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Anisotropy of the thermoelectric power in superlattices

B M Askerov, S R Figarova and V R Figarov

Baku State University, 23 Z Khaliliv Street, Baku AZ-1148, Azerbaijan

E-mail: figarov@bsu.az

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Abstract

Anisotropy of the thermoelectric power in superlattices on the scattering of charge carriers by impurity ions is studied. The thermopower anisotropy is found to be significant at the small degree of band filling. It has been shown that the concentration dependence of the transverse component of the thermopower is nonmonotonic.

1. Introduction

Superlattices (SLs) are attracting much attention because their low dimensionality may improve the thermoelectric figure of merit [1, 2]. The thermoelectric power theories have been developed in [3, 4] where the relaxation time was assumed to be isotropic, which holds true only on the acoustic phonons' scattering, whereas in the low temperature range the scattering of charge carriers by impurity ions dominates the transport and in SLs such a scattering is anisotropic. A number of works are currently dedicated to scattering mechanisms in low-dimensional systems; in a few of them the scattering of charge carriers by impurity ions and its influence on electronic transport phenomena are examined [5–8]. In the majority of the reports the relaxation time and transport phenomena in the basal plane are being treated. In specific cases of SLs and layered crystals the transverse transport exists aside from the longitudinal one: however, no consistent calculation is available on longitudinal and transverse components of the thermoelectric power, as far as we know. Owing to this, under investigation in this paper are the longitudinal (in the cross-plane direction, perpendicular to SL interfaces) and transverse (parallel to SL interfaces, in-plane direction) components of the thermoelectric power of SLs with a degenerate electron gas on the impurity scattering of charge carriers. The anisotropy of the impurity scattering is taken into account through the introduction of the inverse relaxation time tensor in the Born approximation. Proceeding from expressions of the anisotropic relaxation time of conduction electrons with a cosine dispersion law, by the solution for the Boltzmann equation, general expressions for longitudinal and transverse components of the thermoelectric power have been deduced. The thermopower anisotropy depending on the degree of band

filling (i.e. the relation between the Fermi level and mini-band width) is analysed. The concentration dependence of longitudinal and transverse components of the thermoelectric power is discussed. It has been disclosed that the thermopower along the layer plane is a nonmonotonic function of the concentration. The anisotropy of the thermopower is noted to be substantial. The thermopower across the layer is drastically less than that in the layer plane.

2. Longitudinal and transverse components of the thermoelectric power

The anisotropy of electronic properties of quasi-two-dimensional systems is primarily connected with peculiarities of the energy spectrum, which in SLs and layered crystals are

$$\varepsilon(k) = \hbar^2 k_{\perp}^2 / 2m_{\perp} + \varepsilon_0 [1 - \cos(ak_z)], \quad (1)$$

where $k_{\perp} = (k_x^2 + k_y^2)^{1/2}$, k_z being the z component of the wavevector, ε_0 is the mini-band half-width in the direction k_z , a is the lattice constant in the direction perpendicular to the layer plane and m_{\perp} is the effective mass of current carriers in the layer plane.

Another cause of the anisotropy are features of the scattering that in the relaxation time approximation in anisotropic systems are described by the inverse relaxation time tensor.

In order to explain the kinetic coefficient behaviour in SLs and layered crystals proper allowance must be made for both the factors.

Transverse, $\frac{1}{\tau_{\perp}}$, and longitudinal, $\frac{1}{\tau_{\parallel}}$, components of the tensor of the inverse relaxation time on the scattering of current carriers on impurity ions in the case of the small screening

($kr_0 \gg 1$) have the appearance (see the appendix):

$$\frac{1}{\tau_{\perp}} = \frac{1}{\tau_0} \frac{\ln 4k_z r_0}{(2k_{\perp} r_0)^3}, \quad (2)$$

$$\frac{1}{\tau_{\parallel}} = \frac{1}{\tau_0} \frac{1}{4k_{\perp} k_z r_0^2}, \quad (3)$$

where r_0 is the screening radius, $\tau_0 = \frac{(m_{\perp} \chi)}{8\pi N e a^{3/2}}$, χ is the dielectric permittivity, e is the electron charge magnitude and N is the impurity concentration.

It might be pointed out that at the strong screening ($kr_0 \ll 1$) the relaxation time anisotropy does not occur. In this limit case a charged impurity ion behaves as a point defect with the short action δ -like potential.

Based upon the solution for the kinetic equation in the inverse relaxation time tensor approximation for components of the thermopower in the layer plane, α_{\perp} , and in the direction normal to the layer, α_{\parallel} , we have

$$\alpha_{\perp} = -\frac{k_0 k_0 T}{e \varepsilon_F} \frac{5\pi^2}{6} \frac{J_{0,0,1/2}}{J_{0,0,5/2}}, \quad (4)$$

$$\alpha_{\parallel} = -\frac{k_0 k_0 T}{e \varepsilon_F} \frac{\pi^2}{6} \frac{J_{1,2,-1/2}}{J_{1,2,1/2}}, \quad (5)$$

where ε_F is the Fermi energy, k_0 is the Boltzmann constant, T is temperature and J integrals are defined with the formula

$$J_{k,l,m} = \int_0^{Z_0} z^k (\sin z)^l \left(\varepsilon_F^* - 2\varepsilon_0^* \sin^2 \frac{z}{2} \right)^m dz,$$

here $\varepsilon_F^* = \frac{\varepsilon_F}{k_0 T}$, $\varepsilon_0^* = \frac{\varepsilon_0}{k_0 T}$; $Z_0(\varepsilon) = \arccos(1 - \frac{\varepsilon}{\varepsilon_0})$ as $\varepsilon_F < 2\varepsilon_0$ and $Z_0 = \pi$ if $\varepsilon_F > 2\varepsilon_0$.

From formulae (4) and (5) it transpires that on the impurity scattering the thermopower anisotropy (relation of the transverse component of the thermopower to the longitudinal one), in contradistinction to the anisotropy of the electrical conductivity [9], is merely dictated by the Fermi level to the mini-band width ratio and is irrespective of the effective mass anisotropy and superlattice constant.

Using formulae (4) and (5), in figure 1 the longitudinal and transverse components of the thermopower are plotted against the degree of band filling at temperature $T = 4$ K with the parameter $\varepsilon_0 = 12.5$ meV appropriate for GaAs/Al_{0.36}Ga_{0.64}As SLs.

As seen in figure 1 at the lower degree of band filling nonmonotonic properties both longitudinal and transverse components of the thermopower take place. It is evident that the transverse and the longitudinal components have a maximum as a function of the band filling: the transverse component of the thermopower is about four times as much as the longitudinal one.

For the thermopower anisotropy it is indicated in [1], where it was experimentally revealed that the transverse component of the thermopower greatly exceeds the longitudinal one in SiGe SLs.

We now turn to the concentration dependence for the thermopower of a degenerate electron gas.

The transverse thermopower, α_{\perp} , as $\varepsilon_F > 2\varepsilon_0$ (two-dimensional case), obeys the next concentration dependence:

$$\alpha_{\perp} = -\frac{k_0^2 T}{e} \frac{5\pi^2}{6} \frac{g(\varepsilon_F)}{n_0}, \quad (6)$$

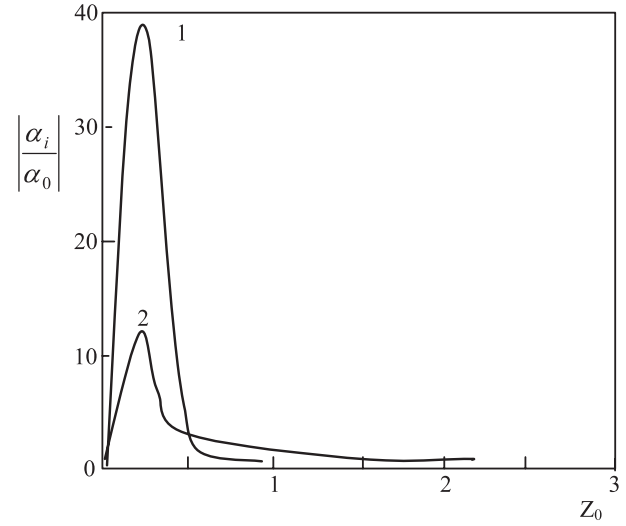


Figure 1. Transverse (curve 1) and longitudinal (curve 2) components of the thermopower versus the band filling.

where $n_0 = \frac{m_{\perp}(\varepsilon_F - \varepsilon_0)}{\pi^2 \hbar^2 a}$, $g(\varepsilon_F)$ is the density of states, $g(\varepsilon_F) = \frac{m_{\perp}}{\pi^2 \hbar^2 a} Z_0$, $Z_0 = \pi$ as $\varepsilon_F > 2\varepsilon_0$ and $Z_0(\varepsilon) = \arccos(1 - \frac{\varepsilon}{\varepsilon_0})$ as $\varepsilon_F < 2\varepsilon_0$ [9]. Formula (6) fits the experimental data in [10] where it was observed that the thermopower of the GaAs/Ga_{1-x}Al_xAs SLs is reduced by the elevated concentration.

As $\varepsilon_F < 2\varepsilon_0$ (quasi-two-dimensional case), for transverse thermopower we obtain:

$$\alpha_{\perp} = -\frac{k_0}{e} \left(\frac{k_0 T}{\varepsilon_0} \right)^2 \frac{5\pi^2}{6} \frac{n}{g(\varepsilon_F)} \frac{1}{\frac{3}{2} - \sin^2 Z_0 - \frac{3}{4} \frac{\sin 2Z_0}{Z_0}}, \quad (7)$$

where $n = \frac{m_{\perp} \varepsilon_0}{\pi^2 \hbar^2 a} (\sin Z_0 - Z_0 \cos Z_0)$ and n is the quasi-two-dimensional electron gas concentration [9].

From the comparison of the two latter formulae it is inferred that the thermopower dependence on the concentration is nonmonotonic: in the concentration region, when the Fermi level lies in the mini-band ($\varepsilon_F < 2\varepsilon_0$), it is detected the growth of α_{\perp} as the concentration is stepped up, and when ε_F is positioned above the mini-band width, $\varepsilon_F > 2\varepsilon_0$, α_{\perp} is in inverse proportion to the concentration at the constant density of states.

For the longitudinal thermopower in the two-dimensional case, $\varepsilon_F > 2\varepsilon_0$, one derives:

$$\alpha_{\parallel} = -\frac{k_0 \pi^2}{e} \frac{\pi^2}{6} k_0 T \frac{g(\varepsilon_F)}{n}. \quad (8)$$

According to formula (8), with increasing the lattice constant the density of states is reciprocally diminished and hence the thermopower drops, too, which is in line with numerical computations in [11] where is calculated the thermopower of a two-dimensional semiconductor with a quantum well structure.

The longitudinal component of the thermopower in the quasi-two-dimensional case, $\varepsilon_F < 2\varepsilon_0$, is of the form:

$$\alpha_{\parallel} = -\frac{k_0 \pi^2}{e} \frac{\pi^2}{6} \frac{k_0 T}{\varepsilon_F - 2\varepsilon_0 \sin^2 \frac{z}{4}}. \quad (9)$$

In this case J integrals were computed in a crude way.

It follows from formula (8) that in the two-dimensional case the longitudinal component of the thermopower declines with the concentration.

By the absolute value the longitudinal component of the thermopower is appreciably smaller than the transverse one.

As $\varepsilon_F > 2\varepsilon_0$, in the two-dimensional case the transverse thermopower for the scattering by phonons as well as by impurity ions can be written as:

$$\alpha_{\perp} = \frac{\alpha_0}{1 - \frac{\varepsilon_0}{\varepsilon_F}}, \quad (10)$$

where $\alpha_0 = -\frac{\pi^2}{6} \frac{k_0}{e} \frac{k_0 T}{\varepsilon_F}$.

This result again agrees that of Kubakaddi *et al* [11].

3. Conclusions

On the scattering of charge carriers by impurity ions the thermopower anisotropy is solely determined by the ratio of the Fermi level to the mini-band width and is independent of the effective mass anisotropy and superlattice constant. At the low degree of band filling the anisotropy is essential; it exhibits a nonmonotonic character. Both transverse and longitudinal components of the thermopower have a maximum as a function of the band filling. With the concentration, the transverse component of the thermopower rises, as the Fermi level is located in the mini-band, and falls, as the Fermi level is above the mini-band, while the longitudinal component of the thermopower varies inversely.

Appendix

Keeping in view the explicit form of energy spectrum (1) in cylindrical coordinates for transverse, $\frac{1}{\tau_{\perp}}$, and longitudinal, $\frac{1}{\tau_{\parallel}}$, components of the inverse relaxation time on the scattering of charge carriers by impurity ions after integrating with respect to φ and ε_{\perp} with the aid of the δ function yields:

$$\frac{1}{\tau_{\perp}} = \frac{m_{\perp} C V a^2}{4\pi^2 \hbar^2 k_{\perp}^2} \int_{-k_z}^{k_z} \frac{B^2 - 2k_{\perp}^2 a^2 A}{(A^2 + B^2)^{3/2}} \theta(\varepsilon - \varepsilon'_z) dk'_z, \quad (A.1)$$

$$\frac{1}{\tau_{\parallel}} = \frac{m_{\perp} C V a^4}{4\pi^2 \hbar^2 k_z} \int_{-k_z}^{k_z} |k_z - k'_z| \frac{A + 2k_{\perp}^2 a^2}{(A^2 + B^2)^{3/2}} \theta(\varepsilon - \varepsilon'_z) dk'_z \quad (A.2)$$

where

$$A = 2\gamma(\cos ak'_z - \cos ak_z) + (k_z - k'_z)^2 a^2 + (a/r_0)^2,$$

$$B = 2k_{\perp} a [(k_z - k'_z)^2 a^2 + (a/r_0)^2]^{1/2},$$

$$\gamma = m_{\perp}/m_{0z}, \quad m_{0z} = \hbar^2/\varepsilon_0 a^2,$$

$$\theta(\varepsilon_z - \varepsilon'_z) = 1 \quad \text{as } \varepsilon_z - \varepsilon'_z > 0$$

$$\text{and } \theta(\varepsilon_z - \varepsilon'_z) = 0 \quad \text{as } \varepsilon_z - \varepsilon'_z < 0$$

is the Heaviside function, $C = \frac{2\pi}{\hbar} \frac{N}{V} (\frac{4\pi e^2}{\chi})^2$, N is the impurity concentration and χ is the dielectric permittivity.

In the approximation when the effective mass across the layer, m_{\parallel} , is many times more than the effective mass in the layer plane ($m_{\parallel} \gg m_{\perp}$), having regard to the weak screening of Coulomb impurity atoms, in the Debye approximation for components of the inverse relaxation time one gets analytical expressions for longitudinal and transverse components of the relaxation time in the shape of (2) and (3), handy for further applications in kinetic coefficient calculations.

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