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LETTER TO THE EDITOR

Influence of Umklapp processes on the sign of phonon-drag thermopower in semiconductor superlattices

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Abstract. The phonon-drag thermopower, S_{gp}, is calculated for semiconductor superlattices, with the temperature gradient parallel to the superlattice axis, taking account of electron–phonon Umklapp processes. S_{gp} changes sign when the Fermi energy reaches the top of the miniband. The anomalous behaviour is attributed to the inclusion of U-processes.

With the remarkable advances in semiconductor technology it has become possible to fabricate nearly perfect superlattices (SLs) consisting of alternating semiconductor layers having different band gaps. From the electronic structure point of view this can be thought of as a sequence of quantum wells separated by energy barriers. With sufficiently thin barrier layers, the wave functions of carriers in the neighbouring wells overlap significantly and energy levels broaden into minibands with extended Bloch-type states. The additional long-range order of the SL results in the reduced Brillouin zone scheme of minibands separated in energy by miniband gaps. The minibands are expected to lead to the transport of carriers parallel to the SL growth axis (Bloch transport). With steady improvement in the quality of SLs, investigation of transport along the SL axis is becoming increasingly important. Very recently, by measuring the subpicosecond time-resolved luminescence spectra in GaAs–AlGaS SL, Deveaud *et al* [1] have shown, unequivocally, that the electron and hole transport along the SL axis is through extended, Bloch-type states.

The thermopower (S), which gives valuable information about electron transport processes in metals and semiconductors, is an interesting property for study in semiconductor SLs. In recent years, although there exists, in literature, lots of experimental and theoretical work on thermopower in GaAs/GaAlAs heterojunctions, very little attention has been given to its study in SLs. Calculations of the diffusion contribution to thermopower (S_d) in SLs exist in the literature [2, 3]. However, in view of the experimental [4–6] and theoretical [7–9] evidence for dominance of the phonon-drag condition, S_g, at low temperatures, in heterostructures, it is of interest and importance to study S_g in SLs.

The thermopower in SLs depends on whether the temperature gradient is parallel or perpendicular to the SL axis. In this letter we present calculations of the phonon-drag thermopower S_{gp}, in the interesting case where the temperature gradient is parallel to the SL axis. More importantly, we include the contributions from the electron–phonon

Umklapp (U) processes also. In this context it may be observed that, in metals, whether the net thermopower is positive or negative depends on the relative probabilities of U to N (normal) processes as well as on the Fermi surface and its proximity to the Brillouin zone boundaries [10, 11]. Physically, a Bragg reflection is involved in an electron–phonon U-process. The associated large change of momentum involved may lead to reversal in the electron velocity, with the result that, rather than movement towards the cold end of the conductor, the movement is towards the hot end, thus contributing to a positive phonon-drag thermopower. In SLs we show that the effect of inclusion of U-processes is to suppress the magnitude of S_{gp} and to change its sign from negative to positive when the Fermi energy reaches the top of the miniband.

We describe the SL in a tight-binding approximation and consider the case for which only the lowest miniband is populated. In the limit of weakly interacting quantum wells the total wave function can be written as

$$\Psi_K(\boldsymbol{r}, z) = A^{-1/2} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r})\Phi(k_z, z) \tag{1}$$

where $\boldsymbol{K} = (\boldsymbol{k}, k_z)$ is the total wave vector, and $\boldsymbol{r}$ and $\boldsymbol{k}$ denote the position and wave vector of the electron in the (x, y) plane, respectively. A is the area of the SL in the (x, y) plane. The part of the wave function in the z-direction is

$$\Phi(k_z, z) = N^{-1/2} \sum_j \varphi(z - jl) \exp(\mathrm{i}jlk_z) \qquad j = 0, \pm 1, \pm 2, \ldots \tag{2}$$

with $\varphi(z - jl)$ describing the solution for the jth well. It is normalized over N periods along the z-axis with periodicity $l = 2(a + b)$, where $2a$ is the well width and $2b$ the width of the barrier. The energy eigenvalues corresponding to (1), in the effective-mass approximation, can be expressed in the form

$$E_k = E(\boldsymbol{k}) + E(k_z) = \hbar^2 k^2/2m^* + E(k_z) \tag{3}$$

where m^* is the effective mass of the electron. The energy dispersion along the z-direction, $E(k_z)$, in the tight-binding approximation, can be described by a sinusoidal form:

$$E(k_z) = t(1 - \cos(k_z l)) \tag{4}$$

with band width $2t$.

Phonon-drag thermopower arises due to drag of electrons by the phonon flux due to electron–phonon interaction. In the following, to calculate S_{gp} in SLs, we assume the electrons to interact with 3D phonons via a screened deformation potential and piezoelectric coupling. Cantrell and Butcher [7] have solved the linearized electron and phonon Boltzmann equations, in the relaxation-time approximation, to obtain an expression for the phonon-drag contribution to the thermopower in heterojunctions. Their equation (42) in [7] can be modified to obtain the expression for the phonon-drag thermopower contribution in a SL when the temperature gradient is along the SL axis:

$$S_{gp} = \frac{2|e|}{V\sigma_p k_B T^2} \sum_{K,K',Q} \hbar\omega_Q f(E_K)(1 - f(E_{K'}))P_Q^a(\boldsymbol{K}, \boldsymbol{K}')\tau(\boldsymbol{Q})F_P(\boldsymbol{K}, \boldsymbol{K}') \tag{5}$$

where σ is the electrical conductivity, V is the volume of the SL, $f(E_K)$ is the Fermi–Dirac distribution function at temperature T with the Fermi energy E_F, $P_Q^a(\boldsymbol{K}, \boldsymbol{K}')$ is the transition probability for scattering of electrons from state $\boldsymbol{K}$ to $\boldsymbol{K}'$ with absorption of a phonon with wavevector $\boldsymbol{Q}$ and energy $\hbar\omega_Q$, and $\tau(\boldsymbol{Q})$ is the phonon relaxation time.

The subscript p is to indicate that the quantities in the equation refer to the direction of the SL axis. The factor $F_p(\boldsymbol{K}, \boldsymbol{K}')$ is

$$F_p(\boldsymbol{K}, \boldsymbol{K}') = (\nabla\omega_Q)_p(\tau_p(E_K)V_p(\boldsymbol{K}) - \tau_p(E_{K'})V_p(\boldsymbol{K}')) \tag{6}$$

where $V_p(\boldsymbol{K})$ is the electron velocity and $\tau_p(E_K)$ is the relaxation time for electrons.

The transition probability is given by

$$P_Q^a(\boldsymbol{K}, \boldsymbol{K}') = (2\pi/\hbar)N_Q|V(\boldsymbol{Q})|^2\Delta(q_z)\delta_{k',k+q}\delta(E_{K'} - E_K - \hbar\omega_Q) \tag{7}$$

where N_Q is the Bose distribution function at T and $|V(\boldsymbol{Q})|^2$ is the square of the matrix element for electron–phonon interaction. The overlap integral $\Delta(q_z)$ including the U-processes due to the periodicity of the SL in the z-direction is

$$\Delta(q_z) = \left|\int_{N\text{periods}} \Phi^*(k_z', z)\Phi(k_z, z)\,\mathrm{e}^{\mathrm{i}q_z z}\,\mathrm{d}z\right|^2$$

$$= \sum_{I=-\infty}^{\infty} \delta_{k_z', k_z+q_z-G}\left|\int \varphi^*(z)\varphi(z)\,\mathrm{e}^{\mathrm{i}q_z z}\,\mathrm{d}z\right|^2. \tag{8}$$

Here $G = I(2\pi/l)$ is the reciprocal-lattice vector along the z-axis. I takes integral values.

To evaluate (5) we proceed as follows. At low temperatures $\hbar\omega_Q \ll E_K$, we write

$$f(E_K)(1 - f(E_K + \hbar\omega_Q)) = \hbar\omega_Q\delta(E_K - E_F)/(1 - \exp(-\hbar\omega_Q/k_B T)). \tag{9}$$

With this, energy integration becomes simple. With regard to the electron relaxation time we suppose that $\tau_p(E_K)$ is constant over an energy range of the order of $\hbar\omega_Q$. Then (6) reduces to

$$F_p(\boldsymbol{K}, \boldsymbol{K}') = -v(q_z/|\boldsymbol{Q}|)\tau_p(E_K)\hbar^{-1}(\nabla_{k_z'}E_{K'} - \nabla_{k_z}\mathrm{E}_K) \tag{10}$$

where v is the phonon group velocity. To proceed further, we assume that the phonon relaxation time is dominated by the boundary scattering, so that $\tau(\boldsymbol{Q})$ can be written as $\tau(\boldsymbol{Q}) = L/v$, where L is the phonon mean free path. Summation over $\boldsymbol{Q}$ is carried out by replacing $\boldsymbol{q}$ by $\boldsymbol{k}' - \boldsymbol{k}$ and q_z by $k_z' - k_z + G$.

Concerning the integration over k_z, there are two cases. The limiting values are

$$k_z d = \begin{cases} \pm\cos^{-1}(1 - E_F/t) & \text{for } E_F \leqslant 2t \\ \pm\pi & \text{for } E_F > 2t. \end{cases} \tag{11}$$

Explicit forms for $|V(\boldsymbol{Q})|^2$ are given by Price [12]. We take the following expression for the screening factor, which is valid in the long-wavelength limit [13]:

$$\varepsilon(\boldsymbol{Q}) = 1 + (4\pi e^2/K_s Q^2)D(E_F) \tag{12}$$

where $D(E_F)$ is the density of states at E_F:

$$D(E_F) = \begin{cases} (m^*/\pi^2\hbar^2 l)\cos^{-1}(1 - E_F/t) & \text{for } E_F \leqslant 2t \\ m^*/\pi\hbar^2 l & \text{for } E_F > 2t. \end{cases} \tag{13}$$

Incorporating expressions (7)–(11) in (5) we have numerically evaluated S_{gp} as a function of temperature, Fermi level and miniband width.

The parameters used are $m^* = 0.067m_0$, deformation potential constant $E_1 = 11.5$ eV, piezoelectric tensor component $h_{14} = 1.2 \times 10^7$ V cm^{-1}, $K_s = 12.9$, mass density $\rho = 5.39$ g cm^{-3}, transverse sound velocity $v_t = 3.04 \times 10^5$ cm s^{-1}, longitudinal

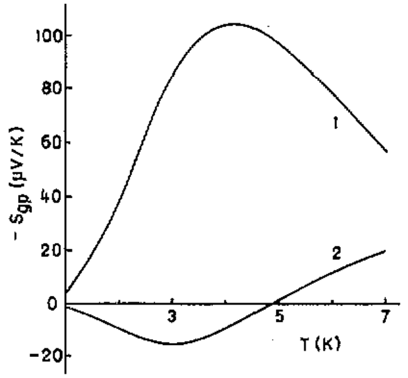

Figure 1. A plot of S_{gp} against temperature. Curve 1: when the Fermi energy is in the middle of the miniband, $E_F = t$, corresponding to an electron concentration $n = 2.84 \times 10^{17}\,\mathrm{cm}^{-3}$. Curve 2: when the Fermi energy coincides with the top of the miniband, $E_F = 2t$, corresponding to $n = 8.9 \times 10^{17}\,\mathrm{cm}^{-3}$.

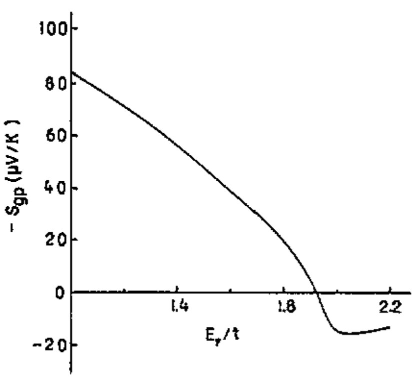

Figure 2. The variation of S_{gp} with E_F/t at $T = 3$ K.

sound velocity $v_l = 5.14 \times 10^5\,\mathrm{cm\,s^{-1}}$ and $L = 0.03$ cm. For a typical GaAs–GaAlAs SL with a periodicity $l = 80$ Å ($2a = 2b = 40$ Å) and barrier height $V_0 = 250$ meV, Kronig–Penney calculations give a bandwidth $2t = 50.8$ meV [14]. With these values S_{gp} has been calculated as a function of T and is shown in figure 1. Curve 1 represents the results when E_F is in the middle of the miniband, $E_F = t$ (corresponding to the carrier concentration $n = 2.84 \times 10^{17}\,\mathrm{cm}^{-3}$), and curve 2 represents the results when E_F coincides with the top of the miniband. $E_F = 2t$ (corresponding to $n = 8.9 \times 10^{17}\,\mathrm{cm}^{-3}$). For E_F well within the miniband there is a maximum in the variation of S_{gp} with T. Calculations with U-processes left out show a monotonic increase of S_{gp} with T in the temperature range considered here. The inclusion of U-processes is found to suppress the magnitude of S_{gp}. From curve 2 it is seen that S_{gp} changes sign with a positive maximum around 3 K. This anomalous behaviour is characteristic of inclusion of U-processes as pointed out at the beginning.

In figure 2 we have shown the variation of S_{gp} with E_F/t at $T = 3$ K. $|S_{gp}|$ is seen to decrease with increase of E_F. This is consistent with what is normally expected and observed in 2D and 3D electron systems [6, 15]. Here, as E_F tends to $2t$ we have the additional effect of U-processes, which suppresses $|S_{gp}|$ and leads to a change in sign of S_{gp}.

The calculation of the diffusion contribution to the thermopower has shown sensitivity to the scattering mechanisms. In some cases a sign reversal (hole-like behaviour) is predicted for Fermi energies near the top of the miniband [2, 3]. Hence, in view of this and our calculations, it would be interesting to study, experimentally, the variation of thermopower with dopant concentration and temperature.

In conclusion, a calculation of phonon-drag thermopower when the temperature gradient is along the SL axis is given. It is shown that the inclusion of U-processes leads to a change in sign of the thermopower. Measurements of thermopower along the SL axis may provide additional evidence for the electron transport through extended, Bloch-type states.

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