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LETTER TO THE EDITOR

The phonon drag and diffusion thermopower of Si inversion layers

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Abstract. New accurate results for the thermopower of Si inversion layers are compared with the calculated screened phonon-drag thermopower. Good agreement is obtained for both the temperature dependence and the magnitude, except at the lowest temperatures, when a change of sign to positive thermopower is observed. This we interpret as being due to the diffusion thermopower associated with surface roughness scattering.

The thermopower, S, of quasi-two-dimensional electrons became a topic of great interest after the discovery of the quantum Hall effect, when it was predicted that the components of the diffusion thermopower, S_d, would, for weak disorder show oscillatory behaviour of a universal nature with maxima quantised in units of k/e, where k is Boltzmann's constant. The first experimental studies seemed to confirm these ideas, but later work led to many contradictory results.

It is now generally accepted that the reason for this is that the phonon-drag thermopower dominates except at the very lowest temperatures. Fletcher *et al* [1] suggested that this was the reason for the very large thermopowers they observed. They produced further strong evidence for this in studies where electron density and phonon MFP were varied [2, 3]. Ruf *et al* [4] were able to see a change from a roughly T^3 dependence at He temperatures to a T dependence below 0.6 K and interpreted this as being due to a phonon drag plus a diffusion contribution. They also observe the effects of second sub-band occupation, as do Syme *et al* [5] for Si on sapphire.

The theory of phonon-drag thermopower for 2D electrons coupled to 3D phonons was developed by Cantrell and Butcher [6]. This enabled Gallagher *et al* [7] to do a quantitative comparison of the thermopower of the 2D electrons in the Si-MOSFET system with theory. They found good agreement with the form of the temperature dependence but that the predicted values were all too large by a factor of about 40. This was attributed to the neglect of screening.

In the present study we have much improved our experimental results and modified the theory to include the screening. We now find excellent agreement in both form and magnitude. We also find that for high electron densities the thermopower changes sign. This we argue is due to a positive diffusion thermopower arising from surface roughness scattering.

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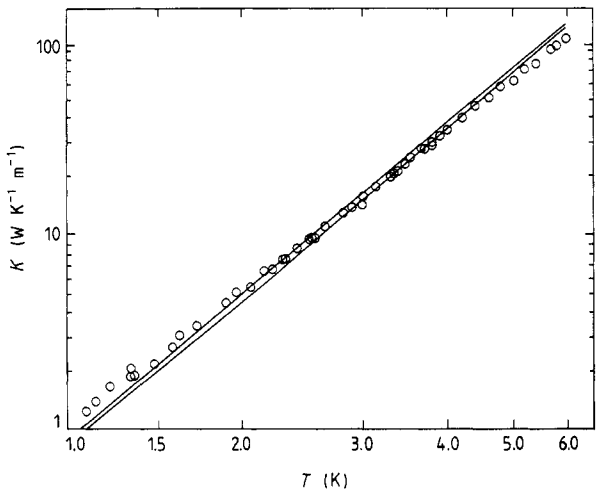

Figure 1. Measured thermal conductivity. The upper line is the theoretical fit without stress. The lower line includes stress. (See text.)

The experimental technique employed is the same as that of Gallagher *et al* [7], the resistances at two points across the sample being used as the 'thermometers'. In our earlier work we measured the difference between the resistances at the two points directly. In the present work we have both measured the ratios directly and the resistance directly using a very high accuracy ASL inductive divider bridge. We find no detectable difference in the temperature gradients obtained. Thus the fact that our 'thermometers' are electrically connected is not of importance. The accuracy of the thermometry is shown by the thermal conductivities obtained (see below). The thermoelectric voltages were measured using an EM Electrons N1A nanovoltmeter, and the whole system shows drifts of only a few nanovolts per hour and noise figures close to the Johnson noise limit. We believe our overall accuracy to be about 5%.

The n-channel (100) MOSFETs used were fabricated on 10 Ω cm B-doped wafers. They were 2 mm by 0.4 mm and the substrates were cut into bars 12 mm long, 1 mm wide and 380 μm thick. The specimens were cut so that the [110] direction was along the length of the specimen.

We can use our measured temperature gradients to obtain the thermal conductivity, K, of the Si bar. Our results, shown in figure 1, are the same within error as those obtained previously [7]. K increases slightly more slowly than the T^3 dependence expected for boundary scattering.

We have performed a detailed calculation of the thermal conductivity of our specimen. We proceeded as follows.

(i) The Casimir boundary scattering length was calculated for the rectangular cross section [8] with a small correction for phonon focusing and length corrections [9].

(ii) An appropriate average of the non-isotropic phonon velocities for heat conduction along the [110] direction was made yielding a transverse velocity v_T of 5,525 m s^{-1} and a longitudinal velocity v_L of 8,872 m s^{-1}.

(iii) The scattering from the B acceptor sites and from isotopes in the Si was calculated using the theory of Suzuki and Mikoshiba [10] but their scattering potentials were

replaced with the more reasonable values of Heraud [11]. A boron density of 1.3×10^{15} cm^{-3}, appropriate to 10 Ω cm Si, is used.

Such a procedure treats the longitudinal and transverse modes separately, avoids any need to define arbitrarily an 'average velocity', and yields the full slightly temperature dependent longitudinal and transverse mean free paths which, in fact, differ by no more than 10%. The calculated behaviour is compared with the experimental results in figure 1. The agreement in magnitude is extremely good; the temperature dependence is however slightly stronger than that found experimentally. This could be due to stress in the specimen. We believe that, because the ends of our specimen were held tightly in indium-faced Cu clamps and because of differential contraction of the support structure, large stresses may be present. This cannot be modelled. However, to see the possible effects we have calculated the scattering from the B sites in the presence of a range of uniaxial stresses up to 3×10^7 N m^{-2} (again using the approach of Suzuki and Mikoshiba [10]) and averaged over these. These calculated values are also shown in figure 1. We see that the magnitude and temperature dependences are altered very little. The discrepancy is therefore probably caused by some other factor, an increasing degree of specular reflection as T is lowered being the most obvious candidate.

Overall, we would conclude that the agreement between experiment and theory is very good: this gives us confidence both in the accuracy of our thermometry and in the derived mean free paths used in the calculations of thermopower.

The measured thermopowers are in very good agreement with our earlier work [7] but the scatter has been greatly reduced and the results extended to lower temperatures and higher electron densities. This extension of the results reveals a dramatic change of sign in the thermopower at low T and at high areal densities, n_A. For phonon-drag thermopower we expect a temperature dependence of the form $T^3 f(T)$, where the cubic term comes simply from the number of phonons and $f(T)$ is a measure of the effectiveness of the momentum transfer from the phonons to the electrons. Figures 2 and 3 therefore show that the rough T^3 dependence holds at higher temperatures but implies that $f(T)$ has distinctive structure and a strong temperature dependence at low T. The peaks observed are a form of the 'Kohn anomaly' and should ocur for $q_D \simeq 2k_F$, the condition for maximum momentum transfer, where q_D is the dominant phonon wavevector and k_F is the Fermi wavevector. For $q_D > 2k_F$ the power of T falls with increasing T, as the electrons can couple with progressively fewer of the additional phonons (though the fall in screening tends to compensate for this somewhat). For $q_D < 2k_F$, S falls rapidly with T as the momentum transfer becomes very ineffective. The expected position of the peaks, T^*, in this simple approach, can then be obtained by writing

$$q_D = 4.96\, kT/\hbar v_s \qquad \text{and} \qquad k_F^2 = \pi n_A$$

thus

$$T^* = (\hbar v_s/4.96k)(2\pi)^{1/2} n_A^{1/2} \qquad v_s = (2v_T^{-2} + v_L^{-2})/(v_T^{-3} + v_L^{-3}).$$

From figure 4 we see that this is surprisingly accurate.

The full calculation of the phonon-drag thermopower is rather complicated. We have used the theory of Cantrell and Butcher with parameters appropriate to our system and without some of the simplifying assumptions of our earlier work [7]. In the present calculation we use the Fang and Howard wavefunctions rather than our previous square well approximation, and replace our previous deformation potentials by the values Ξ_u = 9 eV and $\Xi_d = -6$ eV [12]. These changes have very little effect on the results. We also

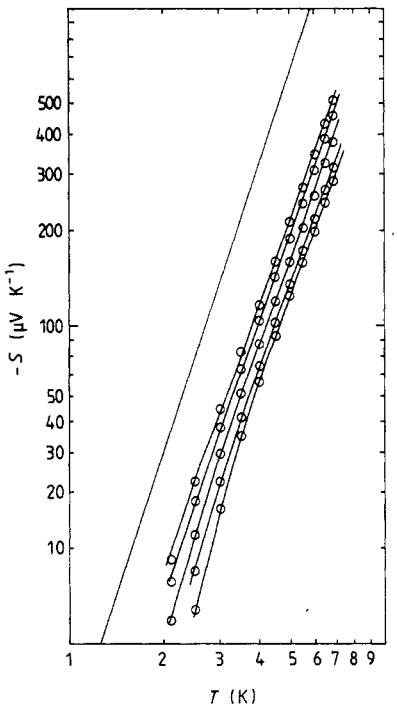

Figure 2. Variation of thermopower with temperature. Charge densities, uppermost line $4.90 \times 10^{15}\ m^{-2}$, second $5.47 \times 10^{15}\ m^{-2}$, third $6.57 \times 10^{15}\ m^{-2}$, fourth $8.35 \times 10^{15}\ m^{-2}$, fifth $10.7 \times 10^{15}\ m^{-2}$. The straight line is proportional to T^3. The curves through the points are a guide to the eye.

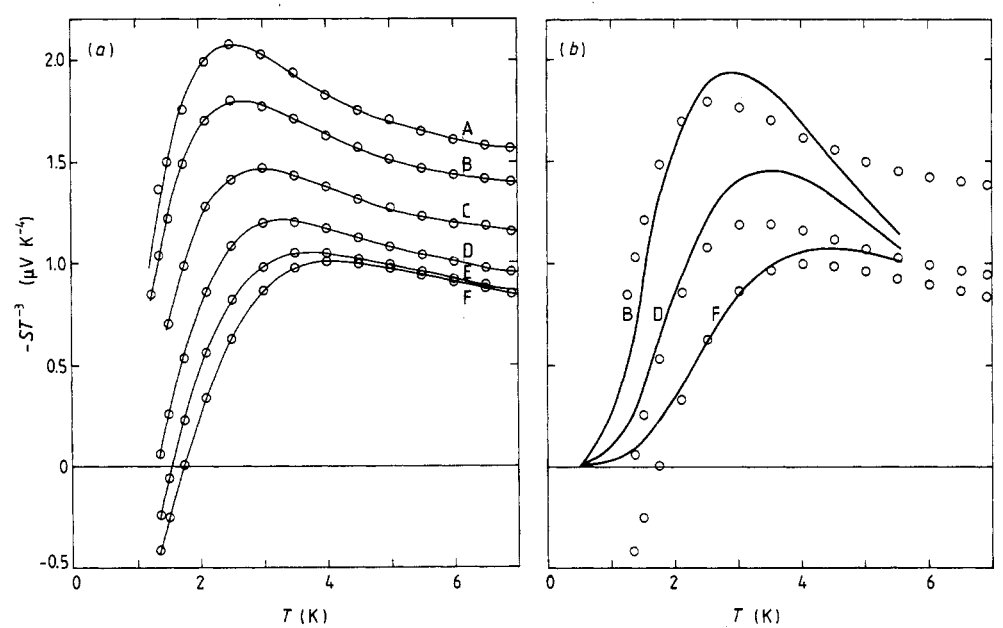

Figure 3. (*a*) Thermopower divided by T^3 for charge densities (A) $4.90 \times 10^{15}\ m^{-2}$; (B) $5.47 \times 10^{15}\ m^{-2}$; (C) $6.57 \times 10^{15}\ m^{-2}$, (D) $8.35 \times 10^{15}\ m^{-2}$; (E) $10.7 \times 10^{15}\ m^{-2}$; (F) $14.1 \times 10^{15}\ m^{-2}$. The curves through the points are a guide to the eye. (*b*) Data and theory curves for (B) $5.47 \times 10^{15}\ m^{-2}$, (D) $8.35 \times 10^{15}\ m^{-2}$, (F) $14.1 \times 10^{15}\ m^{-2}$.

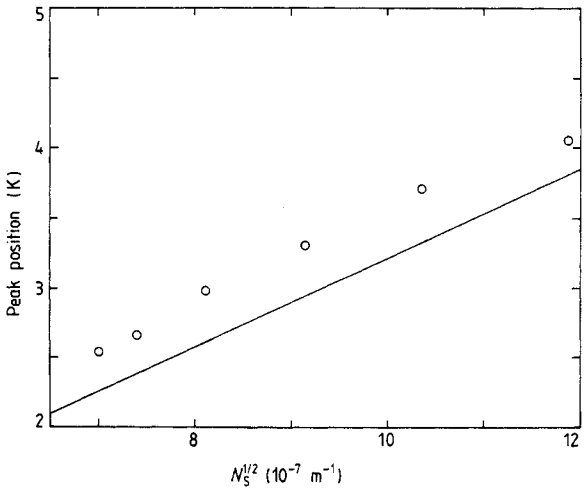

Figure 4. Position of peaks in ST^{-3} curves. The line is the theoretical fit.

employ the phonon velocities discussed in the previous section and the separate slightly temperature dependent longitudinal and transverse phonon mean free paths obtained from the thermal conductivity. These improvements again produce rather small changes. Most importantly, we include the full form of the screening of the electron–phonon interaction recently introduced by Smith and Butcher [6]. We do not, however, include departures from degeneracy of the electron system at finite temperatures and the associated temperature dependence of the screening.

We see from figure 3 that the general agreement is good, except at the lowest temperatures, where clearly a dramatic departure from the expected behaviour is observed. This we attribute to the diffusion thermopower. At higher temperatures the calculated values fall too quickly; this we believe to be due to departure from degeneracy. The dramatic drop in the calculated magnitude is entirely due to the screening. This was predicted in our earlier paper [7], as was the fact that the agreement with the dependence upon n_A would not be destroyed. This seems to us to show conclusively that the thermopower is dominated by phonon drag and also that our model of the electron–phonon coupling is quite good.

Provided that (i) the electrons are reasonably degenerate and (ii) the scattering time, τ, is a smoothly varying function of energy, the diffusion thermopower is given by

$$S_d = -(\pi^2/3)(k/e)[kT/(E_F - E_c)](1 + p)$$

where the scattering time is of the form $\tau(E) \propto E^p$ and E_c is the position of the mobility edge. Detailed calculations in which conditions (i) and (ii) are not assumed lead only to minor modifications to this [13].

The power of E is generally small and positive for most scattering mechanisms [13] but a negative p is required to understand our positive thermopowers if, as we believe, they are due to the diffusion contribution.

Two scattering mechanisms are believed to be important in Si MOSFETs, ionised impurity and surface roughness. Ionised impurity scattering is believed to give a value of $p \simeq +1$ [13] but, to our knowledge, there is no calculation of the energy dependence

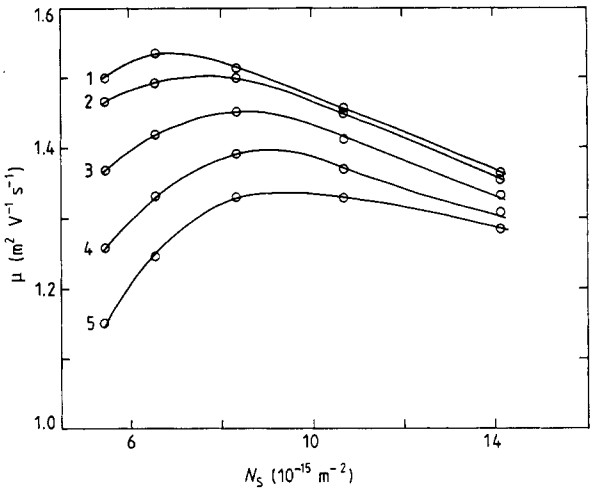

Figure 5. Electron mobility at (1) 1.75 K, (2) 2.1 K, (3) 3 K, (4) 4 K and (5) 5 K.

of surface roughness scattering. One can, however, estimate what the behaviour will be if one assumes that

$$p \equiv \frac{\mathrm{d}(\ln\tau)}{\mathrm{d}(\ln E)}\bigg|_{E=E_F} \cong \frac{\mathrm{d}\ln(\tau)}{\mathrm{d}\ln(E_F)} \equiv \frac{\mathrm{d}\ln(\mu)}{\mathrm{d}\ln(n_A)}$$

in 2D where μ is the mobility.

One cannot generally equate the derivative at E_F with that with respect to E_F, but it is often a reasonable guide to the true behaviour. The measured behaviour of $\mu(n_A)$ (figure 5) shows that μ increases with n_A at low n_A where ionised impurity scattering dominates. It has a maximum when the surface roughness scattering becomes a comparable importance. Then, for larger n_A, μ falls rapidly. Such behaviour is well known, with the peak usually occurring at $n_A \simeq 10^{16}$ m^{-2} and $\tau \propto n_A^{-2}$ when surface roughness scattering totally dominates [14].

This simple picture is completely consistent with our results. At low n_A one expects $p \simeq +1$, but the expected small negative contribution will be masked by the phonon drag, which is always large for small n_A. As n_A is increased, the two scattering rates will become comparable and we will have $p \simeq -1$. The diffusion contribution will then become unobservably small, despite the reduction of S_{drag} at low temperature as the peak in $S_{drag}\,T^{-3}$ moves to higher temperatures. This would then be the explanation for the absence of a measurable contribution in our previous data [7]. Finally, at sufficiently high enough n_A the contribution would become positive, with $p \simeq -2$, and observable at low temperatures.

We feel that the explanation is probably correct; however, this clearly needs further experimental and theoretical examination. The only obvious alternative explanation is that we are starting to occupy the second sub-band. This, however, is highly improbable, since significant occupation is believed not to occur until $n_A \simeq 8 \times 10^{16}$ [14]. Furthermore, our interpretation would explain both the absence of an observable diffusion contribution at lower n_A and a positive contribution at higher n_A.

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