# Monte Carlo calculations of transport parameters of one-dimensional hot electrons in quantum-well wires

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Monte Carlo calculations of hot-electron drift velocity, average energy, and diffusion coefficient are reported for the one-dimensional electron gas in a GaAs quantum-well wire of square cross section with side length $L$. Electron scattering by acoustic and longitudinal polar optic phonons is included. The transport parameters are found to rise more rapidly with electric field for $L=160$ Å than for $L=40$ Å, particularly at a lower ambient temperature. Einstein's relationship is shown to underestimate the hot-electron diffusivity for $L=160$ Å.

The search for high-electron-mobility submicrometer devices in recent years has caused considerable interest in the fabrication and properties of ultrathin wire and related semiconductor structures.[1-14] In such structures, quantization occurs in two transverse directions so that a one-dimensional electron gas (1D EG), free to move in the longitudinal direction, is formed. The 1D EG is characterized by a high-electron mobility resulting from the spatial separation of the electrons from their parent donor atoms due to modulation doping and from the reduced number of final states in a scattering event which consists of either forward or backward scattering in a single subband.[1] As an aid to the work related to the devices using quantum-well wire structures, understanding of the hot-electron kinetics of the 1D EG is essential.[14]

In this paper, we report a Monte Carlo study of the electric field dependencies of the drift velocity, the average energy, and the diffusivity of the 1D EG in a GaAs quantum-well wire of square cross section. Results are presented for different transverse dimensions of the wire structures for different lattice temperatures. The hot-electron diffusivity, calculated from Einstein's relationship with an effective temperature, is found to be much lower than the exact value for a wire of wider cross section.

In the present investigation the conduction band is assumed to be parabolic with subband energies given by the solution of the wave equation for a square-well potential. Scattering of the quantized electrons by intrinsic processes, e.g., deformation-potential acoustic- and longitudinal-polar-optical phonons is considered. Phonon modes are taken to be bulklike and the scattering rates are calculated numerically. The phonon spectrum is likely to be altered and to lead to a reduced electron-phonon interaction in heterostructures.[15,16] Similar effects are also expected in one-dimensional systems although the problem has not yet received attention. While calculations of transport parameters including the modified phonon spectra are needed, the weakening of the electron-phonon interaction would be moderated by remote interaction with phonons in the adjacent material owing to the long-range character of the polar interaction. Thus the assumption of bulklike phonons is not likely to lead to any serious error. In fact, most recent investigations of electronic transport in heterostructures have used bulk-mode phonons.[8-10,14,17,18]

In this initial work, the effects of electron-electron scattering, screening, and degeneracy of the carrier distribution are neglected. It is a formidable task to include these effects explicitly into a Monte Carlo study of electronic transport.[19] While for linear electron densities below $7\times10^5$ cm$^{-1}$ the effects are sufficiently small to be ignored, for higher electron densities our results would help in evaluating the importance of these effects when methods to include them exactly are devised.

The Monte Carlo simulation technique in which the trajectories of charge carriers moving in the applied fields and interacting with the crystal lattice are followed on a time basis has been recently reviewed by Jacoboni and Reggiani.[19] Random numbers are generated to determine the time of free flight between scattering events and the type of scattering terminating the free flight. In our case, the carriers are scattered inelastically by polar-optical phonons and elastically by acoustic phonons. The absorption and the emission of phonons in inelastic scattering events are treated separately. For a 1D EG additional random numbers are not required to determine the final state after scattering due to the reduced dimensionality of the system. The method of calculating the transport parameters in the simulation technique follows that described in Ref. 19.

The material parameters of GaAs used in the computations are listed in Table I. Among these parameters, there is some controversy over the choice of the acoustic deformation potential. While the commonly accepted value of this potential is 7 eV, recent studies[20-22] of the two-dimensional electron gas in GaAs have yielded for the acoustic deformation potential a value of about 11 eV, which we use in the present calculations.

As the high-electron-mobility devices are operated typically at low temperatures, calculations are done here for ambient temperatures ($T$) of 30, 77, and 120 K. The calculated electric field dependencies of the drift velocity, average energy (relative to the bottom of the lowest sub-

 

TABLE I. GaAs material parameters.

| | |
|---|---|
| Effective-mass ratio ($m/m_0$) | 0.067 |
| Longitudinal elastic constant | $14.7\times10^{10}$ N m$^{-2}$ |
| LO-phonon energy | 0.0361 eV |
| Optic dielectric constant | 10.9 |
| Static dielectric constant | 12.8 |
| Acoustic deformation potential | 11 eV |

band), and diffusion coefficient are displayed in Figs. 1, 2, and 3, respectively for $L=40$ and 160 Å, where $L$ represents a side of the square cross section of the quantum-well wire. The transport parameters are found to depend on the value of $L$ which enters into the calculation through the electron wave function. This wave function affects the matrix element for the interaction of the one-dimensional electrons with the three-dimensional phonon field. Although a strictly one-dimensional electron gas is achieved in narrower wires, the transverse phonon field has a chance to oscillate over the confinement length $L$ as the latter increases. As a result, the electron-phonon interaction in a single subband becomes weaker in a wire of wider cross section.[10] The interaction is also weaker at lower ambient temperatures as the phonon occupation number gets smaller. Consequently, the drift velocity and the average energy of the hot electrons are larger for the higher value of $L$ and for lower ambient temperatures. Previously it was shown that the polar-optical scattering tends to establish a saturatory behavior of the drift velocity at low temperatures.[14] The additional inclusion of acoustic scattering in the present calculations is found to destroy this behavior.

For the sake of comparison, we have included in Fig. 1 the results of the Monte Carlo calculations for bulk GaAs at 77 K. It is found that although the drift velocities for $L=40$ Å are smaller, those for $L=160$ Å are larger than

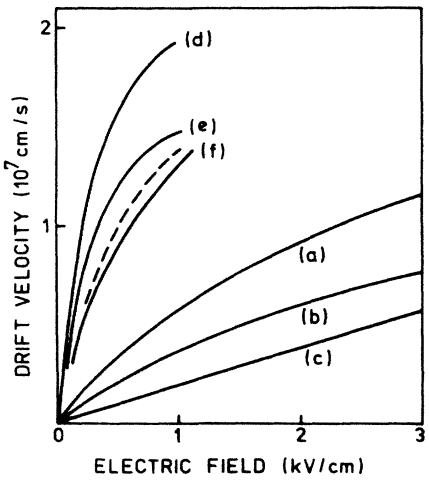


FIG. 1. Variation of drift velocity with electric field. (a) $L=40$ Å, $T=30$ K; (b) $L=40$ Å, $T=77$; (c) $L=40$ Å, $T=120$ K; (d) $L=160$ Å, $T=30$ K; (e) $L=160$ Å, $T=77$ K; (f) $L=160$ Å, $T=120$ K. The dashed curve is for bulk GaAs at 77 K.

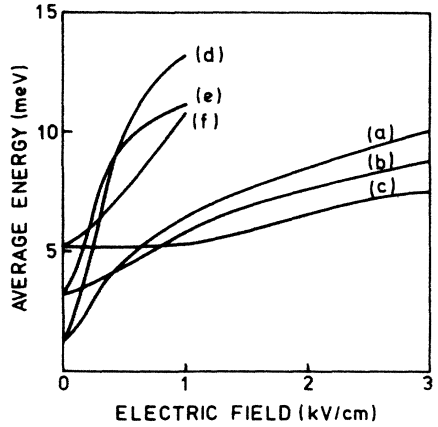


FIG. 2. Variation of the average energy (measured from the bottom of the lowest subband) with electric field. Curves (a)–(f) have the same significance as in Fig. 1.

those in the bulk due to the reduced scattering rate for $L=160$ Å.

The average energies of hot electrons shown in Fig. 2 are less than 15 meV. For $L=40$ Å there is only one subband within the well, while for $L=160$ Å, the separation between the lowest subband and the next-higher subband is 60 meV. As this separation is much larger than the calculated average energies, the occupation of the next-higher subband is negligible for the fields considered here. Also, the calculated energies are much less than the barrier height of 250 meV between GaAs and Ga-Al-As. The electrons thus remain within the quantum-well wire and do not escape into the neighboring bulk material.

The strong electron-phonon interaction for $L=40$ Å at 120 K makes the diffusion coefficient nearly field independent up to the field of about 3 kV cm$^{-1}$ as revealed by curve (c) of Fig. 3. The diffusion coefficient, however,

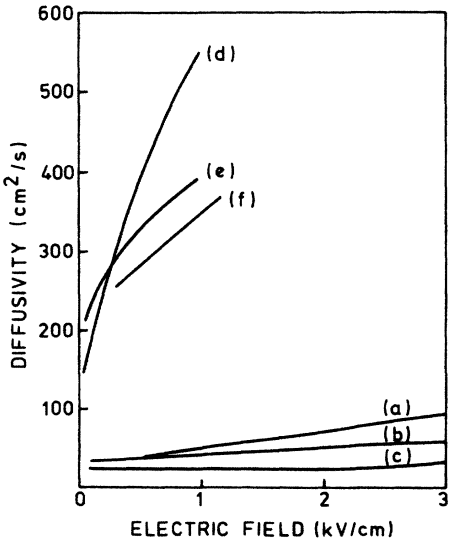


FIG. 3. Variation of the diffusion coefficient with electric field. Curves (a)–(f) have the same significance as in Fig. 1.

rises with electric field when $L$ is increased, and the temperature is decreased due to the weakening of the electron-phonon interaction under such conditions.

The values of the hot-electron diffusivity, calculated from Einstein's relationship, $D_E=\mu k_B T_e/e$, are shown in Table II for an electric field of 1 kV/cm. Here $\mu$ is the mobility, $e$ is the electronic charge, $k_B$ is the Boltzmann constant, and $T_e$ is the effective electron temperature derived from the mean random energy $\bar{E}$ using the relationship $\bar{E}=\frac{1}{2}k_B T_e$: the factor $\frac{1}{2}$ accounts for the one translational degree of freedom of the 1D EG. The values of $D_E$ for $L=160$ Å are found to be significantly smaller than the exact values of the diffusion coefficient $D$, plotted in Fig. 3 and also given in Table II for an easy comparison. The difference in the values of $D_E$ and $D$ is, however, not so great for $L=40$ Å, where strong electron-phonon interactions prevent rapid heating of the carriers.

In conclusion, our Monte Carlo calculations show that the drift velocity and the diffusion coefficient are larger and more strongly field dependent for a quantum-well wire width $L=160$ Å than that with $L=40$ Å, particularly at lower ambient temperatures. Thus the higher value of $L$ is desirable for high-speed devices from mobility considerations, but its performance would be degraded by the higher value of the diffusivity. Einstein's relationship is found to be generally invalid for the hot electrons in quantum-well wires.

TABLE II. Comparison of the exact values of the diffusivity with those obtained from Einstein's relationship.

| Ambient temperature (K) | $D_E$ ($cm^2 s^{-1}$) $L=40$ Å | $L=160$ Å | $D$ ($cm^2 s^{-1}$) $L=40$ Å | $L=160$ Å |
|---|---|---|---|---|
| 30 | 63 | 234 | 50 | 550 |
| 77 | 41 | 205 | 40 | 392 |
| 120 | 21 | 197 | 25 | 348 |


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