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Diffusion thermopower of the two-dimensional electron gas in AlP quantum wells including exchange and correlation effects

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ABSTRACT

We investigate the diffusion thermopower for the quasi-two-dimensional electron gas in a GaP/AlP/GaP quantum well taking into account exchange and correlation effects. We consider the interface-roughness and remote impurity scattering, and study the dependence of diffusion thermopower on the temperature, carrier density and quantum well width using different approximations for the local-field correction. It is shown that at low density many-body effects due to exchange and correlation considerably modify the thermopower. We find that, for system parameters considered in this paper, the diffusion thermopower is mainly determined by the remote impurity scattering. In the case of the interface-roughness scattering and $L > L_c$, the diffusion thermopower as a function of carrier density may change sign at low densities due to strong correlation effects. We also discuss the limitations of Mott formula and the deviation from linear temperature dependence of thermopower.

1. Introduction

GaP/AlP/GaP quantum well (QW) structures, where the electron gas is located in the AlP, have been studied recently both experimentally [1–5] and theoretically [6–9]. In this structure, due to biaxial strain present in the AlP layer, there exists a splitting of the energy minimum to a twofold level and a onefold level. The twofold level is lower in energy than the onefold level. This strain induced energy splitting and gives rise to two bands, one with the valley degeneracy $g_v = 2$ and one with $g_v = 1$. The electron gas in the lowest subband has valley degeneracy $g_v = 1$ for wells of width $L < L_c = 45.7$ Å and valley degeneracy $g_v = 2$ for wells of width $L > L_c$ [1,2,6,7]. Gold and Marty have calculated the transport scattering time, single-particle relaxation time and the magnetoresistance for a GaP/AlP/GaP QW at zero temperature [6,7]. The authors of this paper have extended the calculation of Gold and Marty by taking into account temperature and correlation effects [8,9]. The scattering mechanism, which is responsible for limiting the mobility, can be determined by comparing experimental results for resistivity and mobility with those of theoretical calculations [10–12]. However, the resistivity and mobility are of limited help to distinguish between different scattering mechanisms. On the contrary, the diffusion thermopower, electric field developed per unit temperature gradient, is a very sensitive probe of the scattering mechanism and usually complementary to resistivity as it reflects the energy dependence of the scattering mechanism and details concerning the distribution of the

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scatterers and their type [13,14]. Therefore, in this paper, we calculate the diffusion thermopower of the two dimensional electron gas (2DEG) realized in AlP for interface-roughness scattering (IRS) and remote charged impurity scattering (RIS) taking into account exchange-correlation effects. We hope that our calculations will help sample growers to design samples with interesting physical properties.

2. Theory

We consider a 2DEG, with parabolic dispersion determined by the effective mass m^*, moving in the xy plane with infinite confinement for $z < 0$ and $z > L$. We assume that electrons are only in the lowest subband and described by the wave function $\psi(0 \le z \le L) = \sqrt{2/L}\,\sin(\pi z/L)$ for $0 \le z \le L$ [8,9,15]. Diffusion thermopower S^d, in Boltzmann transport formalism under relaxation time approximation, is given by Refs. [13,14,16],

$$S^d = (1/eT)[-E_F + \langle E\tau(E)\rangle/\langle\tau(E)\rangle] \tag{1}$$

with

$$\langle x\rangle = \int_0^\infty x(-\partial f_0/\partial E)EdE \Big/ \int_0^\infty (-\partial f_0/\partial E)EdE, \tag{2}$$

Here $\tau(E)$ is the relaxation time of the electrons with energy E, $f_0(E)$ is the Fermi-Dirac distribution function and E_F is the Fermi energy. The total S^d can be calculated using total τ given by Matthiessen's rule:

$$\tau^{-1} = \tau_{IRS}^{-1} + \tau_{RIS}^{-1} \tag{3}$$

The relaxation time is given in the Boltzmann theory by Refs. [15],

$$\frac{1}{\tau(k)} = \frac{1}{2\pi\hbar E}\int_0^{2k} \frac{\langle|U(q)|^2\rangle}{[\in(q)]^2}\,\frac{q^2dq}{\sqrt{4k^2-q^2}} \tag{4}$$

where

$$\in(q) = 1 + \frac{2\pi e^2}{\in_L}\frac{1}{q}F_C(q)[1-G(q)]\Pi(q,T), \tag{5}$$

$$\Pi(q,T) = \frac{\beta}{4}\int_0^\infty d\mu' \frac{\Pi 0(q,\mu')}{\cosh^2\frac{\beta}{2}(\mu-\mu')}, \tag{6}$$

$$\Pi^0(q,E_F) = \Pi^0(q) \;= \frac{g_v m^*}{2\pi\hbar^2}\left[1-\sqrt{1-\left(\frac{2k_F}{q}\right)^2}\,\Theta(q-2k_F)\right] \tag{7}$$

$$F_C(q) = \frac{1}{4\pi^2+L^2q^2}\left(3Lq + \frac{8\pi^2}{Lq} - \frac{32\pi^4}{L^2q^2}\,\frac{1-e^{-Lq}}{4\pi^2+L^2q^2}\right) \tag{8}$$

with $\beta = (k_B T)^{-1}$, $E = \hbar^2k^2/(2m^*)$ and $\in_L$ denotes the background static dielectric constant (for AlP we use $\in_L = 9.8$ [5]). Here $k_F = (4\pi n/g_v)^{1/2}$, $E_F = \hbar^2k_F^2/(2m^*)$, $\mu = \ln[-1+\exp(\beta E_F)]/\beta$ and $\Pi(q,T)$ is the 2D Fermi wave vector, Fermi energy, chemical potential and polarizability of 2DEG, respectively. $G(q)$ is the local-field correction (LFC) describing the exchange-correlation effects [15, 17] and $\langle|U(q)|^2\rangle$ is the random potential which depends on the scattering mechanism [15]. For IRS the random potential is given by Ref. [15].

$$\langle|U_{IRS}(q)|^2\rangle = 2\left(\frac{4\pi}{L^2}\right)\left(\frac{m^*}{m_z}\right)^2\left(\frac{\pi}{k_FL}\right)^4(E_F\Delta\Lambda)^2e^{-q^2\Lambda^2/4} \tag{9}$$

where Δ represents the average height of the roughness perpendicular to the 2DEG, Λ represents the correlation length parameter of the roughness in the plane of the 2DEG and m_z is the effective mass perpendicular to the xy-plane.

For RIS, the random potential has the form