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Hot-electron transport in GaAs-AlGaAs heterojunctions

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Hot-electron transport in a GaAs-AlGaAs heterojunction is studied by the use of a non-Boltzmann balance-equation approach recently developed. The occupation of the lowest and next lowest subbands and the Coulomb interactions between intrasubband and intersubband electrons are taken into account. We include the scattering by remote charge impurities, acoustic phonons (via deformation potential and piezoelectric coupling), and polar optical phonons in the force and energy balance equations to give the carrier mobility as a function of drift velocity and/or electric field. Theoretical results are in reasonably good agreement with experiments.

Materials composed of modulation-doped GaAs-AlGaAs heterostructure show extremely high electron mobility.[1,2] This enhanced mobility makes them very useful in fabricating fast-speed field-effect transistors.[3] It was found, however, that the mobility of electrons in a GaAs-AlGaAs heterojunction depends strongly on the electric field, and hot-electron effects were observable at fields as low as 10 V/cm.[4] This means that the peformance of devices made from these materials is greatly subject to their nonlinear transport behavior at "large" electric field. Therefore, an understanding of the physics of high-field transport in heterostructure materials is important both for basic research and for optimization of the design and operation of the devices fabricated from them. Experimentally, several measurements have been made to determine the mobility as a function of electric field.[4-6] A good theoretical explanation, however, is not available at present. Most workers fit their high-field mobility data using the variation of low-field mobility $\mu_0(T)$ with lattice temperature T, replacing T by a "carrier temperature" T_c, which is measured based on the assumption that the conducting electrons can be described by an equilibrium-type distribution function (Boltzmann or Fermi-Dirac) at temperature T_c. This assumption is hardly justifiable. The only high-field theoretical result reported so far for modulation-doped GaAs-AlGaAs systems was a model calculation by Drummond *et al.*[4] according to the theory of Hess and co-workers,[7,8] but seems not in good agreement with experiments.

Recently, a non-Boltzmann balance-equation approach has been developed by Lei and Ting[9] for nonlinear electronic transport in electron-phonon-impurity systems in the presence of a strong electric field. The method has been extended to two-dimensional electron systems, specifically to a GaAs-AlGaAs single heterostructure by Lei, Birman, and Ting.[10] The purpose of this Communication is to report a study of hot-electron transport in GaAs-AlGaAs heterojunctions based on this approach.

The starting point of the approach is a force and an energy balance equation for the steady state in the presence of an electric field $\mathbf{E}$:

$$Ne\mathbf{E}+\mathbf{F}(\mathbf{v})=0 \ , \tag{1}$$

$$\mathbf{v}\cdot\mathbf{F}(\mathbf{v})+W(\mathbf{v})=0 \ , \tag{2}$$

where $\mathbf{v}$ is the center-of-mass velocity, or the average drift velocity of the electrons, and e and N are, respectively, the charge and the sheet density of the carriers. The current density is given by

$$\mathbf{J}=Ne\mathbf{v} \ . \tag{3}$$

In these equations $\mathbf{F}(\mathbf{v})$ is the frictional force experienced by the center of mass when it moves at a constant speed, which is composed of two parts, one due to impurities and one due to phonons, respectively:

$$\mathbf{F}(\mathbf{v})=\mathbf{F}_i(\mathbf{v})+\mathbf{F}_p(\mathbf{v}) \ , \tag{4}$$

and $W(\mathbf{v})$ is the energy transfer rate from the electron system to the phonon system.

In high electric fields, the electron temperature may rise to 200 K even at zero lattice temperature. The variation of electron statistics and the occupation of more than the lowest subband should be taken into account even for low carrier sheet density. The expressions for the frictional forces and energy transfer rate have been given in Eqs. (24)–(26) of Ref. 10, including multisubband structures, and will not be repeated here. We use the same notation as that in Ref. 10. The electron-electron Coulomb interaction is fully included in these expressions through the function $\hat{\Pi}_2(n',n,\mathbf{q},\omega)$, the imaginary part of the density-density correlation function for relative electrons $\hat{\Pi}(n',n,\mathbf{q},\omega)$, in which n and n' are subband indices. Under the random-phase approximation it can be expressed as

$$\hat{\Pi}(n',n,\mathbf{q},\omega)=\Pi(n',n,\mathbf{q},\omega)[1+\tilde{V}_{n'n,n'n}(q)\hat{\Pi}(n',n,\mathbf{q},\omega)] \ . \tag{5}$$

The renormalized potentials $\tilde{V}_{n'n,m'm}(q,\omega)$ satisfy the following equations:

$$\tilde{V}_{n'n,m'm}(q,\omega)=V_{n'n,m'm}(q)+\sum_{l',l}V_{n'n,l'l}(q)\Pi(l',l,q,\omega)\tilde{V}_{l'l,m'm}(q,\omega) \ . \tag{6}$$

In these equations

$$\Pi(n',n,\mathbf{q},\omega)=2\sum_{\mathbf{k}}\frac{f(E_{n'\mathbf{k}+\mathbf{q}})-f(E_{n\mathbf{k}})}{\hbar\omega+E_{n'k+q}-E_{nk}+i\delta} \tag{7}$$

is the density-density correlation function for electrons in the n and n' subbands in the absence of Coulomb interaction between them. Here $E_{nk}=E_n+\hbar^2k^2/2m$ is the electron energy with two-dimensional wave vector $\mathbf{k}$ in subband n and $f(E)=\{\exp[(E-E_f)/k_BT]+1\}^{-1}$ is the Fermi function with E_f as the temperature-dependent Fermi energy, which is to be determined from the total carrier sheet density N by the equation,

$$2\sum_{n,k} f(E_{nk})=N \quad . \tag{8}$$

In Eq. (6)

$$V_{n'n,m'm}(q)=\frac{e^2}{2\epsilon_0\kappa q}H_{n'n,m'm}(q) \tag{9}$$

are the matrix elements of the Coulomb coupling between electrons, κ is the low-frequency dielectric constant of GaAs, and

$$H_{n'n,m'm}(q)=\int dz_1dz_2\zeta^*_{n'}(z_1)\zeta_n(z_1) \times\zeta^*_{m'}(z_2)\zeta_m(z_2)\exp(-q|z_1-z_2|) \quad . \tag{10}$$

The contribution from image changes is neglected in Eq. (9) because of the smallness of the difference of the dielectric constants on both sides of the GaAs-AlGaAs interface.

In discussing Ohmic mobility, Lei[12] used a simpler approximate equation to determine $\hat{\Pi}(n',n,\mathbf{q},\omega)$, which differs from Eqs. (5) and (6) by some extra intersubband terms. However, numerical results show no appreciable corrections for linear mobility if we use more reliable equations (5) and (6).

In most experimental systems, in which carrier sheet density $N<5\times10^{11}$ cm^{-2}, only lowest subband ($n=0$) is occupied at zero temperature. For the case of electron temperature less than 200 K, we can consider only the lowest and next lowest subbands in the calculation. The random-phase-approximation (RPA) equation (6) can thus be truncated by taking n', n, m', $n=0$, 1 only. We will use the Fang-Howard-Stern variational function

$$\zeta_0(z)=\left(\frac{b_0^3}{2}\right)^{1/2}z\exp\left(-\frac{b_0z}{2}\right) \tag{11}$$

and

$$\zeta_1(z)=\frac{3}{2}\left(\frac{b_1^5}{b_0^2-b_0b_1+b_1^2}\right)^{1/2}z\left[1-\left(\frac{b_0+b_1}{6}\right)z\right]\exp\left(-\frac{b_1z}{2}\right) \tag{12}$$

as the envelope wave function for the $n=0$ and 1 subbands, respectively. The parameters b_0 and b_1 are determined by minimizing the energy E_0 and E_1 as usual.[11] The integrations in Eq. (10) are performed to give closed expressions for $H_{n'n,m'n}(q)$. The density-density correlation functions for both intrasubband and intersubband electrons then can be obtained from Eq. (5) and the truncated RPA equation (6).

We assume the remote impurities are the dominant elastic scatterers, which are located within a narrow-space charge layer with a total sheet density N_I at a distance s from the interface in the barrier of the AlGaAs side. The impurity-induced frictional force can be written as

$$F_i(\mathbf{v})=\sum_{n',n,\mathbf{q}}|U_{n'n}(q)|^2\hat{\Pi}_2(n',n,\mathbf{q},\mathbf{q}\cdot\mathbf{v}) \quad , \tag{13}$$

with

$$|U_{n'n}(q)|^2=\left(\frac{Ze^2}{2\epsilon_0\kappa}\right)^2N_Ie^{-2qs}q^{-2}I_{n'n}(q)^2 \tag{14}$$

and

$$I_{n'n}(q)=\int e^{-qz}\zeta^*_{n'}(z)\zeta_n(z)dz \quad . \tag{15}$$

Closed expressions for $I_{n'n}(q)$ are obtained using Eqs. (11) and (12) as wave functions.

The electron-phonon matrix elements $M(n',n,\mathbf{q},q_z,\lambda)$ in the expressions of the frictional force and energy transfer rate share the same form factors as Eq. (15):

$$M(n',n,\mathbf{q},q_z,\lambda)=M(\mathbf{q},q_z,\lambda)I_{n'n}(iq_z) \quad . \tag{16}$$

$M(\mathbf{q},q_z,\lambda)\equiv M(\mathbf{Q},\lambda)$ is the matrix element of the electron-phonon interaction in the three-dimensional plane-wave representation. We consider both the electron–acoustic-phonon interaction (via piezoelectric coupling and deformation potential) and electron–polar-optical-phonon interaction (via Fröhlich coupling). The $M(\mathbf{Q},\lambda)$ expressions for these interactions are well known and have been examined in Ref. 10 [Eqs. (54)–(58)]. The electron–polar-optical-phonon interaction turns out to be effective in energy transfer from the electron system to the phonon system at a temperature as low as 30 K when its contribution to the frictional force is still negligible.

In Fig. 1 we plot the calculated normalized mobility $\mu/\mu_0(T)$ (solid curves) and electron temperature T_e (dashed curves) as functions of drift velocity v for a GaAs-AlGaAs system with carrier sheet density $N=4.0\times10^{11}$

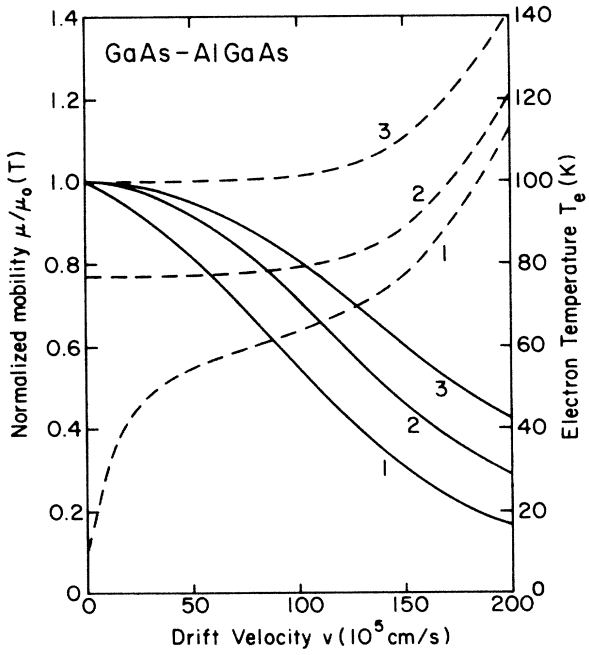

FIG. 1. Calculated normalized mobility $\mu/\mu_0(T)$ (solid curves) and electron temperature T_e (dashed curves) are shown as functions of drift velocity v for a GaAs-AlGaAs system with $N=4.0\times10^{11}$ cm^{-2} and $\mu_0(0)=2.2\times10^5$ cm^2/Vs. The impurities are located at a distance $s=125$ Å from the interface. The lattice temperatures are 1, 10 K; 2, 77 K; 3, 100 K.

cm^{-2} and 0-K Ohmic mobility $\mu_0(0)=2.2\times10^5$ cm^2/Vs at lattice temperatures $T=10$, 77, and 100 K, respectively. Here $\mu_0(T)$ is the Ohmic mobility at temperature T. The mobility curves 1 and 2 for $T=10$ and 100 K are redrawn in Fig. 2 against the applied electric field for comparing with the experimental data reported in Ref. 4. The dashed curve in this figure is the theoretical calculation given in Ref. 4, based on the theory of Hess and co-workers,[7,8] which is, to our knowledge, the only theoretical result so far published on this problem. The present theoretical curves show significant improvement in accordance with experiments for both low- and high-field regions.

In Fig. 3 the calculated normalized mobilities μ/μ_0 (solid curves) and electron temperature T_e (dashed curves) are shown as functions of applied electric field E at lattice temperature $T=4.2$ K for two GaAs-AlGaAs systems with $N=2.5\times10^{11}$ cm^{-2} and $\mu_0=1.0\times10^6$ cm^2/Vs, and $N=3.9\times10^{11}$ cm^{-2} and $\mu_0=7.9\times10^4$ cm^2/Vs, respectively. The crosses are taken from the dark data at 4.2 K of the sample 2 of Höpfel and Weimann.[5] The dots are the experimental results of Shah *et al.*[6] for a multi-quantum-well sample of width 260 Å and layer carrier density $N=3.9\times10^{11}$ cm^{-2} at $T=2$ K. Although the present model is intended specifically for a single-interface heterojunction, it is expected that the predictions for normalized mobility are also qualitatively valid for a multi-quantum-well system with relatively large width and separation.

The material parameters used in the calculations are the following: density $d=5.31$ g/cm^3, effective mass $m=0.07m_e$, transverse sound velocity $v_{st}=2.48\times10^3$ m/s, longitudinal sound velocity $v_{sl}=5.29\times10^3$ m/s, longitudinal-optical-phonon energy $\hbar\Omega_0=35.4$ meV, low-frequency dielectric constants $\kappa=12.9$, optical dielectric constant $\kappa_\infty=10.8$, acoustic deformation potential $\Xi=8.5$ eV, piezoelectric constant $e_{14}=1.41\times10^9$ V/m. These are the values widely used for GaAs-AlGaAs systems.

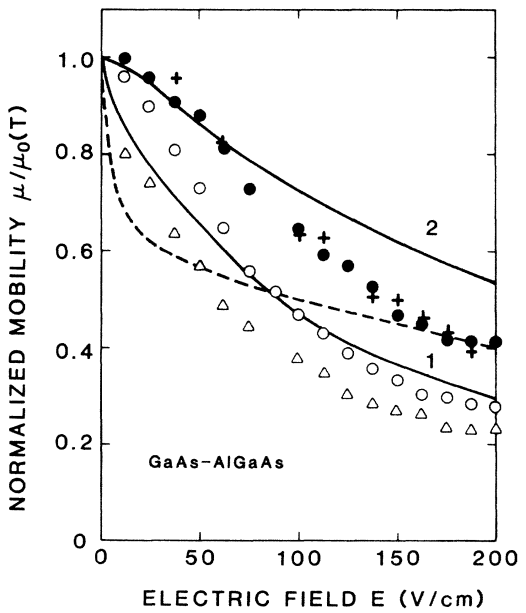

FIG. 2. Normalized mobility μ/μ_0 vs electric field E. Solid curves 1 and 2 are the present theoretical results for $T=10$ and 77 K, respectively. The dashed curve is the theoretical calculation given in Ref. 4 at $T=10$ K. The experimental data are taken from Ref. 4 on sample 367/1: ○, 10 K; +, 77 K; and sample 367/2: △, 10 K; ●, 77 K.

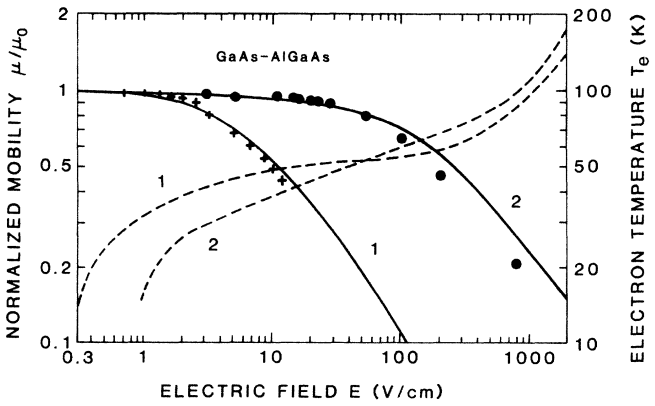

FIG. 3. Calculated normalized mobility μ/μ_0 (solid curves) and electron temperature T_e (dashed curves) vs electric field E at lattice temperature $T=4.2$ K for two systems: (1) $N=2.5\times10^{11}$ cm^{-2}, $\mu_0=1\times10^6$ cm^2/Vs, $s=250$ Å; (2) $N=3.9\times10^{11}$ cm^{-2}, $\mu_0=7.9\times10^4$ cm^2/Vs, $s=125$ Å. The experimental data are taken from Ref. 5 (crosses) and Ref. 6 (dots).

For the normalized mobility μ/μ_0, the agreement between theoretical and experimental values is reasonably good except in the highest-field region, where the experimental data are generally lower than theoretical predictions. This is understandable. The electron-phonon umklapp process and nonpolar-optical-phonon scattering will play roles at high fields and/or at high temperatures. They are neglected in the present model. This may also be responsible for the discrepancy between theory and experiment in Ohmic mobility at high temperatures ($T>200$ K).[12]

It is worth noting that in contrast to the ideas in some carrier temperature models, which attribute the nonlinear effect mainly to the heating of electrons, in the present theory the variation of the electron temperature is not the only source of the nonlinearity of the mobility with electric field. This is obviously seen from the $T=77$ K and $T=100$ K curves in Fig. 1, where the electron temperature is almost unchanged until the drift velocity $v\geqslant6\times10^6$ cm/s; the mobility, however, undergoes a variation of more than 10%. The reason for this is clear: in addition to the electron temperature T_e, the drift velocity v enters the force and energy transfer rate expressions directly via the electron density-density correlation function and the Bose factors. This has an important influence on the nonlinear behavior.

In summary, we have studied the steady-state hot-electron transport in a single GaAs-AlGaAs heterolayer system by a non-Boltzmann balence-equation approach. Although it is a two-parameter theory, this approach is different from the conventional two-parameter models and also different from Monte Carlo simulations.

First, the electron temperature T_e introduced in the present balance-equation approach[9,10] is conceptually different from that in a carrier-temperature model. In the latter the carrier temperature T_c is a parameter in an equilibrium-type distribution function,[13] which is assumed to be valid for the description of electrons transported under the influence of an electric field. Most of the experimental data on carrier temperature are based on the accurate appli-

cability of a Boltzmann- or Fermi-Dirac–type distribution function (with a fixed parameter T_c as temperature) for hot electrons in both low- and high-energy regions, so that, for example, the logarithmic slope of the high-energy tail in luminescence spectra of the system can be identified as $1/T_c$. The real situation, however, is not so simple. The transported electrons, especially at high field, are not in an equilibrium state and generally cannot be described by an equilibrium-type distribution function of any kind in any reference system. Even if an equilibirum-type function is good enough for low-energy electrons in some cases, one cannot be certain that the same form is also valid at high energy. The present model did not assume any distribution function for these electrons. The electron temperature T_e used here is not a parameter in the distribution function, but measures the average energy of the relative movement of the electrons and plays a role mainly in transport. Because the high-energy electrons are a very small percentage of the total, and thus make a very small contribution to the current transport, we can hardly infer the form of their distribution from the T_e value alone. Therefore, it is inappropriate to compare the calculated electron temperature with the one obtained by luminescence measurements. The thermal noise seems to be a more suitable quantity for such a purpose.

Second, the many-body effects of the electrons are fundamentally built into the theory via the density-density correlation function of the relative electrons. Therefore, the full dynamic and temperature-dependent screening and high-field descreening effects, together with electron plasma excitation, are included both in the formulation and throughout the present calculation, within the RPA. This is one of the major differences of the present approach from conventional Monte Carlo simulations and from Thornber-Feynman theory.[14] Furthermore, we have made a full RPA calculation for a two-subband system, including all intrasubband and intersubband interactions between carriers. To our knowledge, this is the first time that many-body effects were considered to such an extent in transport calculations for a heterojunction.

A two-parameter theory certainly has its limitations since for an exact description of a real transport system an infinite number of parameters is needed in order to satisfy an infinite number of balance equations. Also, the exclusion of the umklapp process in electron-phonon scattering is a limitation in the present model. Umklapp scattering is expected to play a growing role with increasing electric field. These should serve as directions for the extension of the theory for the future.

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