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The effect of interface roughness scattering and background impurity scattering on the thermopower of a 2DEG in a Si MOSFET

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Abstract. For a 2DEG in a Si MOSFET the important scattering mechanisms at low temperatures are remote impurity, background impurity and interface roughness scattering. We perform a detailed calculation of the energy dependence of each scattering mechanism in the extreme quantum limit with a view to explaining the observed electron concentration dependence of the thermopower. For N_s less than 8×10^{15} m^{-2}, scattering by remote impurities dominates. A change of sign of the diffusion thermopower is predicted at low T and high N_s, due to the dominance of scattering by background impurities and interface roughness. The total thermopower is calculated by including the phonon drag contribution, the result being in satisfactory agreement with experimental data.

1. Introduction

A great deal of experimental and theoretical work has been carried out recently on the thermoelectric properties of a quasi-two-dimensional electron gas (Q2DEG). The thermopower, S, is defined by (Syme *et al* 1989)

$$S = \Delta V / \Delta T \qquad (1)$$

where ΔV is the potential difference and ΔT is the temperature difference between two points in the inversion layer. 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). There have been experimental measurements both in Si MOSFETs (Gallagher *et al* 1987, 1990) and in GaAs/GaAlAs heterojunctions (Fletcher *et al* 1986, 1988, Ruf *et al* 1988) showing very large values of S compared with the values expected for S^d (Smith and Butcher 1989a). These experiments also show a cubic dependence of S on T in contradiction to Mott's formula (Mott and Davis 1979), but in agreement with the calculations of S_g made by Cantrell and Butcher (1987b). Recently Ruf *et al* (1988) have shown that the T^3 contribution due to the phonon

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drag dominates in heterojunctions in the temperature range 0.6–2.5 K. The more recent experimental results for Si MOSFETs (Gallagher *et al* 1990) indicate that the temperature above which the phonon drag becomes dominant is greater than 1.50 K. A positive thermopower is seen at 1.15 K which can be explained only if the diffusion thermopower dominates the phonon drag component.

In this paper we calculate, in the extreme quantum limit in which only one subband is populated, both S^{d} (following Mott and Davis 1979) and S_{g} (following Smith and Butcher 1989a, b) for the electron densities reported by Gallagher *et al* (1990). We take into account the contribution due to three scattering mechanisms: (i) remote impurity scattering (Stern and Howard 1967, Hess 1979), (ii) background impurity scattering (Stern and Howard 1967) and (iii) interface roughness scattering (Prange and Knee 1968, Matsumoto and Uemura 1974, Ando 1977, 1982, Mori and Ando 1980). We will use Boltzmann transport theory, which we expect to be valid because it satisfies the Peierls criterion even at the lowest electron concentration under consideration ($E_{\mathrm{F}}\tau/\hbar = 16 \gg 1$ for $N_{\mathrm{s}} = 6\times 10^{15}\ \mathrm{m}^{-2}$).

2. Theory

2.1. *Preliminaries*

To deal in concrete terms we consider a degenerate electron gas in a Si MOSFET. Only trivial modifications are necessary to apply the formalism to a GaAs/GaAlAs heterojunction. We take the z axis to be perpendicular to the Si–SiO_2 interface with the origin on the interface and $z > 0$ on the Si side. The dielectric constants are denoted by κ_{ins} for $z < 0$ and κ_{sc} for $z > 0$. The electrons in the inversion layer are supposed to be described by a Fang and Howard (1966) variational wavefunction

$$\Psi(\boldsymbol{r}, z) = X(z)\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}(b^3/2)^{1/2} z \mathrm{e}^{-bz/2} \tag{2}$$

where $\boldsymbol{k}$ is a two-dimensional (2D) wavevector and $X(z)$ is the envelope function. The parameter b is determined by the electric field within the inversion layer and, neglecting the image, exchange, correlation and quadratic terms in the depletion energy, it is given by (Ando *et al* 1982, Smith and Butcher 1989a)

$$b = (48\pi m_z^* e^2 N_{\mathrm{s}}' / \kappa_{\mathrm{sc}}\hbar^2)^{1/3} \tag{3}$$

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

$$N_{\mathrm{s}}' = N_{\mathrm{dep}} + \tfrac{11}{32} N_{\mathrm{s}}. \tag{4}$$

Here N_{s} is the electron concentration in the inversion layer and N_{dep} is the areal concentration of acceptors in the depletion layer. This is given by

$$N_{\mathrm{dep}} = (2\phi_d \kappa_{\mathrm{sc}} \epsilon_0 N_1 / e)^{1/2} \tag{5}$$

where ϕ_d is the electrostatic band bending which is approximated by equating $e\phi_d$ to the Si band gap (Smith and Butcher 1989a). In equation (5) N_1 is the density of the impurities inside the inversion layer.

In all our calculations we assume a parabolic energy band of the form

$$E = E_0 + \hbar^2 k^2 / 2m^* \tag{6}$$

where E_0 is the subband minimum, $k = |\boldsymbol{k}|$ and $\boldsymbol{k} = (k_x, k_y)$ is a 2D wavevector and m^* is the electron effective mass parallel to the plane of the interface.

2.2. *Ionized impurity scattering*

Elastic scattering of degenerate electrons in a Si inversion layer by screened ionized impurities was originally treated by Stern and Howard (1967). Following their approach we write the reciprocal of the relaxation time $\tau(E)$ for this scattering process for an electron state with energy E as (Ando *et al* 1982, Walukiewicz *et al* 1984)

$$\tau_i^{-1}(E) = \frac{2\pi}{\hbar} \int \mathrm{d}z \, N_i(z) \int \mathrm{d}\theta \, \frac{(1-\cos\theta)}{\epsilon^2(q)} |F_i(q,z)|^2 \delta(E_0(\boldsymbol{k}) - E_0(\boldsymbol{k}+\boldsymbol{q})) \tag{7}$$

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

$$q = 2k\sin(\theta/2) \tag{8}$$

and θ is the scattering angle; $i = 1,2$ indicates the location of the ionized impurities (inside or outside the inversion layer), $k = (k_x^2 + k_y^2)^{1/2}$, $N_i(z)$ is the impurity density. For remote impurity scattering ($i = 2$) $F_2(q,z)$ is (Ando et al 1982)

$$F_2(q,z) = \frac{2\pi e^2}{\kappa' q}\left(\frac{b}{b+q}\right)^3 \mathrm{e}^{qz} \tag{9}$$

and for background impurities ($i = 1$) $F_1(q,z)$ is

$$F_1(q,z) = \frac{2\pi e^2}{\kappa_{\mathrm{sc}} q}(P(z) + \delta_\kappa P_0 \mathrm{e}^{-qz}) \tag{10}$$

where

$$\kappa' = \tfrac{1}{2}(\kappa_{\mathrm{ins}} + \kappa_{\mathrm{sc}}). \tag{11}$$

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

At low temperatures we can approximate the dielectric function $\epsilon(q)$ by its value at 0 K. This is given by (Ando *et al* 1982)

$$\epsilon(q) = 1 + (2\pi e^2/\kappa' q) S(q) \Pi_0(q). \tag{12}$$

In equation (12) $\Pi_0(q)$ is the static polarizability in the extreme quantum limit which is given by

$$\Pi_0(q) = g_v m^*/\pi\hbar^2 \tag{13}$$

where g_v is the valley degeneracy and $S(q)$ is the form factor for the electron–electron interaction given by Stern and Howard (1967)

$$S(q) = \frac{1}{16}\left[1 + \frac{\kappa_{\mathrm{ins}}}{\kappa_{\mathrm{sc}}}\right]\left[1 + \frac{q}{b}\right]^{-3}\left[8 + 9\frac{q}{b} + 3\left(\frac{q}{b}\right)^2\right] + \frac{1}{2}\left[1 - \frac{\kappa_{\mathrm{ins}}}{\kappa_{\mathrm{sc}}}\right]\left[1 + \frac{q}{b}\right]^6. \tag{14}$$

2.3. Interface roughness scattering

Let us assume that the Si–SiO_2 interface with or without irregularities can be described by potential barriers $V_0(z-\Delta(x,y))$ and $V_0(z)$ respectively. Here $\Delta(x,y)$ gives the deviation of the interface from the plane $z=0$. We use the usual correlation function for $\Delta(x,y)$ between two points (Matsumoto and Uemura 1974)

$$\langle\Delta(x,y)\Delta(x'y')\rangle = \Delta^2\exp\{-[(x-x')^2+(y-y')^2]/\Lambda^2\} \tag{15}$$

where $\langle\ \rangle$ denotes a system average. In equation (15) Δ is the mean square height of the roughness and Λ is its lateral correlation length. The reciprocal of the relaxation time $\tau_{\rm IFR}^{-1}(E)$ for an electron with a wavenumber k and energy E can be written as (Ando *et al* 1982)

$$\tau_{\rm IFR}^{-1}(E) = \frac{2\pi}{\hbar}\sum_{\boldsymbol{k}'}\langle|\Delta_{\boldsymbol{k}-\boldsymbol{k}'}|^2\rangle\frac{\Gamma(\boldsymbol{k}-\boldsymbol{k}')}{\epsilon(\boldsymbol{k}-\boldsymbol{k}')}(1-\cos\theta)\delta(E(\boldsymbol{k})-E(\boldsymbol{k}')). \tag{16}$$

Here $\boldsymbol{k}$ specifies the initial state, $\boldsymbol{k}'$ specifies the final state and θ is the scattering angle. We find that (Ando 1977)

$$\tau_{\rm IFR}^{-1}(E) = \frac{2\pi m^*\Delta^2\Lambda^2}{\hbar^3}\int_0^{2\pi}\frac{d\theta}{2\pi}\,\frac{1-\cos\theta}{2}\,\frac{\Gamma^2(q)}{\epsilon^2(q)}\exp(-q^2\Lambda^2/4) \tag{17}$$

where $\boldsymbol{q}$ is given from (8) and $\epsilon(q)$ is given from (12).

We are using a variational wavefunction. Consequently we do not employ in our calculations the Prange and Knee (1968) result for the Fourier-transformed potential Γ(q) but we use the Matsumoto and Uemura (1974) result instead. Thus, ignoring the corrections introduced by Ando (1977) we have for the Fourier-transformed potential in (17)

$$\Gamma(q) = \frac{4\pi e^2}{\kappa_{\rm sc}}\left(N_{\rm dep}+\frac{N_{\rm s}}{2}\right). \tag{18}$$

2.4. Mobility

We calculate the total relaxation time $\tau_{\rm t}(E)$ due to all scattering mechanisms using Matthiessen's rule (Aschroft and Mermin 1976):

$$\tau_{\rm t}^{-1}(E) = \tau_2^{-1}(E)+\tau_1^{-1}(E)+\tau_{\rm IFR}^{-1}(E). \tag{19}$$

The three terms in (19) refer to remote, background and interface roughness scattering, respectively. At very low temperatures the electrons with an energy near the Fermi level $E_{\rm F}$ determine the mobility which is given by

$$\mu = e\tau_{\rm t}(E_{\rm F})/m^* \tag{20}$$

where, assuming that the subband minimum $E_0=0$, we have

$$E_{\rm F} = \frac{\pi\hbar^2 N_S}{m^* g_v}. \tag{21}$$

We evaluate $\tau_{\rm t}(E)$, $\tau_{\rm t}(E_{\rm F})$ and the function

$$p(N_{\rm s}) = \frac{E_{\rm F}}{\tau_{\rm t}(E_{\rm F})}\left[\frac{d\tau_{\rm t}(E)}{dE}\right]_{E=E_{\rm F}} \tag{22}$$

which appears in subsequent formulae for both $S^{\rm d}$ and $S_{\rm g}$. It is important to note that N_S is to be held constant in evaluating $d\tau_t(E)/dE$.

2.5. *Diffusion thermopower*

In our calculation of diffusion thermopower at very low temperatures we use Mott's formula (Mott and Davis 1979)

$$S^{\mathrm{d}} = -\frac{\pi^2 k_{\mathrm{B}}^2 T}{\sigma(E_{\mathrm{F}})3e}\left[\frac{\mathrm{d}\sigma(E)}{\mathrm{d}E}\right]_{E=E_{\mathrm{F}}} \tag{23}$$

where e is the electronic charge and k_{B} is Boltzmann's constant and $\sigma(E)$ is the conductivity when the Fermi level is at E, i.e.

$$\sigma(E) = \frac{N_S(E)e^2\tau_t(E)}{m^*} \tag{24}$$

where $N_S = Eem^*/\pi\hbar^2$ is the electron density when $E_{\mathrm{F}} = E$ and $\tau_t(E)$ is given by (19). Using (22) we may write (Smith and Butcher 1989a)

$$S^{\mathrm{d}} = -\frac{1}{3}\frac{\pi^2 k_{\mathrm{B}}}{e}\frac{k_{\mathrm{B}}T}{E_{\mathrm{F}}}(p(N_{\mathrm{s}})+1) \tag{25}$$

where $p(N_{\mathrm{s}})$ is given in (22).

2.6. *Phonon drag thermopower*

The phonon drag contribution to the thermopower when only one electronic subband is populated may be obtained from the solution of coupled electron and phonon Boltmann equations (Cantrell and Butcher 1987a, b). It is given by

$$S_{\mathrm{g}} = \frac{e}{A\sigma k_{\mathrm{B}}T^2}\sum_{\boldsymbol{k}'}\sum_{\boldsymbol{k}}\sum_{\boldsymbol{Q}}\hbar\omega_{\boldsymbol{Q}} f^0(\boldsymbol{k})[1-f^0(\boldsymbol{k}')]P_{\boldsymbol{Q}}(\boldsymbol{k},\boldsymbol{k}') \times \tau(\boldsymbol{Q})v_p(\boldsymbol{Q})[\tau(\boldsymbol{k})v(\boldsymbol{k})-\tau(\boldsymbol{k}')v(\boldsymbol{k}')]. \tag{26}$$

Here $f^0(\boldsymbol{k})$ is the equilibrium distribution function for the electrons, $\boldsymbol{Q}$ is the 3D phonon wavevector, $P_{\boldsymbol{Q}}$ is the equilibrium phonon absorption rate which is given by Fermi's golden rule, $v_{\mathrm{p}}Q)$ is the velocity of phonons with wavevector $\boldsymbol{Q}$ and $\tau(\boldsymbol{Q})$ is the phonon momentum relaxation time. The 2D electron wavevectors $\boldsymbol{k}$ and $\boldsymbol{k}'$ label the initial and final states and A is the area of the 2DEG. We use an approximation introduced by Smith and Butcher (1989b) and write

$$[\tau(E_{\mathrm{F}}+\hbar\omega_{\boldsymbol{Q}})\boldsymbol{v}(\boldsymbol{k}+\boldsymbol{q})-\tau(E_{\mathrm{F}})\boldsymbol{v}(\boldsymbol{k})] = -\frac{\hbar q\tau(E_{\mathrm{F}})}{m^*}\left\{1+\frac{1}{2}p(N_{\mathrm{s}})\left(\frac{\hbar\omega_{\boldsymbol{Q}}}{E_{\mathrm{F}}}\right)\left[1+\left(\frac{k_{\mathrm{F}}}{q}\right)^2\frac{\hbar\omega_{\boldsymbol{Q}}}{E_{\mathrm{F}}}\right]\right\} \tag{27}$$

where $\hbar\omega_{\boldsymbol{Q}}$ is the energy of a phonon with 3D wavenumber $Q = (\boldsymbol{q}, q_z)$ and $p(N_{\mathrm{s}})$ is given by (22). Smith and Butcher take p to be constant; here we make full allowance for its electron concentration dependence. We also use their values for all the material parameters required. The total thermopower is given by

$$S_{\mathrm{t}} = S_{\mathrm{g}} + S^{\mathrm{d}}. \tag{28}$$

3. Results and discussion

We have calculated the energy dependence of the total relaxation time and consequently the diffusion and phonon drag thermopower using Δ, Λ and N_2 as adjustable parameters. The values of the other parameters used are $m_z^* = 0.91$ m, $m^* = 0.19$ m, $\kappa_{sc} = 11.8$, $\kappa_{ins} = 3.8$, $g_v = 2$. The acceptor concentration is $N_1 = 1.7 \times 10^{15}$ cm^{-3}, which is slightly larger than the experimental value of 1.35×10^{15} cm^{-3} (Gallagher *et al* 1990). Since we have no information about the remote impurity concentration we assume simply a constant density N_2. In the following calculations $\Delta = 5.0$ Å, $\Lambda = 22.0$ Å and $N_2 = 2 \times 10^{16}$ cm^{-3}.

In figure 1 we plot $p(N_s)$ versus the electron density N_s for each scattering mechanism. The value of $p(N_s)$ for remote impurities is positive. This happens because, with increasing energy, it becomes more difficult for small-angle dominated scattering to dissipate momentum. On the other hand, for the large-angle scattering mechanisms from scatterers inside the electron gas, one collision is enough to dissipate the momentum. Consequently, at higher energies when collisions become more frequent, the relaxation time goes down and $p(N_s)$ is negative. The value $p(N_s)$ for the background impurities is almost constant (around -2.95) and more than twice as larger as the value due to interface roughness.

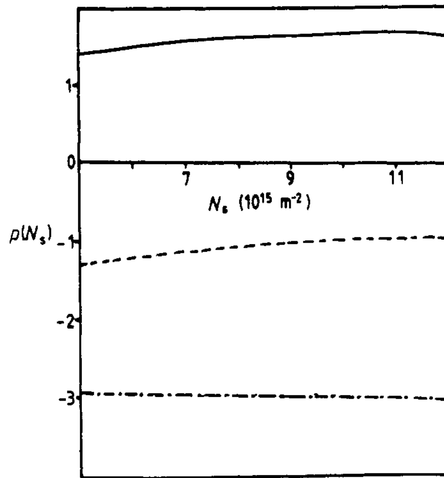

Figure 1. Plots of $p_{RI}(N_s)$ (——), $p_{IFR}(N_s)$ (- - - -) and $p_{BI}(N_s)$ (— · —) against N_s for a 2DEG in a Si MOSFET.

In figure 2 we plot the diffusion thermopower S^d as a function of the electron density N_s for each scattering mechanism separately and also the overall diffusion thermopower at 1.15 K. We see that for $N_s < 8 \times 10^{15}$ m^{-2} remote impurity scattering dominates the overall diffusion thermopower, which is negative. On the other hand when N_s increases large-angle scattering events (background impurity and interface roughness scattering) become more important and S_d changes sign. Thus the sign of thermopower depends on the position of the dominant scatterers. The diffusion thermopower for each scattering mechanism is following a pattern similar to that of $p(N_s)$ in figure 1. This is because from (25) S^d is proportional to the function $-(p(N_s) + 1)$.

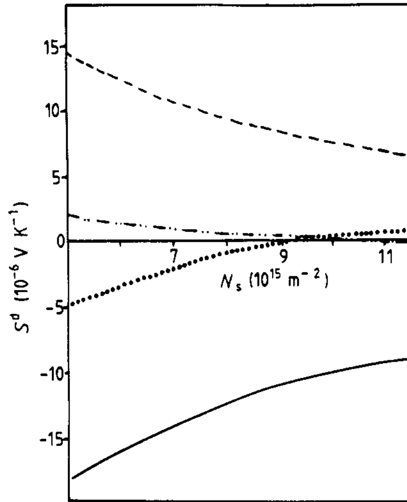

Figure 2. Plots of the overall diffusion thermopower S^d (· · · · · ·), S_{RI} (——), S_{BI} (- - -) and S_{IFR} (— · · —) against N_s at a temperature of 1.15 K.

In figure 3 we compare theoretical (broken curve) and experimental (full curve) plots of the total thermopower $S_t = S^d + S_g$ against N_s at 1.15 K for $\Delta = 5$ Å, $\Lambda = 22$ Å and $N_{RI} = 2 \times 10^{16}$ cm^{-3}. The agreement between the two curves is satisfactory. The discrepancy which appears for small N_s where the remote impurity dominates is due to the lack of information about the oxide charges and the crude interface roughness theory. For higher N_s the agreement is very good. At this temperature the phonon drag contribution is less than 20% of the overall.

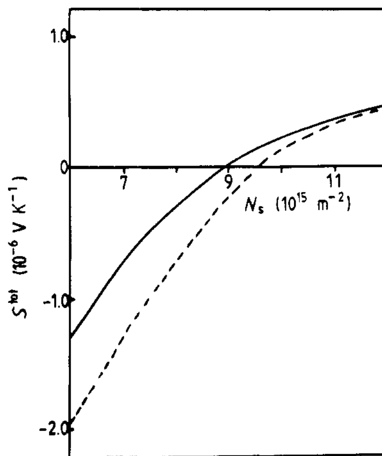

Figure 3. Plot against N_s of calculated S^{tot} (- - -) and experimental data of Gallagher *et al* (1990) (——) at 1.15 K.

In figure 4 the function $p(N_s)$ is plotted against the Fermi wavenumber k_F for remote impurity scattering and also for all the scattering mechanisms combined. At very low k_F, $p(N_s)$ is positive and identical to $p_{RI}(N_s)$. When k_F increases the other

two mechanisms become important and a dramatic change in $p(N_s)$ is observed. When k_F is large enough $p(N_s)$ becomes smaller than -1 and changes the sign of S^d.

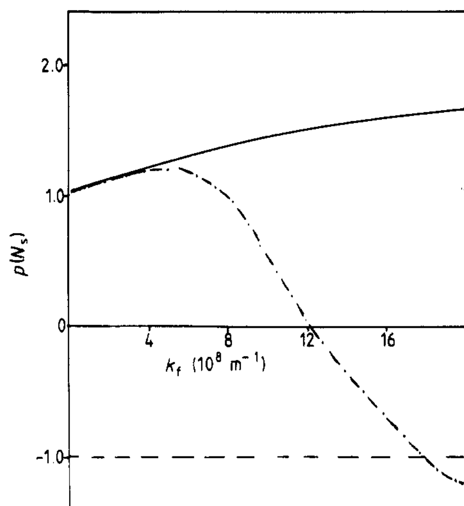

Figure 4. Plots of $p(N_s)$ (— · —) and $p_{RI}(N_s)$ (——) against k_F. The broken line is for $P(N_s) = -1.0$ where the change of sign of the diffusion thermopower is observed. The temperature is again 1.15 K.

In figure 5 we show the influence of the surface roughness parameters on the diffusion thermopower S^d. In figure 5(*a*) we plot S^d versus N_s for three different choices of Δ (5, 6, 7 Å) and for $\Lambda = 14$ Å. For larger values of Δ the diffusion thermopower increases. This happens because a larger Δ means higher surface irregularities which implies greater large-angle scattering and a positive p(N_s). Thus the sign change occurs at lower N_s. A similar plot is given in figure 5(*b*) for the other IFR parameter Λ. As Λ increases S^d for large electron concentration decreases. For small Λ the interface irregularity is sharp resulting in large-angle scattering. Increasing Λ produces smoother interfaces which favour smaller-angle scattering. Thus larger Λ means smaller diffusion thermopower for high N_s. However, for lower N_s we observe an opposite behaviour. The reason for this is that, for smaller N_s, (which is equivalent to smaller momentum for very low temperatures) the momentum is dissipated through even smaller-angle scattering. Thus, by increasing Λ we increase the volume of the surface irregularity and the interface roughness scattering momentum becomes more difficult and we need large-angle scattering to destroy it. That is why we have a change in the behaviour of S^d. The change of sign of the thermopower depends particularly sensitively on this interface roughness parameter. The values of the parameters used to fit the experimental data in figure 3 are not in contradiction with those of other workers (Stern 1980, Ferry 1987).

In figure 6 we plot mobility versus electron concentration for $T = 1.15$ and 3 K using the experimental data reported by Gallagher *et al* (1990) and also our theoretical results using screening appropriate to 0 K. The difference between the observed and calculated mobility arises from two sources. Firstly, the 0 K screening we use increases the mobility. Secondly and more importantly, the existing interface roughness theory is not very satisfactory. To compensate for this Matsumoto and Uemura

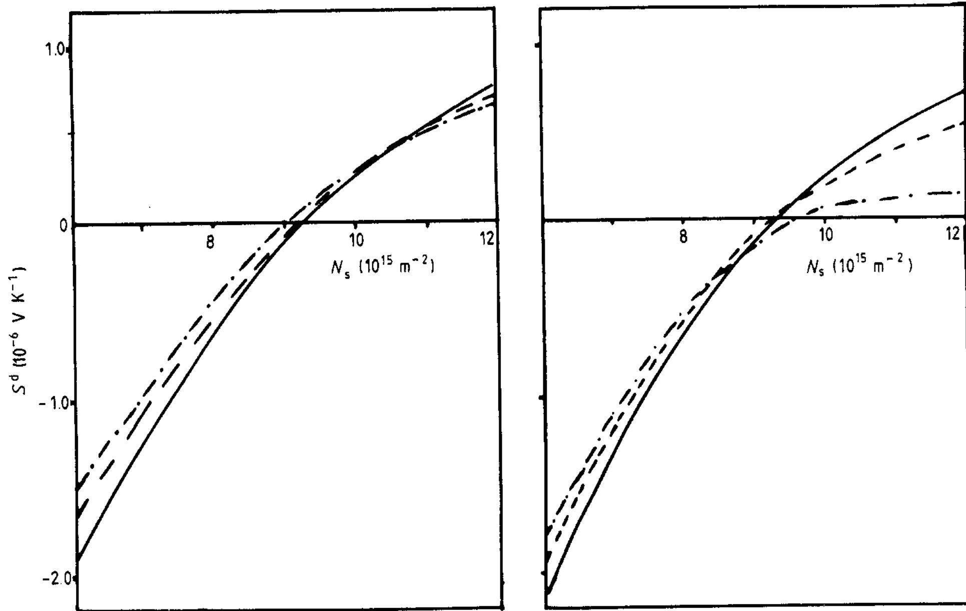

Figure 5. (*a*) Plots of S^d versus N_s for three different values of Δ for $\Lambda = 14$ Å: $\Delta = 5$ Å (——) 6 Å (- - -) and 7 Å (— · —). (*b*) Plots of S^d against N_s for three different values of Λ for $\Delta = 5$ Å: $\Lambda = 17$ Å (——), 22 Å (-----) and 30 Å (— · —).

(1974) therefore introduce an 'imaginary scattering mechanism' in order to obtain better agreement between theory and experiment. A more likely answer to this problem is the current relaxation theory developed by Gold and Götze (Gold and Götze 1981, Gold 1985a, b, 1986). By avoiding the suppression of backscattering which the golden-rule theory produces, they find good agreement between theory and experiment. In order to reduce the number of the unknown parameters by one it is proposed to make measurements of the ratio of the single-particle relaxation time to the scattering time. (Gallagher, private communication). Karavolas and Butcher (1990) have calculated the behaviour of this ratio for a GaAs/GaAlAs heterojunction.

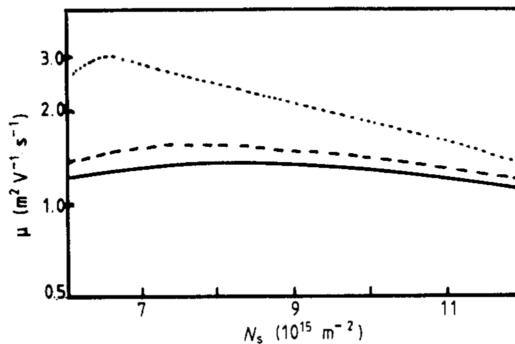

Figure 6. Plot against N_s of theoretical calculated mobility at 0 K (· · · · · ·) and experimental results at 1.15 K (-----) and 3 K (——).

To conclude, our calculations show a change in the sign of thermopower in satisfactory agreement with the experimental data for Si MOSFETs (Gallagher 1990). The reason for this behaviour is the switch of the dominant scattering mechanism from small-angle scattering (remote impurity) to large-angle scattering (interface roughness and background impurity) as the electron concentration increases. In order to achieve better agreement between theory and experiment an improved theory for interface roughness and better knowledge of the various parameters used in this calculations are required.

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