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The thermoelectric effect in a semiconductor superlattice in a non-quantized electric field

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Abstract. The thermoelectric effect in a semiconductor superlattice in a non-quantized electric field is investigated for electrons of the lowest miniband in the linear approximation of ∇T. Analytical expressions for the thermopower and the heat conductivity coefficient are obtained as functions of the superlattice parameters Δ and d, temperature, concentration and electric field E. The results confirm the fact that depending on the relation between Δ and other characteristic energies of the carrier charge (kT, ξ and $\hbar/\tau$) the carrier charges can behave either as a quasi-two-dimensional or as a three-dimensional electron gas. The prospect of using a superlattice as a good-quality and highly efficient thermoelement is also proposed.

1. Introduction

Recent perfection of atomic-scale control over nucleation and growth using modern crystal growth techniques such as molecular beam and liquid-phase epitaxy and chemical vapour deposition has made possible laboratory synthesis of ultrathin layer structures, such as the quantum well structure (QWS) and superlattice (SL).

This has led to the publication of a considerable number of papers, especially on the transport properties of SLs [1, 2]. This includes among other factors the mobility, negative differential conductivity and absolute negative conductivity. There are also papers on phonon polariton modes in a semiconductor SL [3], electron–phonon interactions [4], magnetoplasmons and the quantum Hall effects [5] and so forth.

Few papers have reported on the thermoelectric properties of SLs, even though good knowledge of this effect in SLs can enhance the production of a good-quality and highly efficient thermoelement.

The thermopower of a SL in the situation where $2\Delta \ll k_B T$ (T is the lattice temperature and k_B is Boltzmann's constant) has been calculated [6]. The anisotropic nature of the thermoelectric properties of a SL have been noted [7] and it is said that a study of this can give information about the density of states of the SL. The thermoelectric effects of a SL with the temperature gradient perpendicular to the SL axis has also been considered [8]. The thermopower of a quasi-two-dimensional (Q2D) semiconductor QWS has also been studied [9].

The purpose of this paper is to study thermoelectric effects in a SL in the presence of a non-quantized electric field, with the field and ∇T along the SL axis. Expressions for the thermopower and heat conductivity coefficient were obtained.

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2. Theory

The problem will be considered in the quasi-classical case, i.e. for $2\Delta \gg eEd$, $k_B d\nabla T$, $\tau^{-1}(\hbar = 1)$ (where d is the SL period, 2Δ is the width of the lowest-energy miniband, e is the electron charge and τ is the relaxation time of electron), by means of the Boltzmann kinetic equation

$$\partial f(r,p,t)/\partial t + v(p)\,\partial f(r,p,t)/\partial r + eE\,\partial f(r,p,t)/\partial p = -[f(r,p,t) - f_0(p)]/\tau \qquad (1)$$

where the collision integral is taken in the τ approximation and is further assumed constant [10].

The solution of equation (1) for electrons in the lowest miniband of the SL in the linear approximation of ∇T is given as

$$f(p,t) = \tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right) f_0(p - eEt)\,\mathrm{d}t + \int_0^\infty \exp\left(-\frac{t}{\tau}\right)\mathrm{d}t$$
$$\times\left([\varepsilon(p - eEt) - \xi]\frac{\nabla T}{T} + \nabla\xi\right) v(p - eEt)\frac{\partial f_0(p)}{\partial\varepsilon}. \qquad (2)$$

The current density is defined as

$$j(t) = e\sum_p v(p) f(p,t) \qquad (3)$$

and the density of heat current as

$$q(t) = \sum_p [\varepsilon(p) - \xi] v(p) f(p,t). \qquad (4)$$

Substituting (2) into (3) and (4) and performing the transformation $P - eEt \to P$ the following expressions are found for both the current density and the density of heat current:

$$j(t) = e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\mathrm{d}t \sum_p v(p - eEt) f_0(p) + e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\mathrm{d}t$$
$$\times\sum_p\left([\varepsilon(p) - \xi]\frac{\nabla T}{T} + \nabla\xi\right)\left(v(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right) v(p - eEt) \qquad (5)$$

$$q(t) = \tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\mathrm{d}t \sum_p [\varepsilon(p - eEt) - \xi] v(p - eEt) f_0(p) + \int_0^\infty \exp\left(-\frac{t}{\tau}\right)\mathrm{d}t$$
$$\times\sum_p [\varepsilon(p - eEt) - \xi]\left([\varepsilon(p) - \xi]\frac{\nabla T}{T} + \nabla\xi\right)\left(v(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right) v(p - eEt)$$

$$(6)$$

where

$$\varepsilon(p) = \frac{p_\perp^2}{2m} + \Delta[1 - \cos(p_z d)] \tag{7}$$

(m is the transverse effective electron mass (in the XOY plane)) and

$$v(p) = \Delta d \sin(p_z d). \tag{8}$$

With the help of (5)–(8) the following expressions for j_z and q_z are obtained for a non-degenerate electron gas after a cumbersome calculation:

$$j_z = [\sigma(E)/e]\nabla_z(\xi/e - \varphi) + [\sigma(E)/e][(\Delta - \xi) + 3kT - \Delta(I_0/I_1)]\nabla_z T/T \tag{9}$$

$$\begin{aligned} q_z = {} & [\sigma(E)/e^2][(\Delta - \xi) + kT + 2kT\Theta - \Delta(I_0/I_1)\Theta]\nabla_z(\xi/e - \varphi) + [\sigma(E)/e^2] \\ & \times [4(kT)^2 + 4(\Delta - \xi)kT + (\Delta - \xi)^2 - \Delta(\Delta - \xi)I_0/I_1 \\ & + 4\Delta kT(I_0/I_1)\Theta - \Delta kT(I_0/I_1) + 8(kT)^2\Theta - \Delta(\Delta - \xi)(I_0/I_1)\Theta \\ & + 2(\Delta - \xi)kT\Theta + \Delta^2\Theta]\nabla_z T/T. \end{aligned} \tag{10}$$

The expression for q_z in terms of $\nabla_z(\xi/e - \varphi)$ is not convenient when it comes to comparing theory with experiment; therefore as usual we shall express q_z in terms of j_z and ∇T_z. From (9) and (10) we obtain for q_z the following expression:

$$\begin{aligned} q_z = {} & (k/e)\{[(\Delta - \xi)/kT] + 1 + [2 - (\Delta/kT)(I_0/I_1)]\Theta\}Tj_z \\ & - [\sigma(E)/e^2)\{(kT)^2 + [\Delta kT(I_0/I_1) \\ & + 2(kT)^2 + \Delta^2 - \Delta^2(I_0^2/I_1^2)]\Theta\}\nabla_z T/T \end{aligned} \tag{11}$$

where I_0 and I_1 are the modified Bessel functions of the argument Δ/kT,

$\Theta = [1 + (eEd\tau)^2]/[1 + (2eEd\tau)^2]$ $\qquad$ $\sigma(E) = [e^2\Delta d^2 n\tau/(1 + eEd\tau)^2](I_1/I_0)$.

From (11) the following kinetic coefficients are found:

$$\text{Peltier coefficient} = \alpha T \tag{12}$$

where α is the thermopower given as

$$\alpha = (k/e)\{(\Delta - \xi)/kT + 1 + [2 - (\Delta/kT)(I_0/I_1)]\Theta\}. \tag{13}$$

The heat conductivity coefficient is given as

$$\kappa = [\sigma(E)/e^2]k^2T\{1 + [(\Delta/kT)(I_0/I_1) + 2 + (\Delta/kT)^2 - (\Delta/kT)^2(I^2/I_1^2)]\Theta\}. \tag{14}$$

Considering the weak electric field $eEd\tau \ll 1$ we have

$$\alpha = (k/e)[(\Delta - \xi)/kT + 3 - (\Delta/kT)(I_0/I_1)] \tag{15}$$

$$\kappa = (\sigma_\parallel/e^2)k^2T[3 + (\Delta/kT)(I_0/I_1) + (\Delta/kT)^2 - (\Delta/kT)^2(I_0^2/I_1^2)] \tag{16}$$

where

$$\sigma_\parallel = e^2\Delta d^2 n\tau(I_1/I_0).$$

3. Results, discussion and conclusion

We have obtained an analytic expression for the thermopower and heat conductivity coefficient of a SL. These results can be interpreted in terms of Δ in two ways, as indicated in [11]. In [11] it is noted that the relation between Δ and the characteristic energies (ξ, kT and τ^{-1}) of the carrier charges allow the carriers to behave either as a Q2D or as a three-dimensional (3D) electron gas. For example when $\Delta \ll kT$ the carrier charges behave as a Q2D electron gas and at $\Delta \gg kT$ as a 3D electron gas.

This proposition can be established by our results. For instance when $\Delta \ll kT$ using the well known expressions for I_0 and I_1 at small values of the argument [12] we obtain

$$\alpha = (k/e)(-\xi/kT + 1) \tag{17}$$

$$\kappa = (\sigma_{\parallel}/e^2)k^2 T \tag{18}$$

where

$$\xi = kT \ln(\pi\hbar^2 n_e d/mkT).$$

Equation (17) was first obtained by Shik [6]. A similar expression was obtained for a Q2D semiconductor QWS in [9]. In [9] it is indicated that the thermopower is enhanced above its value in the homogeneous (bulk) semiconductor for lower values of well thickness d and increases with increasing temperature T. Thus enhancement is greater at 77 K than at 300 K.

For $\Delta \gg kT$ using the asymptotic expression for $I_{0,1}$ [12] gives

$$\alpha = (k/e)(-\xi/kT + \tfrac{5}{2}) \tag{19}$$

$$\kappa = \tfrac{5}{2}(\sigma/e)k^2 T \qquad \sigma = ne^2\tau/m. \tag{20}$$

It can therefore be noted from our result that there is a continuous change from a Q2D to a 3D system. Furthermore the presence of the field E in equations (13) and (14) can make it possible to control α and κ.

In conclusion, the thermoelectric effect in a semiconductor SL in a non-quantized electric field has been investigated theoretically.

An excellent analytical expression has been found for α and κ. In our opinion an optimal selection of Δ and d for the SL can allow the use of a SL as a good-quality and efficient thermoelement.

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