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EFFECT OF MAGNETIC QUANTIZATION ON THE THERMOELECTRIC POWER IN HgTe/CdTe SUPERLATTICES WITH GRADED STRUCTURES

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An attempt is made to study the thermoelectric power of the electrons under strong magnetic quantization in HgTe/CdTe superlattices with graded structures and to compare the same with that of the constituent materials by formulating the respective expressions. It is found, that the thermoelectric power increases with decreasing electron concentration and increasing magnetic field, respectively, in an oscillatory manner due to Shubnikov-de Haas effect. In addition, the well-known expressions for bulk specimens of parabolic energy bands have been derived under certain limiting conditions from our generalized relations.

1. Introduction

With recent advances in molecular beam epitaxy, fine line lithography, metal-argamic chemical vapour deposition and other experimental techniques, it has become possible to grow semiconductor superlattices (SLs) composed of alternate layers of two different degenerate materials with controlled thickness. The SL has found wide applications in many new device structures, such as photodiodes[1], tunneling devices[2], transistors[3], light-emitters[4], photodetectors[5], etc. The investigations of the physical properties of narrow-gap SLs have increased greatly[6], because they are important for optoelectronic devices and because the quality of

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heterostructures involving narrow-gap materials has been improved. We wish to note that HgTe/CdTe SLs have raised a great deal of attention since 1979 when they were first suggested as a promising new materials for long wavelength infrared detectors[7]. Interest in Hg-based SLs has further been increased which has revealed new properties with potential device applications[8]. These features arise from the unique zero-band gap material HgTe[9] and the direct band-gap material CdTe where CdTe can be described by three-band Kane model[10]. The combination of the aforementioned materials with specified dispersion relations make HgTe/CdTe SL more attractive due to its ability to tailor material properties for various applications.

We wish to note that the HgTe/CdTe SL has been proposed with the assumption that the interfaces between the layers are sharply defined, as to be devoid of any interface effect. As the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the electrons. Thus the influence of the finite thickness of the interface on the electron dispersion law becomes very important since the electron energy spectrum governs the electron transport in semiconductors. In this paper we shall study the thermoelectric power of the electrons in HgTe/CdTe SL with graded structures under strong magnetic field (TPM).

It is well-known that the analysis of the thermoelectric power gives information about the band structure, the density-of-states function and the effective electron mass[11]. The remarkable property of the TPM is that it is independent of the scattering mechanisms, and in the case of spherical energy surfaces, the shape of the conduction band can be determined from its experimental determination[11]. The TPM can be connected to the Einstein relation for the diffusivity-mobility ratio, the Debye screening length and the carrier contribution to the elastic constants in semiconductors having arbitrary dispersion laws[12]. The discovery of the quantum Hall effect[13] has brought interest to the study of the TPM is semiconductor heterostructures. In recent years, the different modifications of the TPM have extensively been investigated[14–16]. Nevertheless, it appears from the literature that the TPM is HgTe/CdTe SLs has yet to be investigated. In what follows, we shall study the doping and the doping and the magnetic field depedences of the TPM of HgTe/CdTe SL with graded structures and also in the corresponding bulk materials by formulating the respective expressions.

2. *Theoretical background*

The dispersion relations of the conduction electrons in bulk specimens of HgTe/CdTe SL are, respectively, given by[9–10],

$$E = A_0 k^2 + B_0 k \tag{1}$$

and

$$EG(E, E_{g2}, \Delta_2) = \hbar^2 k^2 / 2m^* \tag{2}$$

where E is the energy as measured from the edge of the conduction band in the absence of any quantization, $A_0 = \hbar^2/2m_1^*$, $\hbar = h/2\pi$, h is Planck's constant, m_1^*

is the effective electron mass at the edge of the conduction band of HgTe, $B_0 = 3e^2/128\varepsilon_s$, e is electron charge, ε_s is permittivity of HgTe, $G(E, E_{g2}, \Delta_2) = \left[(E + E_{g2})(E + E_{g2} + \Delta_2) \cdot \left(E_{g2} + \frac{2}{3}\Delta_2\right)\right]\left[E_{g2}(E_{g2} + \Delta_2)\left(E + E_{g2} + \frac{2}{3}\Delta_2\right)\right]^{-1}$ and E_{g2}, Δ_2 and m_2^* are the band-gap, spin-orbit splitting parameter of the valence band and the effective electron mass at the edge of the conduction band of CdTe, respectively. Thus the electron energy spectrum in the presence of a quantizing magnetic field B along z-direction in HgTe/CdTe SL with graded structures can be expressed as

$$k_z = [A(E, n)]^{1/2}/L_0 \tag{3}$$

where $A(E, n) \equiv \left[p(E, n) - 2eB\left(n + \frac{1}{2}\right)\hbar^{-1}L_0^2\right]$, n (=0, 1, 2...) is the Landau quantum number, $p(E, n) = [1/\cos^{-1}\{\psi(E, n)\}]$, $2\psi(E, n) \equiv [2\cos h\{\beta(E, n)\} \cdot \cos\{\gamma(E, n)\} + \varepsilon(E, n), \sin h\{\beta(E, n)\} \cdot \sin\{\gamma(E, n)\} + \Delta_0[(K_0^2(E, n)Q^{-1}(E, n) - 3Q(E, n))\,\mathrm{Cosh}\{\beta(E, n)\}\sin\{\gamma(E, n)\} + (3K_0(E, n) - Q^2(E, n)K_0^{-1}(E, n))\,\mathrm{Cos}\{\gamma(E, n)\}\sin h\{\beta(E, n)\} + 2(K_0^2(E, n) - Q^2(E, n))\cos h\{\beta(E, n)\}\cos\{\gamma(E, n)\} + (1/12)(5K_0^3(E, n)Q^{-1}(E, n) + 5Q^3(E, n)K_0^{-1}(E, n) - 34Q(E, n)K_0(E, n)K_0(E, n))\sin h\{\beta(E, n)\}\sin\{\gamma(E, n)\}]]$ $K_0(E, n) = \left[2E'm_2^*\hbar^{-2}G(E - V_0, a_2, \Delta_2) + 2eB\hbar^{-1}\left(n + \frac{1}{2}\right)\right]^{1/2}$, $\beta(E, n) = K_0(\mathrm{B}, n)(a_0 - \Delta_0)$, $\gamma(E, n) = Q(E, n) \cdot (b_0 - \Delta_0)$, $\varepsilon(E, n) = [K_0(E, n)Q^{-1}(E, n) - Q(E, n)K_0^{-1}(E, n)]$, $E' = V_0 - E$, V_0 is the potential barrier encountered by the electron, $a_2 = E_{g2}$, $L_0 = (a_0 + b_0)$, $Q(E, n) = \left[m_1^*\hbar^4\{-B_0 + \{B_0 + 4EA_0\}^{1/2}\}^2 - 2eB\hbar^{-1}\left(n + \frac{1}{2}\right)\right]^{1/2}$, L_0 is the SL period, Δ_0 is the interface width and a_0 and b_0 are the widths of the barrier and well, respectively. The electron concentration can be expressed, using Eq. (3), as

$$n_0 = (eB/\pi^2\hbar L_0)\sum_{n=0}^{n_{max}}[\psi_1 + \psi_2] \tag{4}$$

where ψ_1 = R. p. of $(A(E_0, n))^{1/2}$, $E_0 = E_F + i\Gamma$, Γ is broadening parameter, $i = \sqrt{-1}$, $\psi_2 = \sum_{r=1}^{1} H[\psi_1]$, r is the set of integers,

$$H = 2(k_BT)^{2r}(1 - 2^{1-2r})\,\zeta(2r)\frac{d^{2r}}{dE_F^{2r}},$$

k_B is Boltzmann constant, T is temperature, $\zeta(2r)$ is the zeta function of order $2r$ and E_F is the Fermi energy in the present case.

The TPM can be expressed[11)]

$$G = S_0/en_0 \tag{5}$$

where S_0 is the magnetoentropy per unit volume in the present case.

We can combine Eqs. (4) and (5) to get the TPM is HgTe/CdTe SL with graded structures as

$$G = C_0 \sum_{n=0}^{n_{max}} [\psi_1' + \psi_2'] \tag{6}$$

where $C_0 = \frac{B k_B^2 T}{3 \hbar n_0 L_0}$ and primes denote the differentiation w. r. t. E_F. The magneto-dispersion laws for bulk specimens can be written as

$$\hbar^2 k_z^2/2m_j^* + \left(n + \frac{1}{2}\right) \hbar w_j = X_j(E) \tag{7}$$

where $j = 1$ and 2, $w_0 = eB/m_j^*$, $X_1(E) = (4A_0)^{-1} [-B_0 + \sqrt{B_0^2 + 4A_0E}]^2$ and $X_2(E) = EG(E, E_{g2}, \Delta_2)$. Thus for bulk specimens of HgTe and CdTe, the electron concentration and the TPM can, respectively, be expressed as

$$n_0 = C_1 \sum_{n=0}^{n_{max}} [\psi_3 + \psi_4] \tag{8}$$

and

$$G = C_2 \sum_{n=0}^{n_{max}} [\psi_3' + \psi_4'] \tag{9}$$

where

$C_1 = eB/\pi^2\hbar$, $\psi_3 =$ R. p. of $\sqrt{p_0(E_0)}$, $p_0(E_0) = \left[X_j(E_0) - \left(n + \frac{1}{2}\right) \hbar w_{0j}\right]$,

$\psi_4 = \sum_{r=1}^{l} H[\psi_3]$ and $C_2 = [\pi^2 k_B T \varepsilon_1/3en_0]$.

Neglecting broadening and under the conditions $\varepsilon_s \to \infty$ and $E_{g2} \to \infty$, the Eqs. (7) to (9) assume the well-known forms[17,10)] as

$$E = \hbar^2 k_z^2/2m_j^* + \left(n + \frac{1}{2}\right) \hbar w_{0j} \tag{10}$$

$$n_0 = N_c \Theta_0 \sum_{n=0}^{n_{max}} F_{-1/2}(\eta) \tag{11}$$

and

$$G = C_3 \sum_{n=0}^{n_{max}} F_{-3/2}(\eta) \tag{12}$$

where $N_c = 2(2\pi m^* k_B T/h^2)^{3/2}$, $\Theta_0 = \hbar w_{0j}/k_B T$, $F_t(\eta)$ is the Fermi-Dirac integral of order t[17)], $\eta = (k_B T)^{-1} \left[E_F - \left(n + \frac{1}{2}\right) \hbar w_{0j}\right]$ and $C_3 = \pi^2 k_B N_c \Theta_0/3en_0$.

3. *Results and discussion*

Using Eqs. (6) and (4) and taking the parameters[18] $m_1^* = 0.025\,m_0$, $\varepsilon_s = 20G_0$, $m_2^* = 0.16m_0$, $\Delta_2 = 0.81$ eV, $E_{g2} = 1.6$ eV, $T = 4.2$ K, $V_0 = 0.81$ eV, $T_D = 3$ K, $\Delta_0 = 10^{-9}$m, $a_0 = 5\cdot10^{-9}$m, $b_0 = 3\cdot10^{-9}$m and $B = 1$ T we have plotted the normalized TPM in HgTe/CdTe SL as a function of n_0 as shown in plot a of Fig. 1. The simplified cases of $\Delta_0 = 0$, bulk materials of HgTe, CdTe and that of parabolic semiconductors are also shown in the plots b, c, d and e, respectively of Fig. 1 by using appropriate equations. With the same parameters as used in obtaining Fig. 1, we have plotted in Fig. 2 all the above cases as functions of B corresponding to an electron concentration 10^{23} m^{-3}.

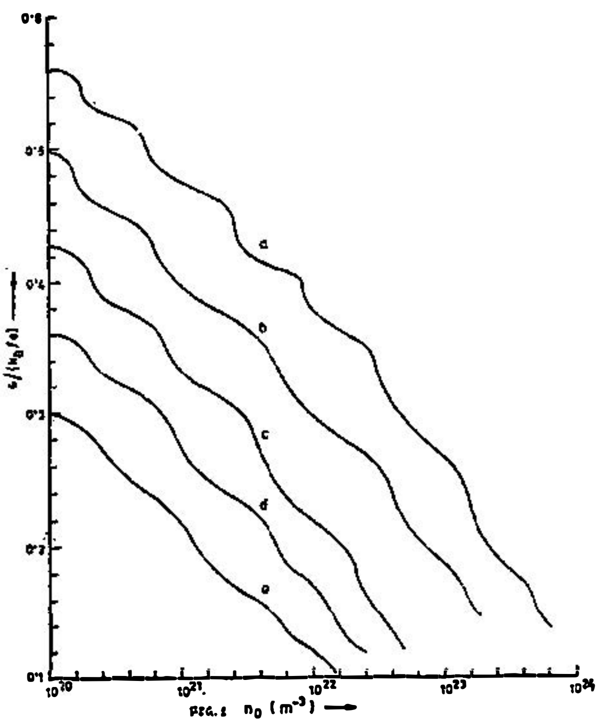

Fig. 1. Plot of $G/(k_B/e)$ as a function of n_0 in (a) HgTe/CdTe SL with $\Delta_0 \neq 0$, (b) HgTe/CdTe SL with $\Delta_0 = 0$, (c) bulk HgTe, (d) bulk CdTe (e), parabolic energy bands.

It appears from Fig. 1 that the TPM increases with decreasing electron concentration in an oscillatory manner and the SL structure exhibit the largest value of the TPM as compared to HgTe or CdTe for a given value of n_0. Besides, the finite value of the interface width enhances the value of the TPM in HgTe/CdTe SL with respect to n_0. From Fig. 2, we observe that the TPM increases with increasing B in an oscillatory way and the appearance of the humps in both the figures is due to Shubnikov-de Haas effect. The variations of TPM with n_0 and B are totally band structure dependent. By knowing the TPM we can also deter-

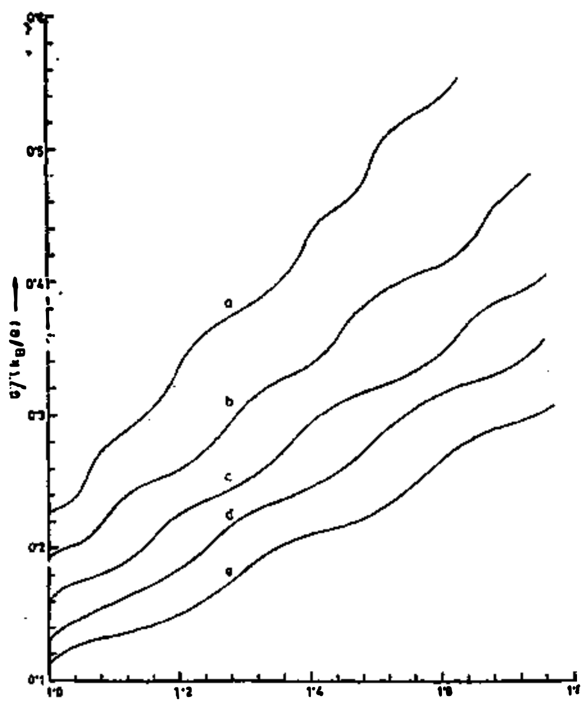

Fig. 2. Plot of $G/(k_B/e)$ as a function of B in (a) HgTe/CdTe SL with $\Delta_0 \neq 0$, (b) HgTe/CdTe SL with $\Delta_0 = 0$, (c) bulk HgTe, (d) bulk CdTe and (e) parabolic energy bands. ($n_0 = 10^{23}$ m^{-3}).

mine the Einstein relation for the diffusivity-mobility ratio (a very important device parameters[19]) for HgTe/CdTe SL and bulk specimens of HgTe and CdTe under magnetic quantization since the same ratio is inversely proportional to the TPM as given elsewhere[12].

We wish to note that the three-band Kane model is valid for III—V semiconductors, in general, but should be used as such for studying the electronic properties of n-InAs where the spin-orbit splitting parameter (Δ) is of the order of band gap E_g[10]. Besides, for many important semiconductors $\Delta \gg E_g$ (e. g. n-InSb, n-$Hg_{1-x}Cd_xTe$ etc.) or $\Delta \ll E_g$ (e. g. GaAs, InP, ZnSe etc.). Under these inequalities, the Eq. (7) gets simplified as

$$E\left(1 + \frac{E}{E_{g2}}\right) = \hbar^2 k_z^2/2m_2^* + \left(n + \frac{1}{2}\right)\hbar w_{02} \tag{13}$$

which is the well-known magneto-dispersion law of two-band Kane model[10]. Also under the conditions $E_{g0} \to a$ and $\varepsilon_s \to \infty$ the equations (7) and (13) assume form

$$E = \hbar^2 k_z^2/2m_j^* + \left(n + \frac{1}{2}\right)\hbar w_{0j} \tag{14}$$

which is the well-known magneto-dispersion relation of the parabolic energy bands. The dispersion relation of HgTe is given by the equation (2) and in formulating the SL energy spectrum we have considered the finite thickness of the interface. Thus we finally note that our simplified theoretical formulation covers various semiconductors under different physical conditions since the study of the transport phenomena and the derivation of the different electronic properties are based on the dispersion relation in such materials.

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EFEKT MAGNETSKE KVANTIZACIJE NA TERMOELEKTRIČKI NAPON U HgTe/CdTe SUPERREŠETKAMA SA STUPNJEVANOM STRUKTUROM

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Učinjen je pokušaj razmatranja termoelektrične elektromotorne sile elektrona u slučaju jake magnetske kvantizacije u HgTe/CdTe superrešetkama i njihova usporedba s konstitutivnim materijalima. Nađeno je da termoelektrički napon raste s opadanjem koncentracije elektrona i rastom magnetskog polja na oscilirajući način kao posljedica Shubnikov-de Haas efekta.