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Low-temperature phonon-drag thermoelectric power in heterojunctions

S. K. Lyo
Sandia National Laboratories, Albuquerque, New Mexico 87185
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The phonon-drag contribution to the thermoelectric power is calculated at low temperatures in polar semiconductor heterostructures. Carriers are assumed to interact with longitudinal acoustic phonons through deformation potential and with both longitudinal and transverse acoustic phonons through piezoelectric field. The magnitude and the temperature dependence of the phonon-drag contribution calculated without any adjustable parameter agree reasonably well with recent data from $Al_xGa_{1-x}As/GaAs$ heterolayer. Both piezoelectric scattering and deformation potential scattering yield comparable contributions in the temperature range studied (i.e., below 10 K), although the former (latter) contribution becomes more important below (above) 3–4 K. Dielectric screening is found to reduce the phonon-drag thermopower significantly.

I. INTRODUCTION

In recent years, there has been increasing interest in the thermoelectric phenomenon in semiconductor heterostructures.[1–4] It is a valuable tool for probing the electronic structure, scattering dynamics of electrons and phonons, and electron-phonon interactions in solids. The thermoelectric power (TEP) is the ratio of the heat current to the charge current per degree under isothermal conditions produced by an external electric field. The heat current arises in part from the motion of the charge carriers, yielding electron-diffusion TEP. This contribution is linear in temperature at low temperatures where the system is degenerate. The carriers impart their momenta to the phonon system through electron-phonon interactions, creating a nonequilibrium phonon distribution and, thus, an additional heat flow. The latter contribution is known as phonon-drag thermoelectric power (PDTEP).

In this paper, we report a theoretical calculation to accurately explain the PDTEP measured for $Al_xGa_{1-x}As/GaAs$ heterostructures. Recent data from $Al_xGa_{1-x}As/GaAs$ heterostructures indicate that the PDTEP is much larger than the electron-diffusion TEP and increases rapidly with temperature.[1,2] The PDTEP peaks around 12–13 K and drops rapidly beyond the maximum due to a short phonon mean free path which decreases with temperature. The phonon mean free path is dominated by temperature-independent boundary scattering[2] below about 5 K and by three-phonon and impurity scattering at higher temperatures.[5] The PDTEP arising from unscreened deformation potential scattering was recently calculated by Cantrell and Butcher.[4] While their work gives an estimate of the size of the effect, it is not adequate for a serious comparison with the data.[1] In this paper, we show that even for a mildly polar material such as $Al_xGa_{1-x}As/GaAs$, the contribution from piezoelectric scattering cannot be ignored. It is comparable to that from the deformation potential scattering in the temperature range studied (i.e., below 10 K) and is actually more important at low temperatures (e.g., below 3–4 K). It causes the PDTEP to increase more rapidly with temperature. Also, a more realistic confinement wave function is employed. Furthermore, the dielectric screening is shown to reduce the PDTEP by a factor as large as 2–3. Because screening is less efficient for a larger momentum transfer (i.e., for higher-energy phonons), it makes the PDTEP rise even more steeply with temperature, yielding good agreement with the data[1] without any adjustable parameter.

II. PHONON-DRAG THERMOELECTRIC POWER

PDTEP equals the heat carried by phonons per charge per degree. In our model, electrons are dominantly scattered by impurities and the relaxation-time approximation is assumed. This approximation is justified for the system[1] to which our theory will be applied, because it has a mobility of 2.27×10^5 cm^2/V sec which is about an order of magnitude smaller than the phonon-limited mobility. On the other hand, phonons are not predominantly scattered by electrons because they are scarce in a single quantum-well structure. Scattering by electrons is important only in multi-quantum-well structures with a large number of quantum wells. The PDTEP is then given in this approximation by[4]

$$S_{\rm ph}=-\frac{2e}{\sigma\Omega k_B T^2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{qs}\hbar\omega_{qs}\tau_{qs}^{\rm ph}f_{\mathbf{k}}(1-f_{\mathbf{k}'})P_{qs}(\mathbf{k},\mathbf{k}')(\tau_{\mathbf{k}'}\mathbf{v}_{\mathbf{k}'}-\tau_{\mathbf{k}}\mathbf{v}_{\mathbf{k}})\cdot\nabla_{\mathbf{q}}\omega_{qs}\,, \tag{1}$$

where e is the electronic charge (negative for electrons and positive for holes), σ the conductivity, Ω the sample volume, k_B Boltzmann's constant, and T the temperature. Factor 2 accounts for spins. The quantities ω_{qs}, $\tau_{qs}^{\rm ph}$, $f_{\mathbf{k}}$, and $\tau_{\mathbf{k}}$ indicate, respectively, the phonon frequency of wave vector $\mathbf{q}$ and of mode s, the phonon scattering time, the Fermi function for the electron of wave vector $\mathbf{k}$ with velocity $\mathbf{v}_{\mathbf{k}}$, and the electron scattering time. The quantity $P_{qs}(\mathbf{k},\mathbf{k}')$ is given

by

$$P_{qs}(\mathbf{k},\mathbf{k}') = \frac{2\pi}{\hbar} |V_{qs}|^2 n_{qs} \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} - \hbar\omega_{qs}) \times \Delta(q_z) \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}_\parallel}, \quad (2)$$

where $\mathbf{q}_\parallel$ is the component of $\mathbf{q}$ in the quantum-well plane, $\varepsilon_{\mathbf{k}}$ is the electronic energy, n_{qs} the boson function for the phonon mode qs, and

$$\Delta(q_z) = \left| \int \phi(z)^2 \exp(iq_z z) dz \right|^2 . \quad (3)$$

Only the ground sublevel with wave function $\phi(z)$ is assumed to be populated at a low density at low temperatures. The square of the electron-phonon interaction in (2) is given in the Debye approximation by

$$|V_{ql}|^2 = \frac{\hbar\omega_{ql}}{2\epsilon(\mathbf{q}_\parallel)^2 \rho c_l^2 \Omega} \left(D^2 + (eh_{14})^2 \frac{A_l}{q^2} \right) \quad (4a)$$

for the longitudinal model and by

$$|V_{qt}|^2 = \frac{\hbar\omega_{qt}}{2\epsilon(\mathbf{q}_\parallel)^2 \rho c_t^2 \Omega} (eh_{14})^2 \frac{A_t}{q^2} \quad (4b)$$

for the transverse modes. The first term in (4a) represents the contribution from deformation potential scattering, while the second term and (4b) are the contributions from piezoelectric scattering. In (4), the quantities $\epsilon(\mathbf{q})$, ρ, c_s, D, and h_{14} are, respectively, the static dielectric constant, the mass density, the sound velocity, the deformation potential coefficient, and the piezoelectric constant. The quantities A_l and A_t (representing anisotropy factors) are given by[6]

$$A_l = 9q_\parallel^4 q_z^2 / 2q^6 , \quad (5a)$$

$$A_t = (8q_\parallel^2 q_z^4 + q_\parallel^6)/4q^6 . \quad (5b)$$

PDTEP is then evaluated using the following approximations. Due to the wave-vector conservation conditions in (2) only those phonons with small q interact with electrons. Therefore, the phonon energy term in the energy delta function is ignored, yielding $f_{\mathbf{k}}(1-f_{\mathbf{k}'})/(k_B T) \simeq \delta(\varepsilon_{\mathbf{k}} - \varepsilon_F)$ where ε_F is the Fermi energy. The conductivity is given in the effective-mass approximation by $\sigma = 2e^2 \varepsilon_F \tau_F \rho_F / (\Omega m^*)$ where $\rho_F = m^* S/(2\pi\hbar^2)$ is the density of states per spin, S is the area of the quantum well, and τ_F is the scattering time for electrons at the Fermi surface. The phonon relaxation time is assumed to be dominated by boundary scattering: $\tau_{qs}^{ph} = \Lambda/c_s$, where Λ is the phonon mean free path due to boundary scattering. The PDTEP is then given by

$$S_{ph} = \frac{k_B}{e} \frac{(2k_F)^3 m^* \Lambda}{\pi\hbar\varepsilon_F k_B T} \frac{2}{\pi} \int_0^{\pi/2} d\theta \int_0^\infty dQ_z \sum_s c_s \Omega |V_{qs}|^2 n_{qs} \Delta(q_z) \sin^2\theta , \quad (6)$$

where $Q_z = q_z/2k_F$, $\sin\theta = q_\parallel/2k_F$, k_F is the Fermi wave number, and 2θ the scattering angle. For the confinement wave function, the Fang-Howard-Stern variational wave function[7] is used:

$$\phi(z)^2 = \tfrac{1}{2} b^3 z^2 e^{-bz} , \quad (7)$$

where $b/2k_F = [33e^2 k_F/(64\kappa_s \varepsilon_F)]^{1/3}$, yielding

$$\Delta(q_z) = [b^2/(b^2+q_z^2)]^3 . \quad (8)$$

The dielectric constant is given in the random-phase approximation by[8]

$$\epsilon(\mathbf{q}_\parallel) = 1 + 2m^* e^2 F(q_\parallel)/(\hbar^2 \kappa_s q_\parallel) , \quad (9)$$

where

$$F(q_\parallel) = \left[8 + 9\frac{q_\parallel}{b} + 3\left(\frac{q_\parallel}{b}\right)^2 \right] \Big/ \left[8\left(1+\frac{q_\parallel}{b}\right)^3 \right] . \quad (10)$$

III. APPLICATION AND DISCUSSION

We now evaluate (6) and compare the result with the data from the $Al_xGa_{1-x}As/GaAs$ heterostructure in Ref. 1. The following parameters are used: N (electron density) $= 1.78\times10^{11}$ cm^{-2} (Ref. 1), $\kappa = 12.9$, $m^* = 0.07 m_0$, $c_l = 5.14\times10^5$ cm/sec, $c_t = 3.04\times10^5$ cm/sec, $\rho = 5.3$ g/cm^2, $h_{14} = 1.2\times10^7$ V/cm (Ref. 9), and $D = -9.3$ eV (Ref. 10). These parameters are reasonably well known and there are no adjustable parameters. The phonon mean free path Λ is expected to be of the order of the smallest dimension of the sample $L_< = 0.36$ mm (Ref. 1) or larger.[11] A recent thermal-conductivity measurement yielded $\Lambda = 0.30$ mm ($\pm 15\%$), somewhat smaller than $L_<$ probably due to Cr doping.[12] The PDTEP is plotted in solid curve A for $\Lambda = 0.36$ mm and curve B for $\Lambda = 0.30$ mm in Fig. 1 and compared with two sets of data from Ref. 1. The data reach maxima in the range 10–12 K and drop rapidly above 12 K (not shown in Fig. 1).[1] A small electron-diffusion TEP is taken out from the data according to (Ref. 1) $S_d = -3.8(1+p)T$ μeV/K (T is in Kelvin) and $p = 1$. The latter choice of p overestimates (underestimates) the absolute value of S_d (S_{ph}) somewhat. The agreement is excellent at low temperatures.

Theoretical values are larger than the data at higher temperatures in Fig. 1 as is expected, because the phonon relaxation time is assumed to be independent of the temperature and energy. Phonons are increasingly scattered by three-phonon processes and also by impurities at higher temperatures. As a result τ_{qs}^{ph} drops rapidly with temperature above 10–12 K.[1] The aforementioned maximum in the PDTEP data arises from the fact that the heat current is proportional to the product of the lattice specific heat (which rises with the temperature) and the scattering time. The thermal conductivity data support a similar conclusion.[2] The theoretical PDTEP arises from piezoelectric scattering (dotted curve) and deformation potential scattering (dashed curve). The former contribution is more important below about 3 K and rises as T^4 with the temperature at low temperatures, whereas the latter contribution is more important above 3 K and rises

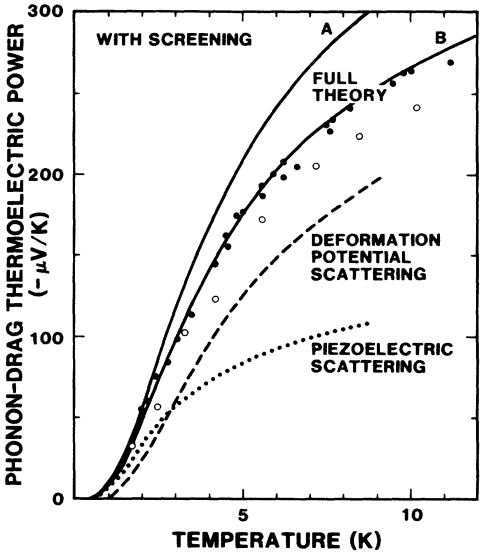

FIG. 1. The phonon-drag thermoelectric power calculated from (6) in the presence of dielectric screening for $\Lambda = 0.36$ mm (curve A) and $\Lambda = 0.30$ mm (curve B). The two sets of data are for two different samples and are quoted from Ref. 1. The dashed and dotted curves are for $\Lambda = 0.36$ mm.

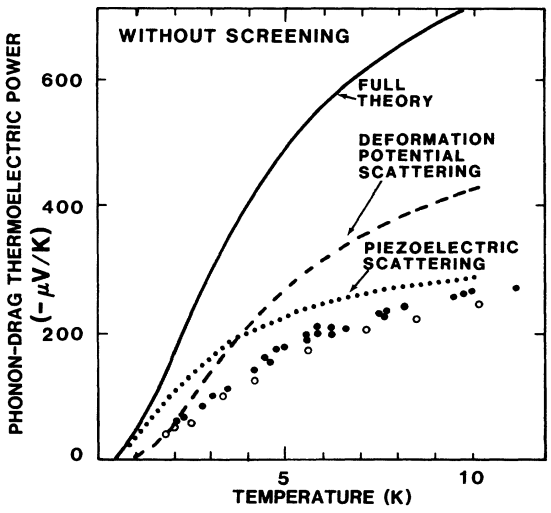

FIG. 2. The phonon-drag thermoelectric power calculated from (6) in the absence of dielectric screening for $\Lambda = 0.36$ mm. The two sets of data are the same as those in Fig. 1.

more rapidly as T^6. The combined effect of these two contributions is to make the PDTEP rise steeply in accordance with the data.

Recently Walukiewicz[13] found that the lattice-scattering mobilities due to deformation and piezoelectric scattering agree better with the data when the screening is ignored. Our result does not support this conclusion. To see the effect of screening, we evaluate the PDTEP in the absence of dielectric screening [i.e., $\epsilon(\mathbf{q}) = 1$], using the same parameters given above and compare it with data in Fig. 2. By comparing the theoretical results in Figs. 1 and 2, it is seen that screening reduces the PDTEP by a factor of 2–3.

The contribution from piezoelectric scattering (dotted curve) in Fig. 2 rises as T^2 at low temperatures, while that from deformation potential scattering (dashed curve) rises more rapidly as T^4. The exponents for the power law here are smaller than those in the presence of screening by two, because screening is more efficient for small transfer yielding an additional temperature-dependent factor $\epsilon(q)^{-2} \propto q^2 \propto T^2$.

IV. CONCLUSIONS

In summary, we studied the PDTEP at low temperatures in polar semiconductor heterostructures. Carriers interact with acoustic phonons through deformation potential and piezoelectric scattering. The result yields good agreement with recent data from doped $Al_xGa_{1-x}As$/GaAs heterostructure without any adjustable parameter. Both piezoelectric scattering and deformation potential scattering yield comparable contributions in the temperature range studied (i.e., below 10 K), although the former (latter) becomes more important below (above) 3–4 K. Dielectric screening is found to reduce the phonon-drag thermopower significantly.

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