region the scattering rate is similar to that of the bulk semiconductor. The decrease in $1/\tau_{ph}$ arises due to the spatial separation of electron wave functions between emitter [region 1 in Fig. 1(a)] and base [region 2 in Fig. 1(a)]. The confinement of the initial wave functions to region 1 is a direct consequence of the velocity mismatch across the abrupt change in potential. The quantum reflection at the heterojunction which tends to localize the initial electron wave function on the emitter side of the heterojunction results in a small probability that the electrons are injected into the base. However, those that are injected scatter at a rate close to the bulk value.

That this is a correct interpretation is best illustrated by calculating $1/\tau_{ph}$ for an electron of energy $E_i$ when the electron velocity in the emitter is the same as in the base [see Fig. 1(a)]. This impedance matching condition[1] (for which the transmission coefficient is unity) is $m_2^*/m_1^* = E_i/(E_i - U_1)$, where $m_1^*$ and $m_2^*$ are the effective electron masses in the emitter and base, respectively. In Fig. 3(a) we plot $1/\tau_{ph}$ for the case of impedance matching for electrons of energy $E_i = (U_1 + \hbar\omega_{LO}/2)$. As can be seen, the impedance matched heterojunction phonon scattering rate is close to half the bulk value since the electron spends half its time in region 2.

To estimate the energy dependence of base current in a unipolar hot-electron transistor (which is related to the current gain $\beta = j_c/j_b$, where $j_c$ and $j_b$ are the collector and base currents), we consider the potential depicted in Fig. 3(b). $U_1$, $U_2$, and $U_3$ are the emitter, base, and collector potentials, respectively. An electron injected from the emitter side is represented by a traveling plane wave, $\psi_i$. Once transmitted

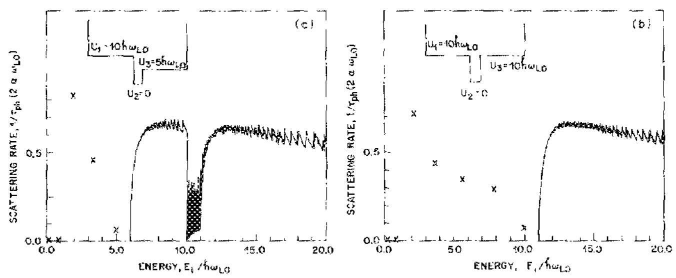

FIG. 2. (a) $1/\tau_{ph}$ for an asymmetric quantum well structure with $U_1 = 10\hbar\omega_{LO}$, $U_2 = 0$, $U_3 = 5\hbar\omega_{LO}$, $m_j^* = 0.021 m_0$, $z_2 = 463$ Å, and $z_1 = z_3 = 24\,510$ Å. (b) $1/\tau_{ph}$ for a symmetric quantum well structure with $U_1 = U_3 = 10\hbar\omega_{LO}$, $U_2 = 0$, $m_j^* = 0.021 m_0$, $z_2 = 463$ Å, and $z_1 = z_3 = 24\,510$ Å.

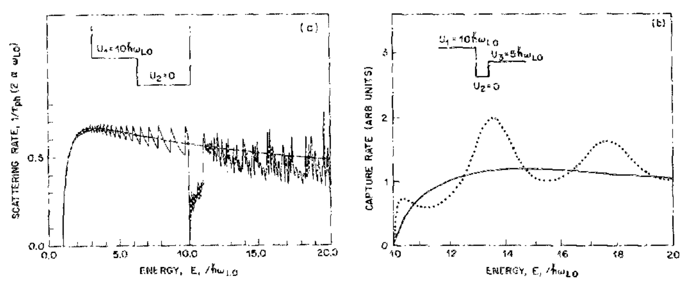

FIG. 3. (a) $1/\tau_{ph}$ for a heterojunction impedance matched at an electron energy $E_i = 10.5\hbar\omega_{LO}$. The smooth curve is the bulk phonon scattering rate. The parameters used in the calculation were $U_1 = 10\hbar\omega_{LO}$, $U_2 = 0$, $m_1^* = 0.048 m_2^*$, $m_2^* = 0.021 m_0$, $z_2 = 463$ Å, and $z_1 = z_3 = 24\,510$ Å. (b) Base capture rate as a function of initial electron energy for an asymmetric quantum well structure. The dotted line corresponds to an impedance mismatched base/collector junction with $m_3^* = 10 m_2^*$. The solid line corresponds to impedance matching with $m_3^* = 0.63 m_2^*$. The other parameters used in the calculation were $U_1 = 10\hbar\omega_{LO}$, $U_2 = 0$, $U_3 = 5\hbar\omega_{LO}$, $m_2^* = 0.021 m_0$, $z_2 = 463$ Å, and $z_1 = z_3 = 24\,510$ Å.

into the collector region the electron is expected to contribute to the collector current. Hence, in our model, the base current is related to a base capture rate obtained by restricting the summation in Eq. (1) to those states $\psi_f$ which are bound to the base region. The result of such a calculation with and without impedance matching at the base/collector interface is shown in Fig. 3(b). Without impedance matching (dotted line) the capture rate peaks at the virtual cavity resonances of the base. We expect these resonances to be detrimental to current gain because, in the transport problem, current flows mainly via resonances where the average velocity of electrons is low and the base capture probability is high. The effect of impedance matching at the base/collector junction is to smoothen the resonance characteristics by reducing the maxima and increasing the minima in the capture rate. In the transport problem the average velocity of electrons is high and the probability of an electron contributing to base current is low.

In conclusion, quantum mechanical reflection at an abrupt semiconductor heterojunction can localize initial and final electron states either side of the junction. This spatial separation, due to scattering from a potential step, strongly reduces inelastic polar optic phonon scattering rates for a limited range of electron energies. However, the influence of this phenomenon on the current gain of hot-electron transistors is small, because the increase in scattering time is canceled by the decrease in transmission probability. Neglect of this phenomenon will cause significant errors in device modeling. We have also demonstrated that resonances in electron scattering rates may be removed by impedance matching electron states across the base/collector junction. The removal of these resonances should increase the current gain of unipolar hot-electron transistors.


[1] A. F. J. Levi and T. H. Chiu, Appl. Phys. Lett. **51**, 984 (1987).

[2] E. M. Conwell, "High Field Transport in Semiconductors," in *Solid State Physics, Advances in Research and Applications*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1967), Vol. 9, p. 156.

[3] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1981).


[4] Consider three regions $j = 1,2,3$, with potential $U_j$ ($U_2 = 0$), width $z_j$ [see Fig. 2(a)], and transverse effective electron mass $m_j^*$, bounded on either side by infinite potential barriers. For simplicity we assume the effective masses parallel to the interface to be equal, i.e., $m_{j,\parallel}^* = m_2^*$. The energy eigenvalues for the system are found by solving for

$$f(k_2) = 0 = \frac{a_2}{a_1}\tan k_1 z_1 + \tan k_2 z_2 + \frac{a_2}{a_3}\tan k_3 z_3 - \frac{a_2}{a_1}\tan k_1 z_1 \tan k_2 z_2 \frac{a_2}{a_3}\tan k_3 z_3,$$

where $a_j = \hbar k_j / m_j^*$ are the transverse velocities and

$$\hbar k_j = \left[2m_j^*\left(\frac{h^2 k_2^2}{2m_2^*} - U_j\right)\right]^{1/2}$$

are the transverse momenta.

[5] It would be interesting to consider the effect dissipative processes, such as phonon scattering, have on this transmission probability. See, e.g., R. Bruinsma and P. M. Platzman, Phys. Rev. B **35**, 4221 (1987).