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LETTER TO THE EDITOR

Hot-electron distribution in the quantum well of a resonant tunnelling diode

Yuming Hu and Shawn Stapleton
School of Engineering Science, Simon Fraser University, Burnaby, BC, Canada V5A 1S6

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Abstract. The incoherent electrons in the quantum well play an important role in resonant tunnelling diodes. The hot-electron distribution, characterized by the electron temperature T_e and the effective Fermi energy μ_e, is proposed to describe the non-equilibrium distribution of the incoherent electrons in the quantum well. These two parameters, T_e and μ_e, can be uniquely determined by the energy conservation law and particle conservation law. We have also calculated the current density tunnelling through the diode. Our results demonstrate that the current peak-to-valley ratio degrades as scattering in the quantum well increases, which is consistent with the current experimental results.

Since Tsu and Esaki first proposed the resonant tunnelling diode (RTD) in 1973 [1], experimental investigations into RTDs have made significant advances due to the improvements in microfabrication technology [2–5]. However, theoretical investigations into RTDs have not kept the same pace and many controversial questions still need to be clarified [6–17]. In this letter, we will only focus on the distribution of electrons in the quantum well, which, to our best knowledge, has not been seriously investigated. This distribution plays a crucial role in RTDs. First, the electron distribution in the well will directly affect the I–V curves of RTDs. Second, electron charges in the quantum well will modify the parasitic capacitance of the RTD. This parasitic capacitance holds an important role in the determination of the maximum obtainable power and oscillating frequency when RTDs are used as microwave oscillators [3]. Third, the electron charges in the quantum well will generate an electric field, which will modify the barrier profile of RTDs. The modified barrier profile will affect total charges in the well, too. This feedback mechanism is believed to be responsible for the hysteresis and shoulder-like behaviour observed in the I–V curves of RTDs [9, 15–16].

We will start with the dampled resonant tunnelling model, which was first introduced by Stone and Lee [10] in disorder-localized one-dimensional systems and, later on, developed for the RTD [11–12]. In this model, the electron waves will be treated exactly the same as the light waves. The contacts with the RTD will be modelled by electron reservoirs which emit thermal equilibrium electrons and absorb completely any incoming electrons. In order to model the effects of scattering due to the phonons, defects, etc., a damping constant, α, is introduced for the electron waves in the quantum well. It is reasonable to assume that electrons lose phase coherence completely after being scattered, so we may partition the total electrons tunnelling through the RTD into two parts:

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(1) The first part is the coherent tunnelling electrons which do not experience any scattering, except by the barriers during tunnelling. For these electrons, the momenta parallel to the walls are conserved and motion perpendicular to the walls are described by quantum mechanics. Since the distribution of the coherent electrons in the well can be relatively easily derived from the results in [13], we will not elaborate on it here.

(2) The second part is the incoherent electrons which are scattered by the phonons, impurities, defects, etc. For these electrons, the momenta parallel to the walls are not conserved during tunnelling because they can be scattered into any direction in 3-dimensional space. The incoherent electrons will redistribute themselves in the well and subsequently escape from the well by tunnelling through the barriers incoherently. In order to calculate the total number of incoherent electrons in the well, it is required to determine the non-equilibrium distribution of the incoherent electrons. Unfortunately, the derivation of this distribution from a kinetic equation is an extremely non-trivial problem. This is because many conceptual problems regarding open systems are not fully understood yet [17]. However, intuitively, we may propose the hot-electron distribution to model the non-equilibrium distribution of the incoherent electrons in the well, i.e.

$$f(k, T_e, \mu_e) = \{\exp[(E - \mu_e)/k_B T_e] + 1\}^{-1} \tag{1}$$

where T_e is the electron temperature and μ_e is the effective Fermi energy. The hot-electron distribution has been used to describe the electron transport in the device of a metal–insulator–metal–insulator–metal structure, which has exactly the same band structure as that of the RTD [18]. The physical arguments for this assumption are as follows. When an electron enters the quantum well from the emitter, it will gain kinetic energy (later on the term 'kinetic energy' will be shortened to just 'energy') and momentum from the external electric field. The electron will transfer, at most, $k_B\Theta$ energy to the lattice (where Θ is the Debye temperature of the lattice) when it is scattered by the phonons, and will not lose energy when it is scattered by the impurities and defects. The momentum of the electron, however, can be randomized immediately by all the scattering mechanisms, no matter whether it is scattered by phonons or impurities. This means that it takes much longer time for the electron to lose its energy than it takes to lose its momentum gained in the electric field. Since the energy relaxation is a slow process (10^{-12} s) while the momentum relaxation is a faster process (10^{-14} s) [19], the energy gained in the field cannot be dissipated quickly enough into the lattice. This energy will be randomized into the thermal energy of the electron itself through carrier-to-carrier interactions, causing the electron temperature to be higher than the lattice. The distribution given by (1) has not been completely specified unless the electron temperature, T_e, and the effective Fermi energy, μ_e, are known. These two parameters may be determined by using the energy conservation equation and the particle conservation equation. Energy and particle conservations are necessary conditions for any distribution used to describe the incoherent electrons in the well.

Our model of the RTD is shown in figure 1, where the trapezoidal barrier has been replaced by a square barrier with the same area for simplicity. This, we believe, will not yield any qualitative difference. The x direction is chosen to be perpendicular to the walls of the RTD (see figure 1). We shall denote the transmission coefficients, t, and reflection coefficients, r, for the barriers by $t_{1l}, r_{1l}, t_{2l}, r_{2l}, t_{1r}, r_{1r}, t_{2r}$ and r_{2r}. The subscripts 1 (2) designate the left (right) barrier and subscripts l (r) designate a wave coming in from the left (right) side. The energies of the electrons in regions 1, 2, 3 will be denoted by

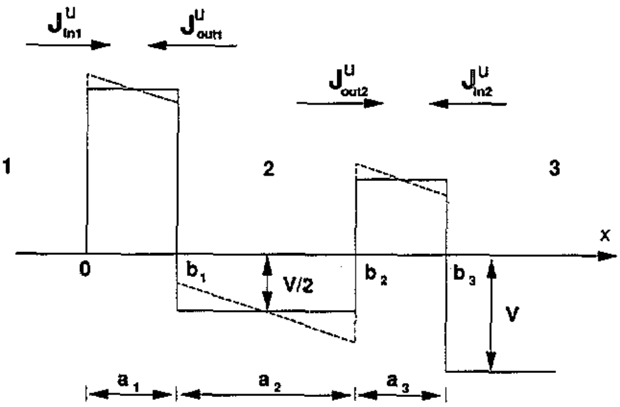

Figure 1. A simplified structure for a double barrier with an applied field, where the trapezoidal barriers have been replaced by square barriers with the same area.

E_1, E_2, E_3, and the magnitudes of the momentum by k_1, k_2, k_3. We also use k_{jx} and $k_{j\perp}$ ($j = 1, 2, 3$) to represent the momentum components parallel and perpendicular to the x direction in region j, respectively. The corresponding velocity in the x direction in region j is denoted by $v_{jx} = \hbar k_{jx}/m$. Following a similar procedure as that for the damped Fabry–Perot resonator [11–13], we can obtain the global transmission, t_G, and reflection, r_G, coefficients for electrons from regions 1 to 3,

$$t_G = t_{1l} t_{2l} \exp(jk_{2x}a_2 - \alpha a_2/2)/[1 - r_{1r} r_{2l} \exp(j2k_{2x}a_2 - \alpha a_2)] \tag{2a}$$

$$r_G = r_{1l} + t_{1l} r_{2l} t_{1r} \exp(j2k_{2x}a_2 - \alpha a_2)/[1 - r_{1r} r_{2l} \exp(j2k_{2x}a_2 - \alpha a_2)] \tag{2b}$$

where a_2 is the width of the quantum well and α is the damping constant which combines the effects of all the scattering mechanisms. The introduction of the damping constant, α, causes a breakdown of unitarity: the incoming electron current will be larger than the sum of the transmitted current and the reflected current. The missing current, mathematically described by $v_{1x}(1 - |r_G|^2 - |t_G|^2 v_{3x}/v_{1x})$, can be interpreted as a transport of the incoherent electrons into the well, which leads to the accumulation of the incoherent electrons in the well. When an electron enters the quantum well from the emitter, the electron will gain an energy $\frac{1}{2}eV$ from the electric field (e is the elementary charge of an electron and V is the applied voltage), so the electron will carry a total energy $E_1 + \frac{1}{2}eV$ to the well. The total energy flux entering the well from region 1 is the integration of the energy carried by each electron times the incoherent electron flux density entering the well, which is

$$J^{u}_{in1} = \frac{2}{(2\pi)^3} \int_0^{\infty} dk_{1x} \int_{-\infty}^{\infty} dk_{1\perp} f(k_1) v_{1x} \left(E_1 + \frac{eV}{2}\right)\left(1 - |r_G|^2 - |t_G|^2 \frac{v_{3x}}{v_{1x}}\right). \tag{3a}$$

Similarly, the incoming energy flux from region 3 can be written as

$$J^{u}_{in2} = \frac{2}{(2\pi)^3} \int_{k_0}^{\sqrt{2}k_0} dk_{3x} \int_{-\infty}^{\infty} dk_{3\perp} f(k_3) v_{2x} \left(E_3 - \frac{eV}{2}\right) |t_{2r}|^2$$
$$+ \frac{2}{(2\pi)^3} \int_{\sqrt{2}k_0}^{\infty} dk_{3x} \int_{-\infty}^{\infty} dk_{3\perp} f(k_3) v_{3x} \left(E_3 - \frac{eV}{2}\right)\left(1 - |r'_G|^2 - |t'_G|^2 \frac{v_{1x}}{v_{3x}}\right) \tag{3b}$$

where $f(k_j)$ ($j = 1, 3$) is the Fermi–Dirac distribution, $k_0 = \sqrt{meV}/\hbar$, and t'_G and r'_G are the transmission and reflection coefficients from regions 3 to 1, respectively. The first part on the right side of (3*b*) represents the contribution from the electrons whose energy, in the x direction, is larger than $\frac{1}{2}eV$ but less than eV. These electrons are able to tunnel through the right barrier but not through the left barrier, thus they all contribute to the energy flux in the quantum well. The second part represents the contribution from the electrons whose energy in the x direction is larger than eV. These electrons can tunnel through the double-barrier structure, and thus only the 'missing' part contributes to the flux. The energy flux going out from the quantum well to regions 1 and 3 can be written as, respectively,

$$J^{u}_{out1} = \frac{2}{(2\pi)^3}\int_{k_0}^{\infty} dk_{2x} \int_{-\infty}^{\infty} dk_{2\perp}\, f(k_2, T_e, \mu_e) E_2 v_{1x} |t_{1r}|^2 \tag{4a}$$

$$J^{u}_{out2} = \frac{2}{(2\pi)^3}\int_{0}^{\infty} dk_{2x} \int_{-\infty}^{\infty} dk_{2\perp}\, f(k_2, T_e, \mu_e) E_2 v_{3x} |t_{2l}|^2. \tag{4b}$$

The energies of the incoherent electrons in the well can also be dissipated into the lattice by the electron–phonon interactions. The dissipation rate may be modelled by the relaxation-time approximation $[E(T_e) - E(T)]/\tau_\varepsilon$, where τ_ε is the energy relaxation time [19]. $E(T_e)$ and $E(T)$ are the total energy of the incoherent electrons per unit volume in the well at the electron temperature T_e and the lattice temperature T, respectively. In steady state, the energy conservation law requires that the energy flux entering the well is equal to the energy flux going out of the well plus the energy flux dissipated into the lattice, i.e.

$$J^{u}_{in1} + J^{u}_{in2} = J^{u}_{out1} + J^{u}_{out2} + a_2[E(T_e) - E(T)]/\tau_\varepsilon. \tag{5}$$

As $\tau_\varepsilon \to 0$, T_e must equal T. In this case, the hot-electron distribution (1) reduces to the Fermi–Dirac distribution. Similarly, the particle conservation law can be written as

$$J^{c}_{in1} + J^{c}_{in2} = J^{c}_{out1} + J^{c}_{out2} \tag{6}$$

where J^{c}_{in1} and J^{c}_{in2} represent the incoherent electron current densities entering the well from regions 1 and 3, while J^{c}_{out1} and J^{c}_{out2} represent the current densities going out from the quantum well to regions 1 and 3, respectively. The formulas for calculating these currents can be derived from (3) and (4) by replacing the energy carried by an electron with the charge carried by the electron. We would like to emphasize that we do not need to write down the energy and particle conservation equations for the coherent electrons, since they are guaranteed by the quantum mechanics. Equations (5) and (6) are implicit equations of T_e and μ_e, which can only be solved numerically.

The parameters in this calculation were chosen as follows. The widths of the barriers and well were taken as $a_1 = a_3 = 17$ Å and $a_2 = 45$ Å. The Fermi energy, μ, at the emitter and collector was chosen as 0.05 eV and the room temperature was set to 300 K. The barrier heights are equal to 1 eV. The effective mass in the barrier was taken to be $0.1m_0$ (m_0 is the free electron mass), while the effective mass in the other regions is $0.067m_0$. The energy relaxation time was chosen as 5×10^{-12} s and the damping constant, α, is 2×10^{6} cm^{-1}. The secant method was used to solve (5) and (6). We found that this method converges for any applied voltages and a unique solution of T_e and μ_e can be obtained from (5) and (6). The results are displayed in figure 2. We can see from figure

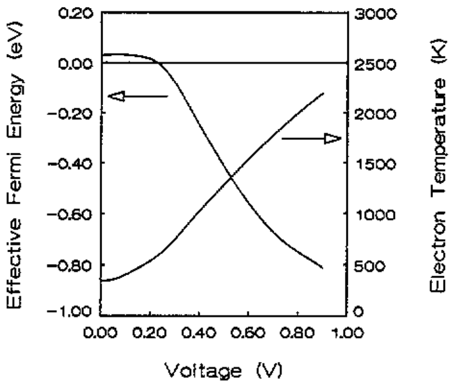

Figure 2. The electron temperature, T_e, and effective Fermi energy, μ_e, are displayed against the voltage across the double-barrier structure. The parameters in this calculation are given in the text.

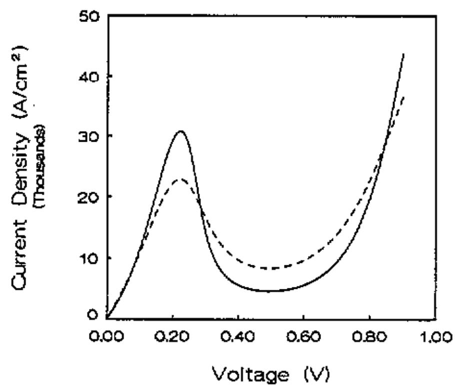

Figure 3. The current densities tunnelling through the RTD are displayed against the applied voltage. The dashed line is for $\alpha = 2 \times 10^6\ \mathrm{cm}^{-1}$ and the solid line is for $\alpha = 10^6\ \mathrm{cm}^{-1}$.

2 that the electron temperature increases as the applied voltage increases. This reflects the fact that the higher the voltage is, the more energy the electron will gain when it enters the quantum well. It is interesting to notice that when the applied voltage is high, say above 0.6 V, the effective Fermi surface is well below the conduction band. Then the distribution given by (1) reduces to the Boltzmann distribution. There is a simple physical explanation for this phenomenon. When the applied voltage is high, the average energy of electrons in the well will be large. This means that the average occupancy of each state will be low and the Pauli exclusion principle becomes insignificant. Since the electrons will not lose energy quickly enough to the lattice, we may approximately think of the total kinetic energy of the electrons in the well as being conserved. Thus, the electrons will adjust their energy and momentum distributions through the electron–electron interaction. This is exactly the same situation as that of the ideal gas and the resultant distribution must be Boltzmann.

We have also calculated the total current density tunnelling through the diode, which is the summation of the coherent current density, J_{coh}, and the incoherent current density, J_{incoh}. The coherent current density can be shown to be given by [20]

$$J_{\mathrm{coh}} = \int_0^\infty \mathrm{d}k_{1x}\, e v_{3x} [f(E_{1x}) - f(E_{1x} + eV)]\, |t_G|^2 \tag{7a}$$

$$f(E_{1x}) = (mk_B T/2\pi^2\hbar^2) \ln(1 + \mathrm{e}^{\beta(\mu - E_{1x})}) \qquad E_{1x} = \hbar^2 k_{1x}^2/2m \tag{7b}$$

and the incoherent current density is given by

$$J_{\mathrm{incoh}} = J^{\mathrm{e}}_{\mathrm{out2}} - J^{\mathrm{e}}_{\mathrm{in2}}. \tag{8}$$

The parameters used in this calculation were exactly the same as that in figure 2, except two damping constants, $10^6\ \mathrm{cm}^{-1}$ and $2 \times 10^6\ \mathrm{cm}^{-1}$ were used. Larger damping constant represent more scattering, which could come from more defects, more impurities, or higher lattice temperature. Our results, as displayed in figure 3, clearly demonstrate that the current peak to valley ratio degrades as the damping constant increases. This is qualitatively consistent with the current experimental results: the current peak-to-valley ratio decreases as the lattice temperature increases [2] or as the density of defects increases. The latter has been analysed by Mao *et al* using fast-neutron irradiation [21].

References

[1] Tsu R and Esaki L 1973 *Appl. Phys. Lett.* **22** 562

[2] Sollner T C L G, Goodhue W D, Tannenwald P E, Parker C D and Peck D D 1983 *Appl. Phys. Lett.* **43** 588

[3] Brown E R, Sollner T C L G, Parker C D, Goodhue W D and Chen C L 1989 *Appl. Phys. Lett.* **55** 1777

[4] Brown E R, Söderström J R, Parker C D, Mahoney L J, Molvar K M and McGill T C 1991 *Appl. Phys. Lett.* **58** 2291

[5] Kesan V P, Mortazawi A, Miller D R, Reddy V K, Neikirk D P and Itoh T 1989 *IEEE Trans. Microwave Theory Tech.* **MTT-37** 1933

[6] Ricco B and Azbel M Ya 1984 *Phys. Rev.* B **29** 1970

[7] Barker J R and Murray S 1983 *Phys. Lett.* **93A** 271

[8] Frensley W R 1986 *Phys. Rev. Lett.* **57** 2853

[9] Kluksdahl N C, Kriman A M, Ferry D K and Ringhofer C 1989 *Phys. Rev.* B **39** 7720

[10] Stone A D and Lee P A 1985 *Phys. Rev. Lett.* **54** 1196

[11] Jonson M and Grincwajg A 1987 *Appl. Phys. Lett.* **51** 1729

[12] Hu Y 1988 *J. Phys. C: Solid State Phys.* **21** L23

[13] Hu Y and Stapleton Shawn 1991 *Appl. Phys. Lett.* **58** 167

[14] Luryi S 1985 *Appl. Phys. Lett.* **47** 490

[15] Goldman V J, Tsui D C and Cunningham J E 1987 *Phys. Rev. Lett.* **58** 1256; 1987 *Phys. Rev. Lett.* **59** 1623
Sollner T C L G 1987 *Phys. Rev. Lett.* **59** 1622

[16] Sheard F W and Toombs G A 1988 *Appl. Phys. Lett.* **52** 1228

[17] Frensley W R 1990 *Rev. Mod. Phys.* **62** 745

[18] Sze S M 1981 *Physics of Semiconductor Devices* (New York: Wiley) p 558

[19] Seeger K 1985 *Semiconductor Physics* (Berlin: Springer) p 102 and Ch 6

[20] Duke C B 1969 *Tunnelling in Solids* (New York: Academic)

[21] Mao J M, Zhou J M, Zhang R L, Jin W M, Bao C L and Huang Y 1990 *Appl. Phys. Lett.* **56** 548