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Low field mobility and thermopower in one-dimensional electron gas

S. Kundu, C. K. Sarkar,[a] and P. K. Basu
Centre of Advanced Studies in Radio Physics and Electronics, Calcutta University, 92 Acharya Prafulla Chandra Road, Calcutta-700009, India

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A scattering theory of one-dimensional electron gas formed in a narrow channel GaAs-AlGaAs high electron mobility transistor has been developed. The mobility values for the different scattering mechanisms have been computed and their variation with temperature has been presented. The various scattering processes include acoustic phonon scattering for both deformation potential and piezoelectric scattering mechanisms, impurity scattering, and surface roughness scattering at lower temperatures and polar optic phonon scattering at higher temperatures. The effect of dynamic screening has also been included. Finally, the temperature variation of thermopower for different 1D electron concentrations has been shown and attempts have been made to interpret the results obtained.

I. INTRODUCTION

The properties of the two-dimensional electron gas (2DEG) formed in the channel of a Si-MOSFET or a GaAs-HEMT (high electron mobility transistors) have been exhaustively studied by a number of research groups.[1] Sakaki[2] first proposed that one-dimensional electron gas (1DEG) could also be realized in ultrathin wires of semiconductors, or by suitable modifications of 2D systems. The 1DEG is also formed in narrow channel FETs made of Si or in heterojunctions made of GaAs and AlGaAs that are used in high electron mobility transistors[3] (HEMT). This system promises even higher mobilities due to the restriction on the scattering angle and therefore improved device potentialities. Much research activity has been directed towards the study of carrier transport in the one-dimensional systems.[3-13]

The mobility of the electrons in the 1DEG is limited by the various scattering processes which have relative importance at different ranges of temperature and carrier concentration. At lower temperatures the acoustic phonon, the piezoelectric, and the impurity (both remote and background) scatterings dominate. The polar-optic-phonon scattering is more important at higher temperatures for the polar semiconductors. Further, the nonplanarity of the semiconductor interface gives rise to surface roughness scattering that plays a very significant role in the one-dimensional system. The various authors[7-13] have studied the effect of individual scattering mechanisms independently in 1DEG electron transport. However, the relative contributions to transport parameters of 1DEG at different temperature ranges have not been analyzed. The present paper proposes a comprehensive analysis of low-field electron transport in 1DEG and it also includes the influence of impurity scattering at different temperatures. In this paper, a realistic model of the one-dimensional electron gas system has been assumed. Here the electrons are confined in a wire where the two-dimensional potential well, that traps the electrons, is obtained by the formation of a nearly triangular potential well in one direction and a square quantum well in the other. The present study deals with the derivation of the expressions for the relaxation times and the calculation of the mobility of the 1DEG. It also estimates the relative importance of the scattering processes at different ranges of temperature and carrier concentration in a GaAs sample. Although attempts have been made to calculate the screening factor in the case of the 1DEG,[14] the effect of screening on different scattering mechanisms has not been studied yet. In the present work the effect of screening on the carrier relaxation time has also been considered. The thermoelectric power is a very important parameter for device characterization and it also gives an idea of the scattering processes operative. Therefore, the theoretical outline for the calculation of one-dimensional thermopower has finally been developed. Attempts have been made in this present paper to explain the results of mobility and thermopower obtained from the theory developed.

[a] Present address: Department of Electronics and Telecommunication Engineering, Jadavpur University, Calcutta-700032, India.

II. THEORY

A. Mobility

1. Unscreened case

We assume that the 1DEG is formed in a narrow channel FET or HEMT and only the lowest subband is occupied. The wave function describing the electrons is[3,13]

$$\psi(x,y,z) = (b^3/La)^{1/2} \sin(\pi y/a) z e^{-bz/2} e^{ikx}, \qquad (1)$$

where L and a are respectively the length and width of the channel, k is the electron wave vector along the x direction, and b is the variational parameter.[1] In the FET, therefore, an approximately triangular potential well is formed along the z axis and a square quantum well of infinite height is present along the y direction. The electron gas trapped within the two-dimensional potential well is constrained to move along the x direction and constitutes the 1DEG.

The matrix element for the transition from k to k' due to electron-phonon interactions[15] is

$$M(k,k') = \int \psi^*(x,y,z)(a e^{i\vec{Q}\vec{R}} - a^+ e^{-i\vec{Q}\vec{R}}) \times \psi(x,y,z)\,dx\,dy\,dz, \qquad (2)$$

where a and a^+ are the annihilation and creation operators,

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$\bar{Q}$ and $\bar{R}$ represent the wave vector and displacement vector in three dimensions, and the integration is over space for both phonons and electrons. The matrix element takes the form

$$M(k,k') = (N_Q + \tfrac{1}{2} \pm \tfrac{1}{2})^{1/2}(C/Q)\partial(k - k' \pm q_x)(2/a) \times \int \sin^2(\pi y/a) e^{\pm iq_y y}\, dy (b^3/2) \times \int z e^{-bz \pm iq_z z}\, dz. \quad (3)$$

The momentum conservation approximation (MCA) proposed by Ridley[16] has been employed for performing the integration over the y axis. The constant C has different expressions for different scattering processes, $q_{x,y,z}$ are the components of the phonon wave vector along the x, y, and z directions, respectively, and N_Q is the phonon number.

On the other hand, the expression for the matrix element for coulomb scattering, as in the case of impurity and surface roughness scattering, is given by

$$M(k,k') = \int \psi^*(x,y,z) V(Q) \psi(x,y,z) dx\, dy\, dz, \quad (4)$$

where $V(Q)$ is the coulomb potential.

Respective expressions for the constant C and the coulomb potential $V(Q)$ for the different scattering mechanisms[17] are substituted in the expressions for the relaxation time, defined as

$$\tau^{-1} = \sum_{k'} P(k,k') \left(1 - \frac{\cos\theta'}{\cos\theta}\right), \quad (5)$$

for nonrandomizing elastic collision, or

$$\tau^{-1} = \sum_{k'} P(k,k') \left(\frac{1 - f_0(E')}{1 - f_0(E)}\right), \quad (6)$$

for randomizing inelastic collision. In the above, k,E are respectively the electron wave vector and energy for the initial state and θ is the angle between k and x. The prime quantities represent the corresponding quantities for the final state. The function $f_0(E)$ is the distribution function of electrons and

$$P(k,k') = (2\pi/\hbar)|M(k,k')|^2 \partial(E_k - E_{k'}), \quad (7)$$

is the transition probability of the electron. $\hbar$ is Planck's constant divided by 2π. For elastic scattering $E_k = E_{k'}$ and $f_0(E') = f_0(E)$. Further, for 1DEG in a thin wire in the quantum limit, the scattering angle θ can only be 180°. The other possibility, i.e., $\theta = 0°$ where initial directions of the electron wave vector are not altered due to scattering, does not contribute to the momentum relaxation time, $(1 - \cos\theta) = 0$.

Considering all these factors, the relaxation times are

$$\tau_{AC}^{-1} = (9/E_1^2 k_B T m^* b)/(8a\hbar^3 C_L k), \quad (8)$$

for deformation potential acoustic phonon scattering;

$$\tau_{PZ}^{-1} = [(K^2 e^2 k_B T m^* b)/(32\pi\hbar^3 \epsilon_s a k)] \times [2f'(k) + f'(k_0)], \quad (9)$$

for piezoelectric scattering;

$$\tau_{BI}^{-1} = (\pi m^* N_B/2\hbar^3 k^3)(e^2/2\pi\epsilon_s)^2 \times \{1 + (ka)^2[K_0^2(ka) - K_1^2(ka)]\}, \quad (10)$$

for background impurity scattering; and

$$\tau_{SR}^{-1} = (35/32\pi)(e^2 N_1 H d/\epsilon_s)^2 \times (m^*/\hbar^3 a^3)(e^{-4k^2 d^2}/k), \quad (11)$$

for surface roughness scattering. The effect of remote impurities can be minimized by introducing spacer layers.

Polar-optic-phonon scattering is neither randomizing elastic scattering nor is the simple expression for finding the relaxation time strictly valid in this case. However, an approximate value for the relaxation time for polar-optic-phonon scattering is obtained using Eq. (6)

$$\tau_{PO}^{-1} = \frac{e^2 \omega b}{128 a \epsilon_p \hbar} \sqrt{\frac{2m^*}{k_B T}} \times \{(X - X_0)^{-1/2}[2f'(q_X) + f'(q_{X_0})](N_Q + 1) + (X + X_0)^{-1/2}[2f'(q'_X) + f'(q'_{X_0})] N_Q\}, \quad (12)$$

where

$$k_0^2 = k^2 + \pi^2/a^2,$$
$$f'(s) = (4b^2 + 9bs + 6s^2)/[s(b + 2s)]^3,$$
$$q_{X_0}^2 = q_X^2 + 4\pi^2/a^2,$$
$$q_{X'_0}^2 = q_{X'}^2 + 4\pi^2/a^2,$$
$$q_X = C_2\sqrt{2X - X_0 - 2[X(X - X_0)]^{1/2}},$$
$$q_{X'} = C_2\sqrt{2X + X_0 - 2[X(X + X_0)]^{1/2}},$$
$$C_2 = (2m k_B T/\hbar^2)^{1/2},$$
$$\epsilon_p^{-1} = \epsilon_0^{-1}[\epsilon_{SI}^{-1} - \epsilon_{SO}^{-1}],$$
$$X_0 = \hbar\omega/k_B T, \quad X = E/k_B T.$$

The symbols are defined as follows: E_1 is the deformation potential constant, C_L is the elastic constant, K is the dimensionless piezoelectric constant, and N_B is the background impurity concentration. k_B is Boltzmann's constant, T is the lattice temperature, m^* is the effective mass, and K_0 and K_1 are the modified Bessel functions of the second kind of order zero and one respectively. H is the mean asperity height, d is the correlation length, ϵ_0 is the absolute permittivity of free space, ϵ_{SO} and ϵ_{SI} are, respectively, the dielectric constants of semiconductor at zero and infinite frequencies, and $\hbar\omega$ is the phonon energy. Gaussian autocorrelation has been assumed for surface roughness scattering.[14]

For an arbitrarily degenerate case, the average relaxation time for 1DEG is obtained by the following equation:[14]

$$\langle\tau\rangle = \frac{\int E^{1/2}\tau(E)(\partial f_0/\partial E) dE}{\int E^{1/2}(\partial f_0/\partial E) dE}, \quad (13)$$

and the mobility $\mu = e\langle\tau\rangle/m^*$ [here f_0 is the distribution function of the electrons and $\tau(E)$ is the relaxation time function of energy E].

2. Screened case

The effect of screening is to reduce the scattering potential by a factor

$$\epsilon(q) = 1 - V(q)P(q), \tag{14}$$

where $V(q)$ is the Fourier component of the potential and $P(q)$ is the polarizability. Now $P(q)$ shows a logarithmic singularity at $q = 2k_F$, where k_F is the wave vector at the Fermi energy. The dielectric function at nonzero temperature is given by the dynamic screening effect[17]

$$\epsilon_T(q) = \int dE\, \epsilon_0(q,E_F) \times \{4k_B T \cosh^2[(E - E_F)/k_B T]\}^{-1} \tag{15}$$

and

$$\epsilon_0(q,E_F) = \epsilon_{BG} + \frac{4e^2 m^*}{\pi\hbar^2}\frac{F(q)}{q}\ln\left|\frac{q+2k_F}{q-2k_F}\right|, \tag{16}$$

and the form factor is

$$F(q) = [2/(qR)^2][1 - 2K_1(qR)J_1(qR)],$$

where $J_n(X)$ and $K_n(X)$ are Bessel function and modified Bessel function, respectively, of order n. R is the radius of the cylindrical wire that approximately replaces the rectangular quantum well (QWW), and ϵ_{BG} is the background permittivity given by $\epsilon_{BG} = 4\pi\epsilon_0\epsilon_s$. The screening function for the cylindrical geometry can be used approximately for the present case of the rectangular quantum well. This would introduce a constant geometrical error without altering the physical concept. However, the requirement of an exact screening function for the present device geometry is not so stringent due to lack of the experimental results. The inverse relaxation time or the scattering rates are divided by the function $|\epsilon_T(q)|^2$ to obtain the corresponding screened values. The average relaxation time and hence the mobility can be obtained as earlier.

B. Thermoelectric power

The thermoelectric power calculation in 1DEG is based on the mobility theory that is derived from the Boltzmann transport equation. The thermoelectric power obtained from the Boltzman transport equation is written as[15]

$$S = (eT)^{-1}(\langle E\tau\rangle\langle\tau\rangle^{-1} - E_F), \tag{17}$$

where $\langle\ \rangle$ means the average defined by expression (13) and E_F is the Fermi energy.

It has been assumed that, at low temperatures, when the acoustic phonon scattering occurs via deformation potential and piezoelectric coupling, the impurity scattering and the surface roughness scattering due to interface irregularities dominate. The total relaxation time for all these processes can be written[16] using Matthiessen rule

$$\tau^{-1} = \sum_i \tau_i^{-1}. \tag{18}$$

We assume the degenerate distribution for electrons and the screening effect is incorporated by dividing all the inverse relaxation times by $|\epsilon_T(q)|^2$. The TEP has been calculated for individual scattering processes including degeneracy at low temperature.

III. RESULTS AND DISCUSSIONS

The following values of parameters are used for calculating the mobility and the thermopower for the 1DEG formed in a narrow channel GaAs-GaAlAs heterostructure:[14,18] $a = 10$ nm, $E_1 = 7$ eV, $K = 0.064$, $C_L = 139.7$ G N m^{-2}, $m^* = 0.067\ m_0$, $\epsilon_{SO} = 12.9$, $H = 0.43$ nm, $d = 1.5$ nm, $N_B = 10^{20}$ m^{-3}, and $\epsilon_S = 10.8$.

The temperature dependence of the mobility, for both the screened and the unscreened conditions are shown in Figs. 1–3 for three different 1DEG densities. In Figs. 1–3, the total mobility is obtained by including the acoustic phonon scattering via the deformation potential, piezoelectric coupling, and impurity scattering. The 1DEG mobility is very high, which increases for the piezoelectric and the surface roughness scattering at low temperatures and then saturates. The deformation potential acoustic phonon scattering becomes more effective at higher temperatures and the total mobility is mainly limited by this scattering as seen from Figs. 1–3. At low temperatures below 10 K, the surface roughness, piezoelectric and impurity scatterings dominate. The acoustic-phonon-limited mobility decreases with temperature and hence the total mobility falls with rise in temperature.

Above 100 K, the polar-optic-phonon scattering takes over. The effect of optical phonon scattering has not been included in the curves labelled "TOTAL" in Figs. 1–3 because it is the only dominant scattering mechanism at high temperatures. At higher temperatures, the occupation of only the lowest subband is not justified and intersubband scattering will be effective. However, the polar-optic-phonon scattering can be included in a straightforward manner. Due to the lack of experimental results on the mobility of 1DEG, the effect has been neglected.

If the polar-optic-phonon scattering is also included to obtain total mobility, then the overall mobility curve should follow the curve for polar-optic-phonon scattering limited mobility above 100 K.

In all cases, the mobility is higher for higher electron

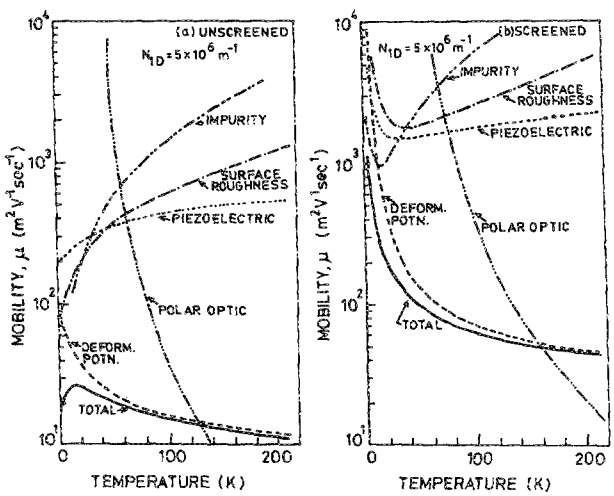

FIG. 1. The variation of electron mobility (μ) vs temperature (T) in GaAs for 1D electron density $N_{1D} = 5.0\times10^{6}$ (a) unscreened, and (b) screened.

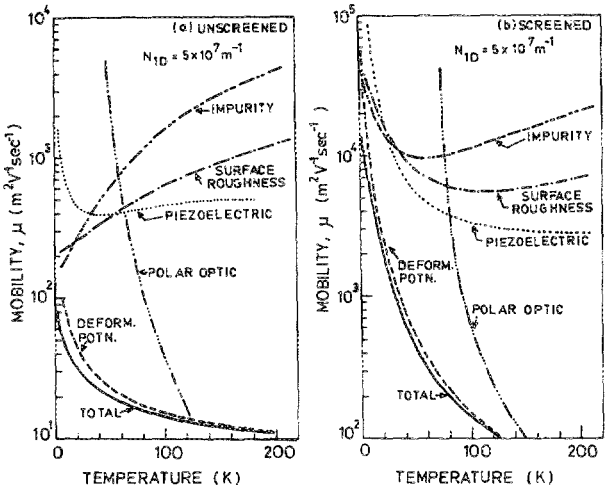

FIG. 2. The mobility (μ) vs temperature (T) in GaAs for 1D electron density $N_{1D} = 5.0\times10^7\ m^{-1}$ (a) unscreened, and (b) screened.

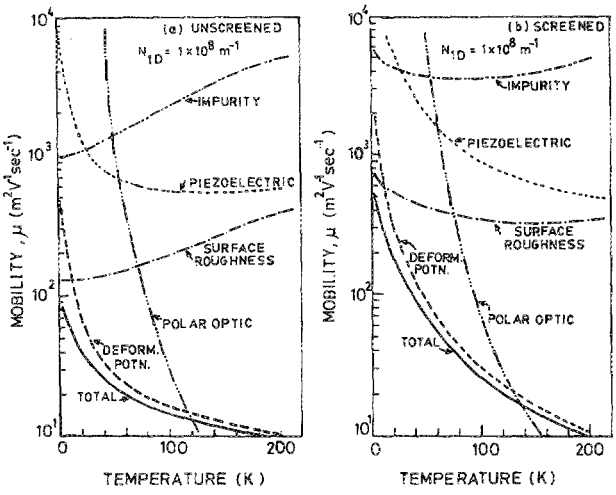

FIG. 3. The mobility (μ) variation in GaAs with temperature (T) for 1D electron density $N_{1D} = 1.0\times10^8\ m^{-1}$ (a) unscreened, and (b) screened.

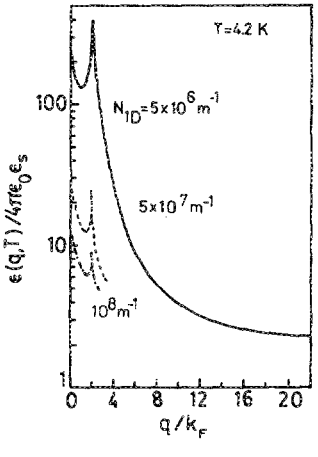

FIG. 4. The variation of normalized permittivity due to screening with normalized phonon wave vector.

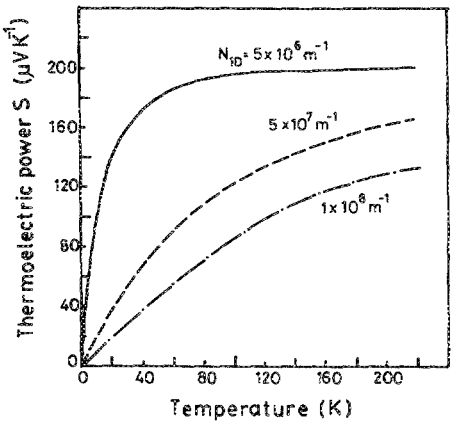

FIG. 5. Thermoelectric power S of 1DEG vs temperature T (screened case) for three different values of 1D electron concentration.

concentration. Screening enhances the mobility values because it lowers the scattering rates. It is apparent from Fig. 4 that the lower the electron concentration, the higher the screening effect. This reduces the scattering rates significantly. The values of one-dimensional thermopower are plotted against temperature in Fig. 5, for different one-dimensional electron concentrations. Screening effects have also been incorporated in the calculations.

The thermopower is found to decrease with increasing electron concentration. This behavior is expected from Eq. (17) since the thermopower is a strong function of the Fermi energy E_F and E_F decreases linearly with 1DEG concentration. The values of thermopower increase with temperature and almost saturate above 100 K.

When the individual contributions to the thermopower due to different scattering processes are compared, it is found that the deformation potential acoustic phonon scattering is the most dominant. However, at the lowest temperatures, i.e., below 10 K, the impurity scattering has a significant contribution. The piezoelectric and surface roughness scatterings are weak.

At higher temperatures, above 100 K, the electron distribution function f_0 becomes nondegenerate. The expression for τ_{AC} indicates that at such high values of temperature $(1/T)(\langle E\tau\rangle/\langle\tau\rangle)$ becomes temperature independent. Thus at higher temperatures the thermoelectric power becomes temperature independent and the curves saturate.

However, above 100 K, both polar-optic-phonon and intersubband scattering should be considered. The present simplified model is therefore inadequate to describe the behavior of thermopower at higher temperatures.

The calculated values cannot be verified due to lack of experimental data, although it is found that the nature of variation of 1DEG thermopower is similar to that for 2DEG.

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