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1992 J. Phys.: Condens. Matter 4 4491

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J. Phys.: Condens. Matter 4 (1992) 4491–4498. Printed in the UK

The thermopower of 2D electron gases in $Al_xGa_{1-x}As/GaAs$ heterostructures over a wide temperature range

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Abstract. This paper presents our results on the thermopower of three heterojunction samples. The thermopower shows a peak in the region of 12 K followed by a rapid decrease at higher temperatures. These features are believed to be due to phonon drag. Above about 100 K, the thermopower becomes relatively constant. We assume that this region is controlled by diffusion effects. A numerical calculation of the diffusion thermopower shows that above 100 K the coefficient is approaching the classical limit and has only a weak variation with temperature.

1. Introduction

In general there are two contributions to the thermopower S of good conductors [1,2], in particular 2D electron gases. At the lowest temperatures (< 1 K for heterojunctions [3]) S is dominated by the diffusion component S^d which is linear in this temperature region. Phonon drag S^g, which, according to both theory [4] and experiment [3], initially increases as T^3, overwhelms S^d in the liquid ^{4}He temperature range. This contribution is caused by the bulk phonons being out of equilibrium due to the temperature gradient. This deviation is transmitted to the electrons by the electron–phonon interaction. Because the phonons are only weakly affected by the presence of the 2D electrons, the magnitude of S^g is a direct measure of the strength of the electron–phonon interaction. As the temperature increases, other phonon scattering mechanisms become increasingly effective in bringing the phonons back into equilibrium. This is expected to result in a peak in S^g and a subsequent rapid decrease in its magnitude. Bulk semiconductors, in particular GaAs [1,2,5], exhibit this behaviour. In this temperature range, restrictions imposed by momentum conservation severely limit the number of phonons which can scatter electrons. Presumably, if bulk semiconductors can be used as a guide, S^d will again become dominant at high temperatures, though the 2D electron gas will no longer be degenerate for the attainable densities and a linear dependence on T will not be appropriate.

The experiments and theories concerning S in 2D electron gases have so far been confined to the low-temperature region where scattering mechanisms other than electron–phonon and phonon–boundary scattering can be ignored ([3,4,6–9] give many references to earlier work). The present experiments were designed to probe the behaviour of S at higher temperatures. We have measured S over the temperature range 5.5–200 K for three $Al_xGa_{1-x}As/GaAs$ heterojunctions and found that the behaviour outlined above actually occurs.

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Table 1. The properties of the samples used in this investigation. In each case the Si doping in the $Al_xGa_{1-x}As$ was about 2.5×10^{24} m^{-3} and the period of the superlattice was about 200 Å. The substrates were all semi-insulating GaAs with nominal dimensions of $12 \times 6.5 \times 0.5$ mm^3.

Sample[a]	n (10^{15} m^{-2})	μ ($m^2V^{-1}s^{-1}$)	Superlattice	GaAs (μm)	$Al_xGa_{1-x}As$			TEP error[b] (%)
					x	undoped spacer (Å)	Si doped (Å)	
1(197)	2.7	19	AlAs/GaAs 4 periods	0.8	0.36	150	400	10
2(349)	4.4	62	AlAs/GaAs 10 periods	1.0	0.32	110	350	16
3(116)	2.1	4.2	AlGaAs/GaAs 10 periods	0.12	0.32	105	525	14

[a] The numbers in brackets are the identifiers of the National Research Council.
[b] Estimated systematic error in the thermopower due to the separation of the thermometer and voltage contacts.

2. Samples and techniques

The three samples which we have used were all grown by molecular beam epitaxy at the National Research Council, Ottawa. Table 1 gives the growth sequences and also the carrier densities n and mobilities μ at 4.2 K. In the case of sample 2, the carrier density was measured from 4.2 K to 200 K, but there was no change to an accuracy of 1%; we expect the others to behave similarly. Each sample was grown on top of a non-conducting superlattice which in turn was grown on a semi-insulating substrate. The samples have a relatively large range of mobility but this is not expected to influence the magnitude of S^g; it may have some effect on S^d at high temperatures, as we shall mention again later.

The experimental techniques were similar to those used in the liquid ^{4}He temperature range [6, 7]. The samples were indium soldered to a copper block whose temperature could be precisely controlled over the range 4–200 K. Heating currents of about 50 mW were applied to the sample producing temperature gradients of up to ≈ 2 K cm^{-1}. Two 2.2 kΩ, $\frac{1}{8}$ W carbon resistors cemented to the sample by epoxy were used as thermometers to measure both the absolute temperatures and the temperature differences. Using a liquid ^{4}He bath as the cold sink, the lowest temperature at which reasonably accurate measurements could be made was about 5.5 K. Liquid N_2 was used for the range $\gtrsim 85$ K. At 200 K the thermometers are becoming too insensitive to be useful, so this determines our upper limit. In fact radiation problems should become increasingly important at higher temperatures, especially since our system does not have a temperature-controlled radiation shield.

Thermometer calibrations were made using either a Ge thermometer, calibrated by the manufacturer up to 65 K, or a Au + 0.03%Fe versus chromel thermocouple. The reference temperature for the thermocouple was a cryogenic bath (either liquid ^{4}He or N_2). All leads to the sample, either for voltage or thermometer connections, were made with 100 μm diameter manganin wire. This wire has a very high thermal resistance, as well as the added advantage that the thermopower is always less than 1 μV K^{-1} and so can be ignored [10].

Voltage differences were measured by a Keithley 182 voltmeter and corrected for any offsets present when the sample had no temperature gradient. The signals were always large enough such that, with a precision of 0.1 μV, the measurement had little random error. Most of the random error is due to the measurement of the temperature gradient. The largest systematic source of error is the measurement of the length between the temperature and the voltage probes, say L_T and L_V. The probe width for L_T was about 0.3 mm, so, with L_T typically equal to 5 mm, this gives rise to an uncertainty of about 6%; this is the main uncertainty in the measurement of the thermal conductivity since the geometrical size of the substrate is relatively well known. The voltage contacts were made by diffusing 0.4 mm diameter Sn balls into the surface. The separation L_V was in the range 2.6–5 mm, giving uncertainties of 8–15%. The combination of these two contributions gives the expected total systematic uncertainties in S, which are listed in table 1.

3. Results and discussion

Figure 1 shows the thermal conductivity λ of all three samples; the three sets of measurements are essentially indistinguishable. Sample 1 tends to show more scatter

than the other two. This does not reflect any physical difference between the samples but is due only to the fact that this was the first sample measured and suffered from our initial lack of expertise. Previous data on λ for GaAs have been published by Holland [11] and Aliev and Shalyt [5]. Above the peak in λ we are unable to discern any differences in the various sets of data to the accuracy with which we can read the published graphs ($\sim$ 5%). Below 20 K, phonon–boundary scattering becomes increasingly dominant and leads to different thermal conductivities for samples of different cross section. In our case the three samples have almost identical geometric factors, so we see no differences between them. Coincidentally, the data for the sample labelled D by Holland follows our results very closely. This good agreement suggests that there are no major errors or problems with the thermometry which we have adopted, especially in the region of 20–200 K.

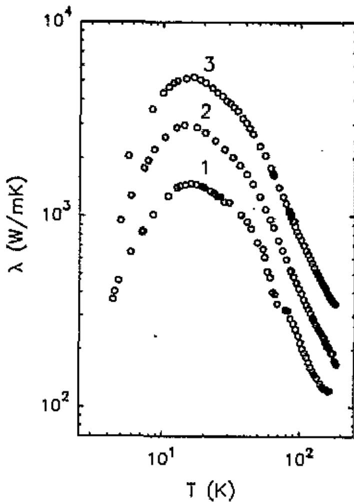

Figure 1. The thermal conductivity λ of the substrates of the three samples as a function of temperature T. For clarity the data for samples 2 and 3 have been multiplied by a factor of two and four, respectively.

At temperatures above $\approx$ 100 K, λ decreases with a dependence close to T^{-1}. At lower temperatures the decrease is more rapid. This general behaviour is consistent with phonon–phonon and phonon–isotope scattering (the latter due to two major isotopes of Ga), but good fits to the earlier experimental data have proved to be difficult to achieve over a wide temperature range [11,12].

The thermopower S of the three samples is shown in figures 2(a)–(c). The results for samples 1 and 2 appear to be identical even though the carrier densities are different. This might be partly coincidental bearing in mind the uncertainties for each of the samples. For sample 3 the peak in S is much higher in magnitude, though above 100 K the data for all three samples are very similar. The thermopower S at low temperatures has previously been measured for two other samples taken from the same wafer as sample 3 [7]. These two previous samples were cut from the same area of the wafer, but this new sample is from another region, though the carrier densities and mobilities are similar. The old and new data do not overlap, since the old data covers the range 1.2–4.2 K and the new data begins near 5.5 K. The new sample was mounted in the cryostat twice so that two sets of data are available to check the reproducibility; there are no significant differences in the results, although the second set was restricted to the temperature range 5.5–80 K. Two independent

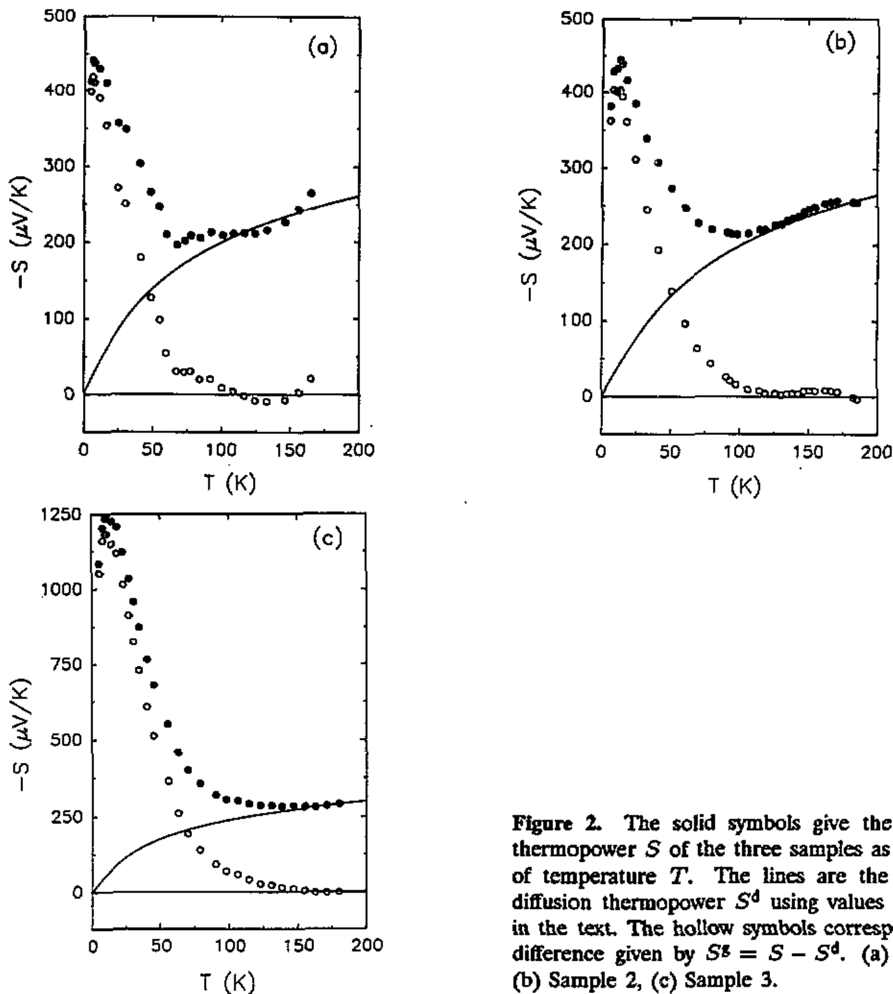

Figure 2. The solid symbols give the measured thermopower S of the three samples as a function of temperature T. The lines are the calculated diffusion thermopower S^d using values of q given in the text. The hollow symbols correspond to the difference given by $S^g = S - S^d$. (a) Sample 1, (b) Sample 2, (c) Sample 3.

pairs of voltage contacts were used in the new data and by roughly extrapolating the weighted mean of S to 4 K we obtain $-780 \pm 100\mu$V K^{-1}. The measured value of S at 4 K for the old data set is -670μV K^{-1} ($\pm$ 15%), which is in substantial agreement. However, although the magnitudes agree, the slopes of the two data sets at the ends of their ranges do not match very well. This discrepancy may be due to the thermometer calibration errors, which tend to be larger at the ends of the ranges; the evaluation of S effectively uses the slope of the thermometer resistance versus temperature. The thermal conductivity for the various data sets shows no obvious discontinuities or slope problems but the magnitude does increase by about a factor of two between 4 K and 5.5 K, so any discrepancies might not be visible. The older samples are no longer available for a direct comparison to be made.

Although we expect the magnitude of S^g to vary roughly inversely with n in the liquid ^{4}He range [4], the relationship at higher temperature is not known. There is no clear correlation betweeen the peak height of S and n for the present results. We have previously noticed this apparent lack of correlation for independent samples,

although particular samples which have been illuminated to change n certainly show a decrease in S [7]. Perhaps other factors are active in changing the magnitude. It is known [6] that impurities in the substrate can cause large variations in both S and λ, but our measurements of λ for these samples show no differences. One possibility is that the presence of different superlattices beneath the heterojunctions affects the phonon distribution in contact with the 2D electron gas, but this is likely to be a small effect.

The rapid decrease of S above 20 K is presumably due to the rapidly increasing phonon–phonon and phonon–isotope scattering, as mentioned earlier. A similar decrease is seen in bulk GaAs [5]. At the present time there are no detailed theoretical predictions for this range of temperatures. However, above $\approx$ 100 K the curves tend to level off and for samples 1 and 2 show a weak increase at higher temperatures—we assume that the data in this region are basically due to S^d. In the relaxation time approximation, S^d is given by [1]

$$S^d = -\frac{1}{eT}\left(\frac{K_2}{K_1} - \mu_c(T)\right) \tag{1}$$

where e is the electron charge, $\mu_c(T)$ is the chemical potential at temperature T and K_m is defined by

$$K_m = \int g(\varepsilon)\tau(\varepsilon)\varepsilon^m \left(\frac{\partial f_0}{\partial \varepsilon}\right) \mathrm{d}\varepsilon. \tag{2}$$

In equation (2), $g(\varepsilon)$ and $\tau(\varepsilon)$ are the density of states and the relaxation time of the electrons at energy ε, f_0 is the Fermi–Dirac distribution function and the integral is evaluated over all energy states. If we assume $\tau(\varepsilon) = \tau_0\varepsilon^q$, with τ_0 and q taken to be constants, then the integrals can be evaluated numerically to give S^d as a function of T. We have assumed that only a single electric subband is populated regardless of T, so that $\mu(T)$ can be evaluated analytically from the equation

$$\mu_c(T) = \mu_c(0) + kT \ln\left[1 - \exp\left(-\mu_c(0)/kT\right)\right] \tag{3}$$

where k is the Boltzmann constant and $\mu_c(0)$ is the chemical potential at zero temperature, i.e. $\mu_c(0) = n\pi\hbar^2/m^*$, where m^* is the electron effective mass. In principle one should weight the thermopower due to different scattering mechanisms using the Nordheim–Gorter relation [13], but the accuracy of our data does not warrant this refinement; furthermore, below 100 K, where the scattering mechanisms might be rapidly changing with T, S is dominated by S^g. Figure 3 shows an example of the calculated S^d as a function of temperature at different values of q. As expected, the fitted curves tend to the degenerate limit at low temperatures, i.e.

$$S^d = -\frac{\pi^2 k^2 T}{3e\mu_c(0)}(q+1) \tag{4}$$

and to the classical limit at high temperatures

$$S^d = -\frac{k}{e}\left(q + 2 - \frac{\mu_c(T)}{kT}\right). \tag{5}$$

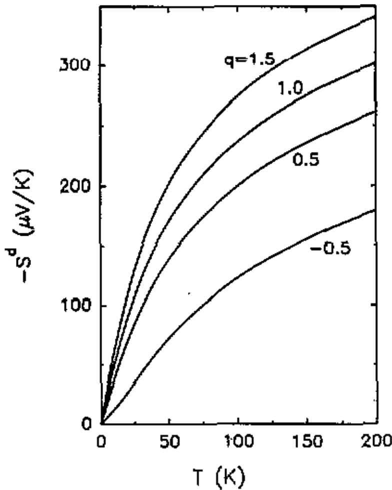

Figure 3. The diffusion thermopower S^d of a sample with $n = 2.75\times10^{15}$ m^{-2} (equivalent to sample 1) as a function of temperature T. The calculations are appropriate to equation (1) in the text with various fixed values of q.

The best fits to the data with a fixed q are shown in figures 2(a)–(c) and yield the following estimates for q: 0.5 ± 0.4 for sample 1, 1.1 ± 0.65 for sample 2 and 0.7 ± 0.6 for sample 3. The uncertainties arise directly from the systematic uncertainties in the magnitude of S, which are given in table 1.

In the temperature range of interest here ($T \geqslant 100$ K), the main scattering source for the electrons in the higher mobility samples 1 and 2 should be provided by optical phonons. If the scattering is assumed to be elastic and similar to that in the bulk, then $q = \frac{1}{2}$ [2]. However, in GaAs the longitudinal optic branch has an energy (near the centre of the zone) of $\hbar\omega_L \simeq 37$ meV [14] so that at 200 K, $\hbar\omega_L/kT \sim 2$. This result appears to be too low for the elastic scattering approximation to be valid and in bulk GaAs under these conditions we would find $q \sim -\frac{1}{2}$ [2]. Acoustic phonon scattering might also be relevant, the appropriate q in this case again being $-\frac{1}{2}$ [2]. Clearly these values are in poor agreement with our results. With sample 3, impurity scattering still accounts for half the resistivity at 180 K. Calculations appropriate to low temperatures are available for both remote and background impurities [15, 16]; both appear to yield values of q in the range 1–1.5. (The calculations of [16] are for electron densities above 6×10^{15} m^{-2}, which are higher than for any of our samples). The variation of electronic screening with temperature may have some effect, but the similarity with the bulk value of $\frac{3}{2}$ [2] for ionized impurity scattering suggests that this is small. For all three samples, we see no obvious differences in the required value of q, perhaps suggesting that the behaviour of bulk GaAs is not necessarily an accurate guide to the appropriate values of q for 2D electron gases.

4. Conclusions

The behaviour of the thermopower of 2D electron gases at $Al_xGa_{1-x}As/GaAs$ heterojunctions is qualitatively in accord with our expectations. The coefficient appears to be dominated by phonon drag at temperatures below about 40 K, and by diffusion above this temperature. We have had some success in fitting the experimental data above 100 K to a theoretical model of the diffusion thermopower, but we are unable

to explain the lack of variation that we find in the exponent of the energy dependence of the relaxation time. There is no theory which is appropriate to the phonon-drag component in the temperature range of interest here and with which we can compare our results.

Acknowledgments

The work was partially funded by a grant from the Natural Sciences and Engineering Research Council of Canada.

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