Phonon-drag effects on thermoelectric power

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We carry out a calculation of the phonon-drag contribution $S_g$ to the thermoelectric power of bulk semiconductors and quantum well structures for the first time using the balance equation transport theory extended to the weakly nonuniform systems. Introducing wavevector and phonon-mode dependent relaxation times due to phonon-phonon interactions, the formula obtained can be used not only at low temperatures where the phonon mean free path is determined by boundary scattering, but also at high temperatures. In the linear transport limit, $S_g$ is equivalent to the result obtained from the Boltzmann equation with a relaxation time approximation. The theory is applied to experiments and agreement is found between the theoretical predictions and experimental results. The role of hot-electron effects in $S_g$ is discussed. The importance of the contribution of $S_g$ to thermoelectric power in the hot-electron transport condition is emphasized.

72.15.Jf, 72.20.Pa, 72.20.Ht, 72.10.Bg

I. INTRODUCTION

Recently the study of thermoelectric power has attracted intensified interest both theoretically and experimentally in various systems: mesoscopic quantum dots, quantum wires, heterojunctions and quantum well structures as well as bulk materials. Almost all of the earlier theoretical treatments were based on the Boltzmann equation in analyzing the diffusion component of thermoelectric power in macroscopic systems and the phonon-drag component of it. In a recent letter Lei pointed out that thermoelectric power can be conveniently analysed entirely within the framework of balance equation approach. He discussed thermoelectric power of both bulk materials and quantum wells in the presence of carrier heating with a strong applied electric field using balance equations for weakly nonuniform systems. His calculation indicates that hot-electron effects on thermoelectric power may not only change its magnitude, but also may change its sign at higher electric field. His result was confirmed very recently by Xing, Liu, Dong, and Wang using the non-equilibrium statistical operator method of Zubarev jointly with the Lei-Ting balance equation approach. However in assuming that the phonon-drag contribution to thermoelectric power may be neglected in the range of electron temperatures of interest for hot-electron transport, both of their treatments missed this contribution, which is known to be very important in linear transport in both bulk semiconductors and two-dimensional (2D) systems. It is usually so large that the diffusion contribution would not be discernible unless measurements were extended to very high or very low temperatures.

In our opinion this assumption is questionable. The analysis reported here includes the phonon-drag component $S_g$ of thermoelectric power using the balance equation approach, which has the advantage of easy inclusion of hot electron effects. In this, we clarify the importance of the contribution of $S_g$ to thermoelectric power in the hot-electron transport condition. Our consideration are applicable to the regime in which the electron drift velocity is lower than the sound velocities, for materials having high impurity concentrations and/or intermediate electric field strength. In fact, our result shows that contrary to the assumption of Xing et al., $S_g$ is markedly enhanced at low lattice temperature under the indicated conditions. As the calculations of Lei and Xing et al. both show that the hot-electron effect does not change the absolute value of the diffusion component of thermoelectric power very much, it is therefore clearly important to include $S_g$ in the hot-electron transport condition, provided that the lattice temperature is not too high.

This paper is organized as follows. In Sec. II, we present hydrodynamic balance equations with the phonon-drag effect included. In Sec. III, we compare our theoretical prediction of $S_g$ with experiments in the linear transport limit. Finally, in Sec. IV, we discuss hot-electron effects on $S_g$ and present our conclusions.
II. HYDRODYNAMIC BALANCE EQUATIONS INCLUDING PHONON-DRAG

The balance equations for electron transport under the influence of an electric field $E$ and in the presence of a small lattice temperature gradient $\nabla T$, can be written as:

$$\frac{\partial n}{\partial t} + \nabla \cdot (vn) = 0, \quad (1)$$

$$\frac{\partial v}{\partial t} + v \cdot \nabla v = -\frac{2}{3mn} \frac{\nabla u}{m} + \frac{eE}{m} + \frac{f_i + f_{ep}}{mn}, \quad (2)$$

$$\frac{\partial u}{\partial t} + v \cdot \nabla u = -\frac{5}{3} \nabla (\nabla \cdot v) - w - v \cdot (f_i + f_{ep}). \quad (3)$$

In these equations the carrier drift velocity $v$, the electron temperature $T_e$, the average relative electron energy $u$, the carrier density $n$ and the chemical potential $\mu$ are all weakly dependent on spatial coordinates due to the small lattice temperature gradient, so that their spatial gradients are all small. Eqs. (1)-(3) are accurate to the first order in these small quantities (all the second and higher orders of spatial derivatives are neglected). The frictional forces due to impurity scattering $f_i$ and due to phonon scattering $f_{ep}$, and the energy transfer rate from the electron system to the phonon system $w$, are all functions of local quantities $n, v, T_e$ and $T$. $f_i$ has exactly the same expression as in the uniform case. $f_{ep}$ and $w$ can be written as ($\hbar = k_B = 1$)

$$f_{ep} = -4\pi \sum_{kq\lambda} |M(q, \lambda)|^2 q \delta(\varepsilon_{k+q} - \varepsilon_k + \Omega_{q\lambda} - q \cdot v) \times \{n_{q\lambda}[f(\varepsilon_k, T_e) - f(\varepsilon_{k+q}, T_e)] - f(\varepsilon_k, T_e)[1 - f(\varepsilon_{k+q}, T_e)]\}, \quad (4)$$

$$w = 4\pi \sum_{kq\lambda} |M(q, \lambda)|^2 \Omega_{q\lambda} \delta(\varepsilon_{k+q} - \varepsilon_k + \Omega_{q\lambda} - q \cdot v) \times \{n_{q\lambda}[f(\varepsilon_k, T_e) - f(\varepsilon_{k+q}, T_e)] - f(\varepsilon_k, T_e)[1 - f(\varepsilon_{k+q}, T_e)]\}, \quad (5)$$

where $\varepsilon_k = k^2/2m$ is the energy dispersion of an electron for an isotropic parabolic band system, $\Omega_{q\lambda}$ denotes the energy of a phonon of wavevector $q$ and branch $\lambda$, and $f(\varepsilon_k, T_e) = 1/[\exp(\varepsilon_k - \mu)/T_e + 1]$ is the Fermi distribution function at the electron temperature. $n_{q\lambda}$ is the occupation number (distribution function) of phonons in mode $q\lambda$, which is weakly nonequilibrium due to the existence of the small thermal gradient. It is just this gradient that leads to a net flow of phonons in one preferred direction, which then imparts momentum to electrons via electron-phonon scattering. Therefore, in the balance equation approach, the phonon-drag contribution to thermoelectric power is embedded in the nonequilibrium phonon distribution function $n_{q\lambda}$ and thereby in the electron-phonon-scattering frictional force $f_{ep}$, which was previously taken to be the equilibrium Bose distribution function $n(\Omega_{q\lambda}/T_e) = 1/[\exp(\Omega_{q\lambda}/T_e) - 1]$ in Refs. [24] and [1]. $M(q, \lambda)$ stands for the dynamically screened electron-phonon matrix element.\[24\]\[24\] Considering the relation

$$\delta(\varepsilon_{k+q} - \varepsilon_k + \Omega_{q\lambda} - q \cdot v) f(\varepsilon_k, T_e)[1 - f(\varepsilon_{k+q}, T_e)]$$

$$= \delta(\varepsilon_{k+q} - \varepsilon_k + \Omega_{q\lambda} - q \cdot v) [f(\varepsilon_k, T_e) - f(\varepsilon_{k+q}, T_e)] n \left(\frac{\Omega_{q\lambda} - q \cdot v}{T_e}\right), \quad (6)$$

Eqs. (4) and (5) can be rewritten as

$$f_{ep} = -2 \sum_{q\lambda} q|M(q, \lambda)|^2 \Pi_2(q, \Omega_{q\lambda} - q \cdot v)[n_{q\lambda} - n(\Omega_{q\lambda} - q \cdot v)/T_e], \quad (7)$$

$$w = 2 \sum_{q\lambda} \Omega_{q\lambda} |M(q, \lambda)|^2 \Pi_2(q, \Omega_{q\lambda} - q \cdot v)[n_{q\lambda} - n(\Omega_{q\lambda} - q \cdot v)/T_e], \quad (8)$$

in which $\Pi_2(q, \Omega_{q\lambda} - q \cdot v)$ stands for the imaginary part of the density-density correlation function

$$\Pi(q, \omega) = 2 \sum_k \frac{f(\varepsilon_{k+q}, T_e) - f(\varepsilon_k, T_e)}{\varepsilon_{k+q} - \varepsilon_k + \omega + i0^+}. \quad (9)$$

The phonon distribution function $n_{q\lambda}$ for the nonuniform system can be determined as follows. Its total rate of change can be written as
\[
\frac{d}{dt} n_{q\lambda} = \left( \frac{\partial n_{q\lambda}}{\partial t} \right)_d + \left( \frac{\partial n_{q\lambda}}{\partial t} \right)_{ep} + \left( \frac{\partial n_{q\lambda}}{\partial t} \right)_{pp},
\]

where the diffusion term is

\[
\left( \frac{\partial n_{q\lambda}}{\partial t} \right)_d = -v_p(q, \lambda) \cdot \nabla n_{q\lambda}.
\]

To the lowest order in the thermal gradient, the distribution function \( n_{q\lambda} \) on the right hand side of Eq. (11) can be replaced by the equilibrium Bose distribution function:

\[
\left( \frac{\partial n_{q\lambda}}{\partial t} \right)_d = -v_p(q, \lambda) \cdot \nabla n(q, \lambda, \Omega, T). \]

In these equations the dependence of \( n_{q\lambda} \) on spatial coordinate \( r \) has been suppressed and is understood; \( v_p(q, \lambda) \) stands for the group velocity of a phonon in mode \( q, \lambda \), and is given by \( \nabla q \Omega_{q\lambda} \). The second term on the right hand side of (11) is the rate of change of \( n_{q\lambda} \) due to electron-phonon interaction, which describes the absorption and emission of phonons by electrons in transport. It has been proved that this term reads

\[
\left( \frac{\partial n_{q\lambda}}{\partial t} \right)_{ep} = 2|\bar{M}(q, \lambda)|^2 \Pi_2(q, \Omega, \lambda, \Omega_{q\lambda} - q \cdot v)[n_{q\lambda} - n\left( \frac{\Omega_{q\lambda} - q \cdot v}{T_e} \right)].
\]

This effect, together with the diffusion of phonons, tends to drive the phonon system out of equilibrium. On the other hand, there is a trend to drive these nonequilibrium phonons back towards equilibrium, which is described by the last term in Eq. (10):

\[
\left( \frac{\partial n_{q\lambda}}{\partial t} \right)_{pp} = \frac{1}{\tau_p(q, \lambda)}[n_{q\lambda} - n\left( \frac{\Omega_{q\lambda}}{T_e} \right)].
\]

Here \( \tau_p(q, \lambda) \) is a wavevector and mode-dependent relaxation time, which is assumed to be determined by (a) boundary scattering

\[
1/\tau_B = v_s L,
\]

(where \( v_s \) denotes the speed of sound in mode \( \lambda \), and \( L \) is of the order of the macroscopic dimension of the specimen), and by (b) phonon-phonon processes:

\[
1/\tau_{pp}(q, \lambda) = A_\lambda T^3 \Omega_{q\lambda}^2,
\]

whence

\[
1/\tau_p(q, \lambda) = 1/\tau_B + 1/\tau_{pp}(q, \lambda).
\]

In the steady state, the occupation number for each phonon mode is constant, i.e. \( dn_{q\lambda}/dt = 0 \), and Eqs. (10)-(14) lead to

\[
n_{q\lambda} = \frac{\left( \frac{\partial n_{q\lambda}}{\partial t} \right)_d + \frac{1}{\tau_p(q, \lambda)} \left[ n_{q\lambda} - n\left( \frac{\Omega_{q\lambda}}{T_e} \right) \right]}{1 + \frac{1}{\tau(q, \lambda)} n\left( \frac{\Omega_{q\lambda} - q \cdot v}{T_e} \right) + \frac{1}{\tau(q, \lambda) n\left( \frac{\Omega_{q\lambda} - q \cdot v}{T_e} \right)}},
\]

in which we have introduced a phonon-mode dependent and electron-drift-velocity dependent inverse electron-phonon scattering time

\[
\frac{1}{\tau(q, \lambda)} n\left( \frac{\Omega_{q\lambda} - q \cdot v}{T_e} \right) = -2|\bar{M}(q, \lambda)|^2 \Pi_2(q, \Omega, \lambda, \Omega_{q\lambda} - q \cdot v),
\]

and the phonon drift component \( \left( \frac{\partial n_{q\lambda}}{\partial t} \right)_d \) has been replaced by Eq. (12). Substituting the distribution function \( \bar{f} \) into Eqs. (5) and (8), and taking the definition \( \bar{f} \) into account, we have

\[
f_{ep} = f_g + f_p, \quad w = w_p,
\]
where \( f_g \) is the frictional force due to phonon drag; \( f_p \) and \( w_p \) are the frictional force and energy transfer rate due to the phonon absorption and emission. They are defined by

\[
f_g = \sum_{q\lambda} q \left( \frac{\partial n_{q\lambda}}{\partial t} \right)_d \frac{1}{\tau_{1d}^{-1}(q, \lambda)} \left[ n \frac{\Omega_{q\lambda}}{T} - n \frac{\Omega_{q\lambda} - q \cdot v}{T_e} \right],
\]

\[
f_p = \sum_{q\lambda} q \frac{1}{\tau_p(q, \lambda)} \left[ n \frac{\Omega_{q\lambda}}{T} - n \frac{\Omega_{q\lambda} - q \cdot v}{T_e} \right],
\]

\[
w = w_p = - \sum_{q\lambda} \Omega_{q\lambda} \frac{1}{\tau_p(q, \lambda)} \left[ n \frac{\Omega_{q\lambda}}{T} - n \frac{\Omega_{q\lambda} - q \cdot v}{T_e} \right].
\]

We consider a small lattice temperature gradient along the \( x \) direction: \( \nabla T = (\nabla_x T, 0, 0) \). Then, in addition to the drift velocity (current flow) and the applied external electric field along the \( y \) direction, there will be a small drift velocity (current) and a small electric field in the \( x \) direction: \( \mathbf{v} = (v_x, v_y, 0) \) and \( \mathbf{E} = (E_x, E_y, 0) \). Here, \( v_x \) and \( E_x \) are small and the spatial variations of all quantities are assumed to be along the \( x \) direction only. Following the same scheme as Lei\textsuperscript{11} by considering the particle number, force and energy balance equations \((21)-(23)\) to first order in the small quantities, we obtain, in the steady state

\[
\frac{2}{3mn} \nabla_x u + \frac{f_x}{m} + eE_x = 0,
\]

\[
neE_y + f_y = 0,
\]

\[
w + v_y f_y = 0,
\]

which state the force balances in the \( x \) and \( y \) directions, together with the energy balance, respectively, and \( \mathbf{f} = \mathbf{f}_g + \mathbf{f}_p \). For small \( v_x \), \( f_x \) is proportional to it, and \( \rho = -f_x/(ne^2v_x) \) is the resistivity in the \( x \) direction in the presence of drift velocity \( v_y \) in the \( y \) direction. Then Eq. \((24)\) may be rewritten as

\[
j_x = \frac{E_x}{\rho} - \frac{2}{3ne\rho} \nabla_x u + \frac{f_x}{ne\rho}.
\]

Noting that the energy \( u \) and number \( n \) densities are given separately by

\[
u = 2 \sum_k \varepsilon_k f \left( \frac{\varepsilon_k - \mu}{T_e} \right),
\]

\[
n = 2 \sum_k f \left( \frac{\varepsilon_k - \mu}{T_e} \right),
\]

we can rewrite Eq. \((21)\) in the form

\[
j_x = L^{11}(E_x - \nabla_x \mu/e) + L_d^{12}(-\nabla_x T_e) + L_g^{12}(-\nabla_x T),
\]

in which \( L^{11} = 1/\rho \). \( L_d^{12} = \frac{1}{\tau_p \Omega_{12}}(\xi_{12}^{12} - \zeta) \) denotes the coefficient of the electron diffusion contribution to the current with \( \zeta = \mu/T_e \) and \( F_{12}(y) = \int_0^\infty x\nu [\exp(x - y) + 1]^{-1} dx \). \( L_g^{12} \) is the coefficient of the phonon drag contribution which is obtained from Eq. \((21)\) as

\[
L_g^{12} = - \frac{1}{ne\rho} \sum_{q\lambda} \frac{q^2}{\Omega_{q\lambda}} \frac{\tau_{1d}^{-1}(q, \lambda)}{T} \left[ n \frac{\Omega_{q\lambda}}{T} - n \frac{\Omega_{q\lambda} - \omega_0}{T_e} \right],
\]

where we have used the Debye-type spectrum for acoustic phonons: \( \Omega_{q\lambda} = v_{s\lambda} q \) with \( v_{s\lambda} \) being the longitudinal sound speed in \( \lambda \) mode and \( \omega_0 = eE_y/\rho \). The thermoelectric power \( S \) of hot electrons in the presence of a strong current flow in the \( y \) direction is then

\[
S = L_d^{12} \left( \frac{\delta T_e}{\delta T} \right) + L_g^{12} \left( \frac{\delta T_e}{\delta T} \right) = S_d + S_g.
\]

The diffusion component \( S_d \) has already been obtained by Lei\textsuperscript{11} and Xing \textit{et al.}\textsuperscript{12} When there is no current flow in the \( y \) direction \((\delta T_e/\delta T = 1)\), it matches the result obtained from the Boltzmann equation with a constant relaxation time assumption in Ref. 3. Furthermore,
\begin{equation}
S_g = -\frac{1}{2e} \sum_{q,\lambda} \frac{q^2 \Omega_q^2}{T^2} \left[ \frac{1}{1 + \tau(q\lambda,\Omega_q\lambda - \omega)} \right] \frac{\Omega_q\lambda}{T} \tag{32}
\end{equation}

is the phonon-drag component of thermoelectric power. Thus, Eqs. (31)-(32) yield the thermoelectric power directly.

The hydrodynamic balance equations (11)-(13) for weakly nonuniform systems are also applicable to 2D systems (quasi-2D electrons coupled to bulk phonons) if the prefactor $\frac{2}{3}$ in Eq. (11) and $\frac{2}{3}$ in Eq. (13) are replaced by unity and 2, respectively. Moreover $|M(q,\lambda)|^2$ in Eqs. (11) and (13) is replaced by $|I(q,\lambda)|^2|I(qz)|^2$. Here, $I(qz)$ stands for a form factor associated with confinement of the sample in the $z$ direction. Specifically, for a quantum-well structure it reads

\begin{equation}
|I(qz)|^2 = \pi^4 \sin^2 y/\left[ y^2(y^2 - \pi^2)^2 \right] \tag{33}
\end{equation}

with $y \equiv q_z a/2$ and $a$ is the width of the quantum well. Thus, the diffusion component of thermoelectric power $S_d$ for a 2D system takes the form

\begin{equation}
S_d = \frac{1}{e} \left[ \frac{2F_1(\zeta)}{F_0(\zeta)} - \zeta \right] \frac{\delta T_c}{\delta T}. \tag{34}
\end{equation}

The phonon-drag component $S_g$ shares the same expression as that of Eq. (32). We may put this equation in a more symmetrical form when there is no current flow in $y$ direction, and correspondingly $\omega_0 = 0$:

\begin{equation}
S_g = -\frac{1}{2e} \sum_{q,\lambda} \frac{q^2 \Omega_q^2}{T^2} \left[ \frac{1}{1 + \tau(q\lambda,\Omega_q\lambda)} \right] \frac{\Omega_q\lambda}{T}, \tag{35}
\end{equation}

with $q = (q_x, q_z) = (q_x, q_y, q_z)$. This equation can be shown to be equivalent to that derived from the Boltzmann equation by Cantrell and Butcher if “1” in the denominator of Eq. (35) is omitted. This correspondence arises because Cantrell and Butcher use an approximation (ie, see Eq. (41) in the first paper of Ref. 7) which is analogous to neglecting the electron-phonon scattering time $1/\tau(q\lambda,\Omega_q\lambda - q \cdot v)$ in our formula (35). If we eliminate this approximation in their derivation, then their final result may be proved to be equivalent to Eq. (33). In our opinion, this approximation is valid only at low temperature. If temperature is high, this approximation yields a result that is too large.

III. COMPARISON WITH EXPERIMENTS IN THE LINEAR TRANSPORT LIMIT

In this section we apply the present theory to GaAs/GaAlAs quantum wells. Both longitudinal and transverse acoustic phonon modes are coupled to electrons via deformation potential and piezoelectric interactions. Only the longitudinal mode gives rise to deformation potential coupling, whereas both longitudinal and (two branches of) transverse modes contribute to piezoelectric interaction. Their matrix elements are given in Ref. 21. The GaAs/GaAlAs material parameters used in our calculations are as follows: volume density $d = 5.31$ g/cm$^3$, effective mass $m = 0.07 m_e$, transverse sound velocity $v_{sT} = 2.48 \times 10^3$ m/s, longitudinal sound velocity $v_{sl} = 5.29 \times 10^3$ m/s, acoustic deformation potential $\Xi = 8.5$ eV, piezoelectric constant $e_{14} = 1.41 \times 10^9$ V/m and low-frequency dielectric constant $\kappa = 12.9$. We note that some of the values of these parameters are still uncertain (eq. in the literature the values for $\Xi$ range from 7 to 16 eV). Nevertheless the above listed values have been used frequently in balance-equation theory in a variety of transport problems and the results obtained are in good agreement with experiments. The coefficients $A_\lambda$ in Eq. (14) can be obtained by fitting to experimental data, and a particular choice will be identified below.

In Fig. 1 we first fit Eqs. (31), (34) and (33) to the experimental data of Sample 1 of Fletcher et al. The electron sheet density is $N = 1.78 \times 10^{11}$ m$^{-2}$, and the length between the contacts used to determine the thermoelectric power is $L = 0.98$ mm. As there is no external electric field in the experiment, $\delta T_c/\delta T = 1$, $\omega_0 = 0$ and $T_c = T$. In our fitting we take $A_1 = 1.68 \times 10^{-21}$ s K$^{-3}$ for longitudinal phonons and $A_4 = 4.36 \times 10^{-22}$ s K$^{-3}$ for transverse modes in Eq. (14). For comparison purposes, the thermoelectric power components due to deformation potential coupling $S_{gT}$, those due to longitudinal piezoelectric interaction $S_{gP}$ and those due to transverse piezoelectric interaction $S_{gPT}$ are also plotted in the same figure. We then apply the same parameters to the calculation of $S$ for the other two samples of Fletcher et al. The plot of $S$ vs. $T$ in Fig. 2 is for electron sheet density $N = 4.8 \times 10^{15}$ m$^{-2}$, with length between the contacts $L = 0.63$ mm, and in Fig. 3 it is for $N = 6.82 \times 10^{15}$ m$^{-2}$, with $L = 2.98$ mm. The widths of the quantum wells in Figs. 1-3 are all 100 Å. From the figures we can see that our theory is in good qualitative agreement with the experimental data. Furthermore, our results in Fig. 1-3 show that, at low
temperature, the two branches of transverse phonons dominate the drag effect through piezoelectric interaction with electrons, whereas the longitudinal phonons contribute to $S_g$ mainly through the deformation potential coupling. It is also seen that the phonon-drag component dominates thermoelectric power in the experiments.

We also apply our theory to a very recent experiment\cite{FletcherPRB10} where the electron density is $N = 3.6 \times 10^{16}$ m$^{-2}$, which is of an order of magnitude larger than that of the previous samples. The width of the quantum well is $a = 100$ Å and $L = 2.5$ mm, as determined in Ref. \cite{FletcherPRB10} using experimental data for thermal conductivity. We use the same material parameters and coefficients $A_l$ as in the previous cases. Figure 4 exhibits a comparison of the experimental data with our theoretical results\cite{FletcherPRB10}. Again the theory fits well qualitatively with experiment. However, this time the theoretical prediction is smaller than the experimental data even at low temperature.

This experiment has also been explained by Fletcher et al. in the same paper\cite{FletcherPRB10} using a formula derived from the Boltzmann equation by Cantrell and Butcher. The material parameters they used are chosen to fit the experimental data at low temperature. However these parameters fail to fit the earlier experimental results shown in Figs. 1-3 at low temperature. In the calculation of Fletcher et al.,\cite{FletcherPRB10} the relaxation time of phonons is treated as a constant and is determined from the thermal conductivity measured in their experiment. Even though the temperature in the experiment ranges from low temperature to very high values, they continue to adopt the approximation of Cantrell and Butcher\cite{FletcherPRB10} throughout, whereas we believe it to be valid only at low temperature. In Fig. 5 we compare our theory with that of Fletcher et al., wherein the chain curve is calculated from our theory and the dotted curve is the theoretical prediction of Fletcher et al.\cite{FletcherPRB10}. It is seen that the peaks predicted by the two theories occur at almost the same temperature. Nevertheless, the approximation used by Fletcher et al.\cite{FletcherPRB10} yields the height of the peak of their theory to be larger than it should be, because this approximation fails at high temperatures. This may be understood from the fact that if we include the same approximation in our formula (ie. omitting “1” in the denominator of Eq. (32)), the result obtained (ie. solid curve) predicts the same peak height found by Fletcher et al.\cite{FletcherPRB10}.

IV. HOT-ELECTRON EFFECTS ON THE PHONON-DRAG COMPONENT $S_G$ AND CONCLUSIONS

This theory may be easily used to calculate thermoelectric power in the presence of a strong external electric field. In fact, although the diffusion component $S_d$ may be negative within a small low-lattice-temperature range at higher electric field\cite{XingPRB9}, the phonon-drag component $S_g$ is still positive. Moreover, it should be even more important to include the phonon-drag contribution to thermoelectric power in the hot-electron transport regime. Actually, $S_g$ is markedly enhanced at low lattice temperature as shown in Fig. 6, for the sample $N = 1.78 \times 10^{15}$ m$^{-2}$ and in Fig. 7 for the much higher electron density sample $N = 3.6 \times 10^{16}$ m$^{-2}$. Our calculated results shown in Fig. 6 and 7 assume high impurity density, such that the electron drift velocity in hot electron transport is smaller than the sound velocities (ie. we discard $\omega_b$ in Eq. (32)). In Fig. 6, $S_g$ is plotted against lattice temperature $T$ as a solid curve for hot-electron temperature $T_e = T + 200$ K, as a dashed curve for $T_e = T + 100$ K and as a chain curve for $T_e = T + 10$ K, with all the other material parameters being the same as those used in Fig. 1. For comparison, $S_g$ in the linear transport limit is also plotted in the same figure (Fig. 6) as a dotted curve, with part of it obtained in Fig. 1. From the figure one can see that $S_g$ is markedly enhanced by hot-electron effects in the low lattice-temperature regime (LLTR) with $T < 20$ K. However, in the high lattice-temperature regime (HLTR) with $T > 20$ K, $S_g$ is slowly reduced as $T_e$ increases. Another feature to be noted is that for $T < 6$ K and $T > 10$ K, $S_g$, for $T_e = T + 200$ K (solid curve), is a bit smaller than it is for $T_e = T + 100$ K (dashed one). These properties can be well understood from the inset of Fig. 6, where $S_g$ is plotted as a function of $\Delta T = T_e - T$ for two fixed typical lattice temperatures $T = 4$ and 40 K of the two regimes. It is seen that in LLTR, the hot-electron effect first increases $S_g$ very rapidly as $T_e$ rises from $T$ to about several hundred degrees Kelvin (104 K in the inset for $T = 4$ K) and then gradually reduces it if $T_e$ goes on increasing. Nevertheless, even though $T_e$ is as high as 1004 K as shown in the inset of Fig. 6, $S_g$ is still so large at low lattice temperature that it can not be neglected as suggested by Xing et al.\cite{XingPRB9} However in HLTR, $S_g$ decreases slowly as $T_e$ increases. The results for $S_g$ in regard to hot electron effects are somewhat different at higher density for the sample of Fig. 7 with $N = 3.6 \times 10^{16}$ m$^{-2}$. In this case, $S_g$ is plotted versus $T$ as a solid curve for $T_e = T + 100$ K and as a dashed one for $T_e = T + 10$ K, with all the other material parameters being the same as those used in Fig. 4. For comparison we also plot $S_g$ in the linear transport condition as a dotted curve in the same figure, which has been obtained in Fig. 4. Again $S_g$ is markedly enhanced in HLTR for $T < 10$ K. However, for $T_e = T + 100$ K (solid curve), $S_g$ is now very close to the plot for $T_e = T + 10$ K (dashed curve) in LLTR and $S_g$ seems to be almost unchanged in HLTR. This is further illustrated in the inset of Fig. 7, where $S_g$ is plotted as a function of $\Delta T = T_e - T$ for three fixed lattice temperatures $T = 3, 6$, and 15 K. It is seen that $S_g$ increases to “saturation” steeply in LLTR as $T_e$ increases and then rises very slowly as electron temperature goes up to several hundred degrees Kelvin. As $T_e$ further increases, $S_g$ begins to decrease slowly. Notwithstanding the fact that $T_e$ is as high as $T + 1000$ K and $S_g$ is slowly decreasing, the absolute value of $S_g$ is still much higher than that in the linear-transport limit ($\Delta T = 0$). In
HLTR, $S_g$ is almost unchanged as $T_e$ rises to several hundred degrees Kelvin before it begins to decrease. These new features result from the high density of the electron gas.

It is well known that the phonon-drag component of thermoelectric power is very important in the linear transport limit and is usually so large that the diffusion contribution would not be discernible unless measurements were extended to very high or very low temperatures. Both the theoretical calculations of Lei and Xing et al. show that the hot-electron effect does not change the absolute value of the diffusion component of thermoelectric power significantly. However, our results show that it is necessary to include the phonon-drag component $S_g$ under hot-electron transport conditions, provided that the lattice temperature is not too high, and the electron drift velocity is smaller than the sound velocities, to accurately calculate the thermoelectric power.

In summary, we have determined the role of phonon-drag in thermoelectric power under hot electron transport conditions using balance equation theory for weakly nonuniform systems. Having introduced wavevector- and phonon-mode-dependent relaxation times due to phonon-phonon interactions, the formula obtained can be used not only at low lattice temperature (where the phonon relaxation time is determined by boundary scattering), but also at high temperatures where phonon-phonon scatterings are dominant in determining the phonon relaxation time. Our results compare well with experimental data in the linear transport limit for a wide range of electron densities and are in good correspondence with the earlier theoretical predictions of the Boltzmann equation, appropriately modified. The role of hot-electron effects on the phonon-drag contribution to thermoelectric power has been clarified, and the importance of the contribution of $S_g$ to thermoelectric power under hot-electron transport conditions was stressed. In fact, the sign of the total thermoelectric power $S$ in the presence of a sufficiently strong external electric field depends on competition between the negative $S_d$ and positive $S_g$ values for high impurity-density materials. For such materials, at least for the low lattice temperatures, the negative $S_d$ value may be entirely counteracted by $S_g$, so that the total thermoelectric power remains positive.

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FIG. 1. Variation of thermoelectric power $S$ as a function of temperature $T$. The black dots are the experimental data of Sample 1 in Ref. 6. The solid curve is the theoretical result obtained from Eqs. (31), (35) and (34) with $A_{\lambda}$ in Eq. (16) chosen to fit the experiment. The components due to transverse piezoelectric coupling $S_{gpt}$ (short-dashed curve), longitudinal deformation potential coupling $S_{gl}$ (dotted curve) and longitudinal piezoelectric interaction $S_{gpl}$ (long-dashed curve), together with the diffusion component $S_d$ (chain line), are plotted in the same figure. The parameters we employ are listed in the text.

FIG. 2. Thermoelectric power $S$ vs. temperature $T$. The black dots are the experimental data of Sample 2 in Ref. 6. The solid curve is our theoretical prediction using the same values of $A_{\lambda}$ in the calculation as those obtained from Fig. 1. The components of $S$ are represented by the other curves in the same way as in Fig. 1.

FIG. 3. Thermoelectric power $S$ is plotted as a function of temperature $T$. The black dots refer to the experimental data of Sample 3 in Ref. 6. The other curves represent components of $S$ as in Fig. 1.

FIG. 4. Comparison of thermoelectric power as given by the theoretical prediction with experimental data. The open circles are the recent experimental data of Fletcher et al. 10. The curves represent $S$ and its components as in Fig. 1.

FIG. 5. Comparison of the Boltzmann equation predictions of Fletcher et al. 10 (with the approximation explained in the text) with our balance equation predictions for $S$. In the figure the chain curve is the theoretical prediction of our balance equation formulation; the solid curve is obtained from our formulas (31), (33) and (34), however, with the approximation of Cantrell and Butcher 7 installed as explained in the text, following Fletcher et al.; and the dotted curve is taken from Ref. 10 as the theoretical prediction of Fletcher et al.

FIG. 6. Phonon-drag component $S_g$ vs. lattice temperature $T$ for the sample $N = 1.78 \times 10^{15}$ m$^{-2}$. Solid curve: in the hot-electron transport condition $T_e = T + 200$ K; dashed curve: $T_e = T + 100$ K; chain curve: $T_e = T + 10$ K; and dotted curve: in the linear transport limit. Inset: $S_g$ is plotted as a function of $\Delta T = T_e - T$ for two fixed lattice temperatures $T = 4$ K and 40 K. The material parameters are the same as those used in Fig. 1, as described in the text.

FIG. 7. Phonon-drag component $S_g$ vs. lattice temperature $T$ for the sample $N = 3.6 \times 10^{16}$ m$^{-2}$. Solid curve: in the hot-electron transport condition $T_e = T + 100$ K; dashed curve: $T_e = T + 10$ K; and dotted curve: in the linear transport limit. Inset: $S_g$ is plotted as a function of $\Delta T = T_e - T$ for three fixed lattice temperatures $T = 3$ K, 6 K, and 15 K. The material parameters are the same as those used in Fig. 4 as described in the text.