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1991 J. Phys.: Condens. Matter 3 2597

(http://iopscience.iop.org/0953-8984/3/15/016)

J. Phys.: Condens. Matter 3 (1991) 2597–2602. Printed in the UK

LETTER TO THE EDITOR

Diffusion thermopower of a 2DEG

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Received 26 October 1990

Abstract. We investigate the effect of the background impurity concentration N_{BI} on the thermopower of a GaAs/AlGaAs heterojunction. A comparison between a GaAs/AlGaAs heterojunction and a Si MOSFET is also given. For the heterojunction we always find a negative sign for the thermopower, in contrast to the Si MOSFET for which the sign sometimes changes with increasing N_{BI}. This different behaviour is due to the difference of the confining potentials of the two systems.

The thermoelectric properties of a quasi-two-dimensional electron gas has attracted the attention of many workers. Both experimental results (Gallagher *et al* 1987, 1990, Fletcher *et al* 1986, 1988, Ruf *et al* 1988, Syme *et al* 1989) and theoretical work (Cantrell and Butcher 1987a, b, Smith and Butcher 1989a, b) confirm that, at liquid He temperatures, the phonon drag contribution to the thermopower (S_g) dominates over the diffusion part (S_d). However for even lower temperatures of the order of 1.0 K the diffusion part dominates and changes sign in a Si MOSFET (Gallagher *et al* 1990). This behaviour has been explained by considering background impurity scattering and interface roughness scattering (Karavolas *et al* 1990). A sign change seen in a GaAs/AlGaAs heterojunction has been attributed to the movement of the Fermi level into the second subband (Ruf *et al* 1989). It is of interest to see if the mechanism investigated by Karavolas *et al* (1990) might also be effective in GaAs/AlGaAs heterojunctions. In this letter similar calculations for a GaAs/AlGaAs heterojunction are reported and a comparison is made of our results for both systems.

The diffusion thermopower assuming a degenerate 2DEG is given by the well known formula (Mott and Davis 1979)

$$S^{d} = -\frac{\pi^2 k_B^2 T}{\sigma(E_F)3e}\left(\frac{d\sigma(E)}{dE}\right)_{E=E_F} \tag{1}$$

where e is the magnitude of the electronic charge and k_B is the Boltzmann constant. Here, σ(E) is the conductivity when the Fermi level is at E

$$\sigma(E) = \frac{N_S(E)e^2\tau_t(E)}{m^*} \tag{2}$$

where $N_S = Eem^*/\pi\hbar^2$ is the electron density when $E_F = E$ and $\tau_t(E)$ is the scattering time involved from the Boltzmann equation (Karavolas *et al* 1990).

0953-8984/91/152597+06$03.50

We suppose that the 2DEG is confined in the z direction and is described by Fang and Howard (1966) envelope functions. We consider the following three scattering mechanisms.

(i) Remote impurity scattering (Stern and Howard 1967, Hess 1979) with a scattering time given by (Ando 1982)

$$\tau_{\mathrm{RI}}^{-1}(E) = \frac{2\pi}{\hbar}\int_{-\infty}^{0} \mathrm{d}z\, N_{\mathrm{RI}}(z) \int \mathrm{d}\theta\, \frac{(1-\cos\theta)}{\epsilon^2(q)} |F_{\mathrm{RI}}(q,z)|^2 \delta(E_0(k) - E_0(k+q)) \tag{3}$$

where $E = \hbar^2 k^2/2m^*$

$$q = 2k\sin(\theta/2) \tag{4}$$

in which θ is the scattering angle and $N_{\mathrm{RI}}(z)$ is the remote impurity concentration. Finally for $z < 0$

$$F_{\mathrm{RI}}(q,z) = \frac{2\pi e^2}{\kappa' q}\left(\frac{b}{b+q}\right)^3 \mathrm{e}^{qz} \tag{5}$$

where z is the impurity position, $\kappa' = \frac{1}{2}\kappa_{\mathrm{sc}} + \kappa_{\mathrm{ins}}$ and b is

$$b = \left(\frac{48\pi m_z^* e^2 N_s'}{\kappa_{\mathrm{sc}}\hbar^2}\right)^{1/3} \tag{6}$$

where m_z^* is the z component of the electron effective mass and

$$N_s' = N_{\mathrm{dep}} + \tfrac{11}{32}N_s \tag{7}$$

in which N_s is the electron concentration and $\mathrm{N_{dep}}$ is the areal concentration of acceptors in the depletion layer.

(ii) Background impurity scattering (Stern and Howard 1967) with a scattering time

$$\tau_{\mathrm{BI}}^{-1}(E) = \frac{2\pi}{\hbar}\int_{0}^{\infty} \mathrm{d}z\, N_{\mathrm{BI}}(z) \int \mathrm{d}\theta\, \frac{(1-\cos\theta)}{\epsilon^2(q)} |F_{\mathrm{BI}}(q,z)|^2 \delta(E_0(k) - \mathrm{E}_0(k+q)) \tag{8}$$

where q is given by (2) and

$$F_{\mathrm{BI}}(q,z) = \frac{2\pi e^2}{\kappa_{\mathrm{sc}} q}(P(z) + \delta_\kappa P_0 \mathrm{e}^{-qz}). \tag{9}$$

Analytical expressions for $P(z)$, P_0 and δ_κ are given by Ando *et al* (1982).

(iii) Interface roughness scattering (Prange and Knee 1968, Matsumoto and Uemura 1974, Ando 1977, 1982) with a scattering time

$$\tau_{\mathrm{IFR}}^{-1}(E) = \frac{2\pi}{\hbar}\sum_{k'}\langle|\Delta_{k-k'}|^2\rangle \left(\frac{\Gamma(k-k')}{\epsilon(k-k')}(1-\cos\theta)\delta(E(k) - E(k'))\right) \tag{10}$$

where Δ is the mean square height of the roughness, Λ is its lateral correlation length and

$$\Gamma(q) = \frac{4\pi e^2}{\kappa_{sc}}(N_{dep} + \tfrac{1}{2}N_s). \tag{11}$$

We calculate the total scattering time $\tau_t(E)$ due to all scattering mechanisms using Matthiessen's rule.

It is convenient to write

$$\tau_t = \tau_0 E^{p(N_s)}. \tag{12}$$

Then we easily obtain for $p(N_s)$ (Karavolas *et al* 1990)

$$p(N_s) = E_F \frac{[d\tau_t(E)/dE]_{E=E_F}}{\tau_t(E_F)} \tag{13}$$

so that (1) may be put in the form

$$S^d = -\tfrac{1}{3}(p(N_s) + 1)\frac{\pi^2 k_B}{e}\frac{k_B T}{E_F}. \tag{14}$$

In the calculations reported here for a GaAs/AlGaAs heterojunction we put Δ= 5.0 Å, Λ=22.0 Å, N_{RI}=2×10^{16} cm^{-3} (as in Karavolas *et al* 1990). For the other parameters we take $m_z = 0.067m$, $\kappa_{sc} = \kappa_{ins} = 12.9$ and $g_v = 1$ and the acceptor concentration is $N_A = 1.7 \times 10^{15}$ cm^{-3}. We also assume a constant density of remote impurities and zero-spaced layer thickness.

In figure 1(a), $p(N_s)$ is plotted against the electron density N_s for each scattering mechanism separately and also for all the scattering mechanisms combined. For remote impurities (full curve) and background impurities (broken curve) $p(N_s)$ is positive, i.e. small-angle scattering characterizes both of these scattering mechanisms. Only interface roughness scattering (chain curve) shows large-angle scattering behaviour as we discuss in full below. Figure 1(b) shows similar results for a Si MOSFET (Karavolas *et al* 1990).

In figure 2(a) the diffusion thermopower S^d for a GaAs/AlGaAs heterojunction at 1.15 K is plotted as a function of the electron density N_s for each scattering mechanism separately and also for all the scattering mechanisms combined. S^d remains negative over the whole range of N_s. The diffusion thermopower for each scattering mechanism follows a similar pattern to that shown in figure 1(a). Figure 2(b) shows corresponding results for a Si MOSFET which exhibit a sign change.

To explain this contradictory behaviour we have to go back to (5) and (9). In these equations the Fourier–Bessel transform of the screened potential, integrated over all z, is given. We see that an exponential factor exists that limits the number of background impurities which actually have a strong affect on the electrons. This imposes the following condition for effective scattering by an impurity located on the plane at z_i (Ando *et al* 1982)

$$|z_i| < k_F^{-1}. \tag{15}$$

(Here we assume that $\langle z\rangle < k_F^{-1}$. When $\langle z\rangle > k_F^{-1}$ and $z_i > 0$ the thickness of the inversion layer $\langle z\rangle$, determines the effective values of z_i instead of k_F^{-1}. However,

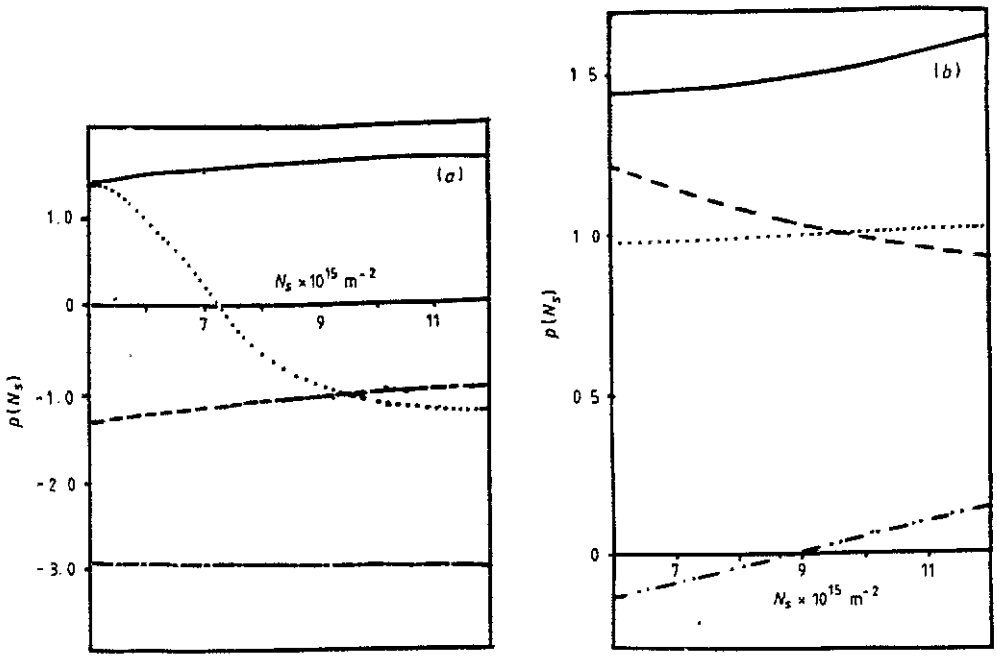

Figure 1. (*a*) Plots of the overall $p(N_s)$ (dotted line), $p_{RI}(N_s)$ (full line), $p_{IFR}(N_s)$ (chain line) and $p_{BI}(N_s)$ (dashed line) against N_s for a GaAS/AlGaAs heterojunction. (*b*) Plots of overall $p(N_s)$ (dotted line), $p_{RI}(N_s)$ (full line), $p_{IFR}(N_s)$ (dashed line) and $p_{BI}(N_s)$ (chain line) for a Si MOSFET.

usually $\langle z \rangle < k_F^{-1}$ (Ando *et al* 1982). We see from (15) that many charged centres contribute to scattering at low N_s, but only a small number, near to the interface, contribute at high N_s.

For Fang and Howard wavefunctions

$$\langle z \rangle = \frac{3}{b}. \tag{16}$$

In figure 3 we plot $|\zeta(z)|^2$ against z for a Si MOSFET (figure 3(*a*)) after Ando (1977) and a GaAs/AlGaAs heterojunction (figure 3(*b*)) after Ando (1982). The parameters used in figure 3(*a*), are close to those appropriate to the MOSFET used by Gallagher *et al* (1990). We see that in the MOSFET, the electron confinement is far stronger than in the heterojunction. From the Fang and Howard wavefunction we can calculate the probability of finding an electron in any range of z. For the MOSFET in figure 3 we have $\langle z \rangle = 30.00$ Å and $k_F^{-1} = 56.4$ Å so that almost all the electrons are near the effective background impurities. This implies a small impact parameter scattering mechanism and thus large-angle scattering is observed. On the other hand, in the heterojunction we have $k_F^{-1} = 56.4$ Å and $\langle z \rangle = 100$ Å. From figure 3(*b*) we see that the majority of the electrons are far away from the effective impurities with a large impact parameter and thus show small-angle scattering behaviour.

A secondary difference between the two cases lies in the interface roughness contribution to the thermopower. In the MOSFET, $p(N_s)$ for interface roughness is close

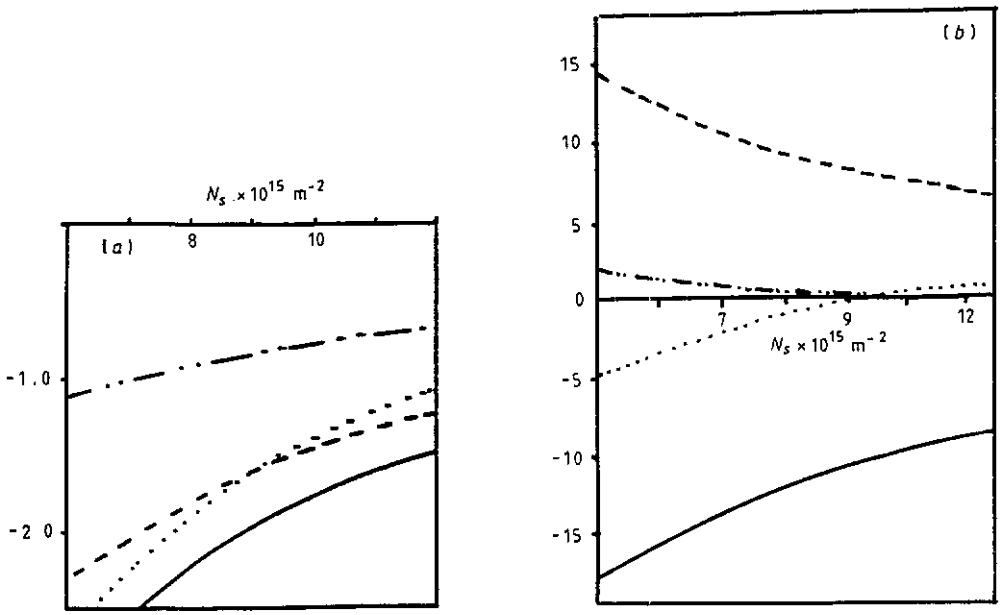

Figure 2. (*a*) Plots of the overall diffusion thermopower S^{d} (dotted line), S_{RI} (full line), S_{BI} (dashed line) and S_{IFR} (chain line) against N_s for a GaAs/AlGaAs heterojunction. (*b*) Same as (*a*) for a Si MOSFET. The temperature is 1.15 K.

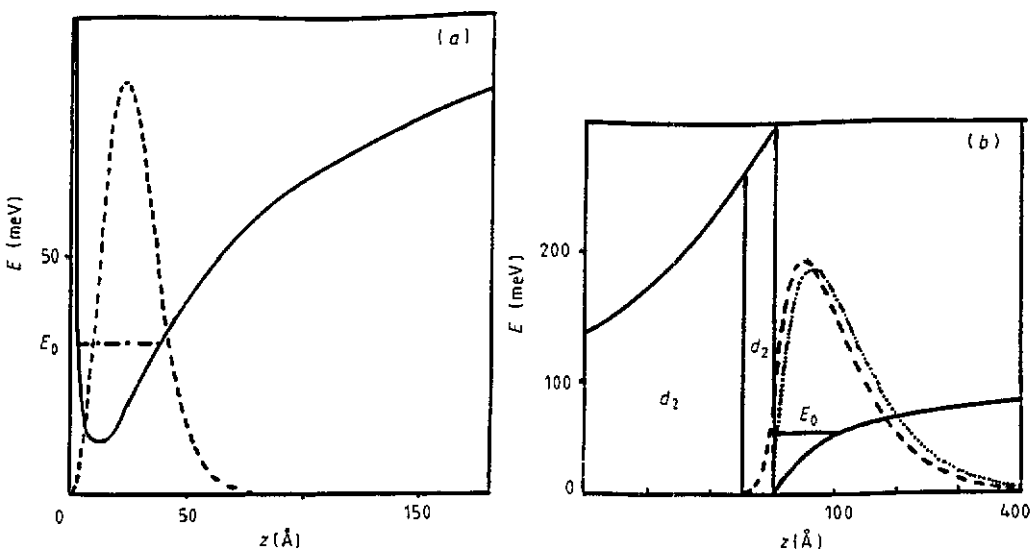

Figure 3. (*a*) Confining potential of a Si MOSFET. The dashed line is the Fang and Howard wavefunction. (*b*) Same as (*a*) for a GaAs/AlGaAs heterojunction. The dashed line is the Ando wavefunction while the dotted line is the Fang and Howard wavefunction.

to -1 (figure 1(*b*)). However, in the heterojunction it is close to 0. There are two reasons for this. Firstly, the electrons in GaAs/AlGaAs are more energetic (because $E_{F_{GaAs}} > E_{F_{Si}}$ for the same N_s) than in Si MOSFET and, as we move to higher energies

for the same N_s, the screening becomes less important. Secondly, using the Fang and Howard envelope functions we ignore the AlGaAs envelope function penetration. For better results we would need to perform a self-consistent calculation of the electron envelope functions.

One of the authors (VCK) wishes to thank the Public Benefit Foundation 'Alexander S Onassis' for its financial support.

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