ELSEVIER

Physica B 316–317 (2002) 276–278

PHYSICA B

www.elsevier.com/locate/physb

Phonon drag in disordered films and structures

A. Sergeev*, V. Mitin

Department of ECE, Wayne State University, Detroit, MI 48202, USA

Abstract

Employing the quantum transport equation, we investigate the effect of electronic disorder on the phonon-drag thermopower. We consider the electron–phonon interaction via the deformation potential, which is strongly renormalized due to elastic electron scattering. The scattering potential of impurities, boundaries and defects is modeled by quasistatic scatterers and vibrating scatterers, which move in the same way as host atoms. In thin films, micro and nanostructures of the phonons relax mainly in a substrate, and the phonon-drag thermopower substantially depends on the character of electron scatterers. Vibrating scatterers decrease thermopower, while quasistatic scatterers (e.g. rigid boundaries) increase it. These changes in thermopower correlate to the disorder-induced modification of the electron–phonon relaxation rate.

PACS: 72.10.Di; 72.15.Jf

Keywords: Phonon-drag thermopower; Disorder

The electron–phonon interaction is strongly modified in disordered conductors. If impurities and boundaries vibrate in the same way as the host lattice, the electron–phonon relaxation rate is decreased by a factor of $q_T l$ ($q_T l \ll 1$, $q_T = T/u$ is the wave vector of a thermal phonon, u is the sound velocity, and l is the electron mean free path) compared with the rate in a pure bulk material [1,2]. On the contrary, in the presence of a quasistatic scattering potential the relaxation rate is enhanced by the same factor [3,4].

The effects of elastic electron scattering on the phonon-drag thermopower are studied in the current work. In the pure case ($q_T l \gg 1$), the thermoelectric coefficient ($\eta = -J_e/\nabla T$) is given by [5]

$$\eta_0 = -\frac{b_n}{3\pi}\frac{e\beta\tau\tau_{ph}(T)T^4}{p_F u^2}, \tag{1}$$

where τ is the electron momentum relaxation time, τ_{ph} is the lifetime of a thermal phonon with frequency $\omega_q = T$, β is the dimensionless electron–phonon coupling constant, p_F is the Fermi momentum, n the exponent in the frequency dependence of the phonon relaxation rate ($\tau_{ph}^{-1} \propto \omega_q^n$), and b_n is the numeric coefficient,

$$b_n = \int_0^\infty \mathrm{d}x\, x^{5-n}\frac{\partial N(x)}{\partial x}, \tag{2}$$

where $N(x) = (\exp(x) - 1)^{-1}$. In a degenerate conductor, the electron–phonon coupling constant is given by

$$\beta = \left(\frac{2\varepsilon_F}{3}\right)^2 \frac{v}{2\rho u^2}, \tag{3}$$

*Corresponding author. Tel.: +1-313-577-5507; fax: +1-313-5 77-1101.

E-mail address: sergeev@ciao.eng.wayne.edu (A. Sergeev).

0921-4526/02/$ - see front matter
PII: S0921-4526(02)00484-2

where ε_F is the Fermi energy, ν is the electron density of states, and ρ is the density.

To investigate effects of elastic electron scattering on the phonon-drag thermopower we use the following methods. First, we employ the quantum transport equation based on the Keldysh diagram technique [2,3]. This approach deals only with electron self-energy diagrams, while the Kubo method requires more complicated diagrams to be considered. Second, we calculate the electric current of electrons as a response to the temperature gradient in the phonon subsystems. The symmetric problem of the phonon thermal flux due to the electric field turns out to be significantly more difficult, because one should take into account specific terms in the form of Poisson brackets. According to the Onsager relation, both approaches give the same result for the thermoelectric coefficient. Third, in considering the vibrating potential, we employ the Tsuneto transformation [1], which allows one to simplify the electron–phonon-impurity Hamiltonian.

In the presence of the temperature gradient in the phonon subsystem, the phonon distribution function is given by

$$F(\mathbf{q},\omega) = F_0(\omega) + F_1(\mathbf{q},\omega), \tag{4}$$

$$F_0(\omega) = 2N_\omega + 1 = \coth(\omega/2T), \tag{5}$$

$$F_1(\mathbf{q},\omega) = \frac{\omega}{T}\frac{\partial(2N_\omega+1)}{\partial\omega}\tau_{ph}\mathbf{u}\nabla T, \tag{6}$$

where τ_{ph} is the phonon momentum relaxation time.

The nonequilibrium electron distribution function $\phi(\mathbf{p},\varepsilon)$ is determined from the transport equation. Assuming that the elastic electron scattering from impurities, boundaries and defects dominates in the electron momentum relaxation, one can linearize the transport equation in the following way:

$$I_{e-imp}[\phi] + I_{e-ph}[S_0, F_1] = 0, \tag{7}$$

where I_{e-imp} and I_{e-ph} are the collision integrals which correspond to the electron–impurity and the electron–phonon interactions, and S_0 is the equilibrium electron distribution function. Thus, the correction $\phi(\mathbf{p},\varepsilon)$ is given by

$$\phi(\mathbf{p},\varepsilon) = \tau I_{e-ph}[S_0, F_1], \tag{8}$$

where the electron–phonon collision integral takes into account all processes of electron–phonon scattering in a disordered conductor. The collision integral is expressed through the electron self-energies as [2,3]

$$I_{e-ph} = -i[\Sigma^C - S(\Sigma^A - \Sigma^R)]. \tag{9}$$

The nonequilibrium corrections in the form of the Poisson bracket are absent, because we consider the response to the temperature gradient in the phonon subsystem.

Considering effects of quasistatic scatterers, we take into account renormalization of the electron–phonon vertex by elastic electron scattering [2–4]. Employing the Keldysh technique, we calculate the nonequilibrium electron distribution function (Eq. (8)), which is used to find the electric current. Calculations show that the thermoelectric coefficient in the disordered conductor with quasistatic scatterers is given by

$$\eta_{st} = \frac{e\beta_l\tau}{6\pi p_F u^2 T}\int d\omega_q \omega_q^5 \frac{\partial N(\omega_q)}{\partial\omega_q} \times \tau_{ph}(\omega_q) W_{st}(ql), \tag{10}$$

where

$$W_{st}(x) = \frac{2}{\pi}\frac{(x^2-1)\arctan(x)+x}{x(x-\arctan(x))}. \tag{11}$$

In the limiting cases, this function is given by

$$W_{st} = \begin{cases} 1+\pi/(2x), & x \gg 1, \\ 8/(\pi x), & x \ll 1. \end{cases} \tag{12}$$

Therefore, in the pure limit, $q_T l \gg 1$, the correction to the thermoelectric coefficient due to elastic electron scattering is

$$\frac{\eta_{st}-\eta_0}{\eta_0} = \frac{\pi}{2}\frac{b_{n-1}}{b_n}\frac{u}{Tl}, \tag{13}$$

where numeric coefficients b_n are given in Eq. (2).

In the impure limit, $q_T l \ll 1$, the thermoelectric coefficient is given by

$$\frac{\eta_{st}}{\eta_0} = \frac{8}{\pi}\frac{b_{n-1}}{b_n}\frac{u}{Tl}. \tag{14}$$

Considering the vibrating potential, it is convenient to treat the electron–phonon interaction in

the frame of reference which moves locally with the lattice [1]. After this transformation, electron scatterers are motionless. Taking into account renormalization of the electron–phonon vertex, we calculate the electron distribution function and electric current. Finally, the thermoelectric coefficient in the conductor with vibrating electron scatterers is given by

$$\eta_{\rm vb} = \frac{e\beta\tau}{6\pi p_{\rm F} u^2 T} \int {\rm d}\omega_q \omega_q^5 \frac{\partial N(\omega_q)}{\partial \omega_q} \times \tau_{\rm ph}(\omega_q) W_{\rm vb}(ql), \quad (15)$$

where

$$W_{\rm vb}(x) = 2[(-5x^6 - 11x^4 + 39x^2 + 15) \times (\arctan(x))^2 + (5x^7 + 17x^5 - 78x^3 - 90x) \times \arctan(x) - 11x^6 + 39x^4 + 45x^2]/[\pi x^3(1+x^2) \times (x - \arctan(x))^2]. \quad (16)$$

In the limiting cases, this function is given by

$$W_{\rm vb} = \begin{cases} 1 + (\pi/2 - 32/(5\pi))/x, & x \gg 1, \\ 104x/(\pi 175), & x \ll 1. \end{cases} \quad (17)$$

In the pure limit, $q_T l \gg 1$, the correction to the thermoelectric coefficient due to elastic electron scattering is

$$\frac{\eta_{\rm vb} - \eta_0}{\eta_0} = \left(\frac{\pi}{2} - \frac{32}{5\pi}\right) \frac{b_{n-1}}{b_n} \frac{u}{Tl}, \quad (18)$$

where numeric coefficients b_n are given in Eq. (2). For $n = 0$, the ratio b_{-1}/b_0 is 5.89.

In the impure limit, $q_T l \ll 1$, the thermoelectric coefficient is

$$\frac{\eta_{\rm vb}}{\eta_0^g} = \frac{104}{175\pi} \frac{b_{n+1}}{b_n} \frac{Tl}{u}. \quad (19)$$

Thus, we have shown that the phonon-drag thermopower in thin films, micro- and nanostructures is strongly affected by elastic electron scattering from boundaries, impurities and defects. The vibrating electron scattering potential substantially decreases thermopower. In the impure limit, $q_T l \ll 1$, the thermoelectric coefficient is of the order of $(Tl/u)\eta_0$ (Eq. (19)). On the contrary, static scatterers, such as rigid boundaries, increase thermopower by a factor of $u/(Tl)$ (Eq. (14)). Such modification correlates to the effect of elastic electron scattering on the electron–phonon relaxation [1–4].

While our results are not directly applicable to the electron–phonon interaction via the piezoelectric potential, we may evaluate disorder-induced modification of thermopower in the following way. According to Ref. [6] the renormalization of the piezoelectric vertex by elastic electron scattering is exactly the same as the renormalization of the electron–phonon vertex by static scatterers. Diffusion enhancement of the piezoelectric interaction increases the energy loss rate by the factor $u/(Tl)$ [6]. Our results show that in the presence of static scatterers the phonon-drag thermopower is also increased by the same factor. Thus, correlated disorder-induced changes in the energy loss and in thermopower are also expected for the piezoelectric potential. Very recently, the effect of elastic scattering on the energy loss rate has been observed in gated GaAS/$Ga_{1-x}Al_x$ δ-doped quantum wells [7]. It would be interesting to investigate the phonon-drag thermopower in these structures.

The research was supported by NASA and NSF grants.

References

[1] A. Schmid, Z. Physik 259 (1973) 421.
[2] M.Yu. Reizer, A.V. Sergeev, Zh. Eksp. Teor. Fiz. 90 (1986) 1056 [Sov. Phys. JETP 63 (1986) 616].
[3] B.L. Altshuler, Zh. Eksp. Teor. Fiz. 90 (1978) 1330 [Sov. Phys. JETP 48 (1978) 670].
[4] A. Sergeev, V. Mitin, Phys. Rev. B 61 (2000) 6041.
[5] F.J. Blatt, P.A. Schroeder, C.L. Foiles, D. Greig, Thermoelectric Power of Metals, Plenum Press, New York, London, 1976.
[6] D.V. Khveshchenko, M.Y. Reizer, Phys. Rev. Lett. 78 (1997) 3531.
[7] R. Fletcher, Y. Feng, C.T. Foxon, J.J. Harris, Phys. Rev. B 61 (2000) 2028.