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THEORETICAL STUDY OF THE THERMOELECTRIC POWER IN ULTRATHIN FILMS OF $A_3^{II}B_2^{V}$ SEMICONDUCTORS IN THE PRESENCE OF A QUANTIZING MAGNETIC FIELD

KAMAKHYA PRASAD GHATAK, ARDHENDU GHOSHAL and BHASWATI MITRA

Department of Electronics and Telecommunication Engineering, Faculty of Engineering & Technology, University of Jadavpur, Calcutta-700032, India

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An attempt is made to study theoretically the thermoelectric power in ultrathin films $A_3^{II}B_2^{V}$ semiconductors in the presence of a quantizing magnetic field by formulating a new magneto dispersion law, within the framework of $\vec{k} \cdot \vec{p}$ formalism incorporating the anisotropies in the band parameters. It is found, taking ultrathin films of n-Cd_3P_2 as an example, that the same power decreases with increasing surface electron concentration and also changes in an oscillatory manner with film thickness and quantizing magnetic field, respectively. In addition, the well-known results for parabolic energy bands in the absence of any quantization have been also obtained from our expressions as special cases.

1. Introduction

The remarkable developments in fine line lithography and new epitaxial technologies of MBE and MOCVD have generated significant possibilities of fabricating various types of $2D$ structures, viz. ultrathin films inversion layers etc.[1-3]. In ultrathin films where the width of the films are comparable to the de Broglie wavelength of the carriers, the restriction of the motion of the carriers in the direction normal to the film (say, the z-direction), may be viewed as carrier confinement in an infinitely deep $1D$ square potential well, leading to the quantization (known as quantum size effect (QSE)) of the wave vector, allowing the $2D$ electron transport parallel to the surface representating new characteristics not exhibited in bulk semiconductors. Heterostructures of different materials are currently widely investigated because of the enhancement of carrier mobility[4]. These properties make such $2D$ structures suitable for applications in high speed

digital network[5-6], optical modulators[7], switching systems and other devices. In the presence of a quantizing magnetic field parallel to the direction of size quantization, the free surface motion becomes quantized and $3D$ quantization occurs. Though many new effects associated with magnetic size quantization have already been reported there still remain scopes in the investigations made, while the interest for further researches of the different other aspects of such systems is becoming increasingly important.

It is well-known that thermoelectric power of the electrons in semiconductors strong magnetic field is a very important parameter and has been studied under different physical conditions[8-11]. The above power is independent of scattering mechanisms[8-9] and in the case of spherical energy surfaces, the shape of the conduction band can be determined from its experimental determination[8]. Nevertheless, it appears from the literature that the thermoelectric power of the electrons under strong magnetic quantization (TPM) in ultrathin films of $A_3^{II}B_2^{V}$ semiconductors has yet to be theoretically investigated by taking spin and broadening into account together with the formulation of new magneto-sized dispersion relation.

It would therefore be of much interest to study the TPM in ultrathin films of $A_3^{II}B_2^{V}$ materials by considering various types of anisotropies in the energy bands. $A_3^{II}B_2^{V}$ semiconductors are being increasingly used as nonlinear elements[12] and light emitting diodes[13]. Rowe and Shay[14] have demonstrated that the quasi-cubic model[15] can be used to explain the symmetry properties and the observed splitting of the conduction and valence bands at the zone center in $\vec{k}$-space of $A_3^{II}B_2^{V}$ materials. By incorporating the crystal field potential in the Hamiltonian, Kildal[16-17] proposed an $E - \vec{k}$ dispersion relation of the conduction electrons in the same materials together with the assumptions of isotropic momentum-matrix elements and isotropic valence band orbit splitting parameters, respectively, though the anisotropies of the aforementioned band parameters are significant physical parameters of $A_3^{II}B_2^{V}$ materials[18].

In what follows we shall formulate the generalized magnetosized energy spectrum by using the generalized dispersion relation, taking into account the anisotropies in these two band parameters, of the conduction electrons of $A_3^{II}B_2^{V}$ semiconductors in the absense of any quantization as given elsewhere[19]. We shall then derive the TPM by incorporating spin and broadening, respectively. We shall also formulate the same expression for three band Kane model, two band Kane model and parabolic energy bands as special cases of our generalized relations. We shall study the concentration, magnetic field and film thickness dependences of the TPM in ultrathin films of $A_3^{II}B_2^{V}$ materials, taking n-Cd_3P_2 as an example.

2. *Theoretical background*

The $E - \vec{k}$ dispersion of the conduction electrons in $A_3^{II}B_2^{V}$ materials can be expressed[19], in the absence of any quantization, as

$$\gamma(E) = f_1(E)\, k_s^2 + f_2(E)\, k_z^2 \tag{1}$$

where the notations are the same as in the above reference.

In the presence of a quantizing magnetic field along z-direction, the modified electron energy spectrum can be written following Wallace[20], as

$$\gamma(E) = D_{\pm}(n, E) + f_2(E) k_z^2 \tag{2}$$

where

$$D_{\pm}(n, E) = \frac{2eH}{\hbar}\left(n + \frac{1}{2}\right) G(E) - \left[E(E + E_g)\frac{2}{9}(\Delta_{\parallel}^2 - \Delta_{\perp}^2)\right] \pm$$

$$\pm \left[\frac{eB\hbar E_g \Delta_{\parallel}}{6}\right]\left[\left(E + E_g + \delta + \frac{\Delta_{\parallel}^2 - \Delta_{\perp}^2}{3\Delta_{\perp}}\right)\frac{E_g + D_{\perp}}{m_{\perp}^*\left(E_g + \frac{2}{3}\Delta_{\perp}\right)}\right],$$

e is the electron charge, n is the Landau quantum number and

$$G(E) = f_1(E) + \frac{\hbar^2 E_g}{18 m_{\perp}^*}(\Delta_{\parallel}^2 - \Delta_{\perp}^2)\frac{E_g + \Delta_{\perp}}{\left(E_g + \frac{2}{3}\Delta_{\perp}\right)}.$$

In an ultrathin film the carriers are assumed to be confined in a $1D$ infinitely deep square potential well of width d_0, leading to the quantization of the wave vector in a direction perpendicular to the film (i. e. the z-direction in the present case). Therefore the modified dispersion relation in the presence of magnetosize quantization can be written as

$$\gamma(E) = D_{\pm}(n, E) + f_2(E)(l\pi/d_0)^2 \tag{3}$$

where $l (= 1, 2, 3, \ldots)$ is the size quantum number.

Thus using equation (3) and following Tsidilkovskii[8], the expressions for surface electron concentration and TPM in the present case can, respectively, be expressed as

$$n_0 = \frac{eH}{2\pi\hbar}\sum_{n=0}^{n_{max}}\sum_{l=1}^{l_{max}} x\,[x^2 + y^2]^{-1} \tag{4}$$

and

$$S(H) = \frac{1}{eT}\left[\frac{\sum_{n=0}^{n_{max}}\sum_{l=1}^{l_{max}} \varepsilon' f(x, y)}{\sum_{n=0}^{n_{max}}\sum_{l=1}^{l_{max}} f(x, y)} - E_F\right] \tag{5}$$

where $x = 1 + A\cos(\eta_2)$, $A = \exp(-\eta_{nl})$, $\eta_{nl} = \dfrac{E_F - \varepsilon'}{k_B T}$, E_F is the Fermi energy in the presence of magnetosize quantization as measured from the edge of the conduction band in the absence of any quantization, ε' is the root of equa-

tion (3), $\eta_2 = [\Gamma/k_B T]$, Γ is the broadening parameter[21], k_B is Boltzmann's constant, T is temperature, $y = A \sin \eta_2$ and

$$f(x, y) = [(x - 1)(x^2 - y^2) + 2xy^2]\,[(x^2 - y^2)^2 + 4x^2y^2]^{-1}.$$

In the absence of broadening, the equations (4) and (5) assume the forms

$$n_0 = \frac{eH}{2\pi\hbar} \sum_{n=0}^{n_{max}} \sum_{l=1}^{l_{max}} F_{-1}(\eta_{nl}) \tag{6}$$

and

$$S(H) = \frac{1}{eT}\left[\frac{\sum_{n=0}^{n_{max}} \sum_{l=1}^{l_{max}} \varepsilon' F_{-2}(\eta_{nl})}{\sum_{n=0}^{n_{max}} \sum_{l=1}^{l_{max}} F_{-2}(\eta_{nl})} - E_F\right] \tag{7}$$

where $F_j(\eta_{nl})$ is the Fermi-Dirac integral of order j as defined by Blakemore[22].

Under the conditions $\delta = 0$, $\Delta_{\parallel} = \Delta_{\perp} = \Delta$ (the isotropic spin-orbit splitting parameters) and $m^*_{\parallel} = m^*_{\perp} = m^*$ (the isotropic effective electron mass at the edge of the conduction band), equation (2) assumes the form

$$\frac{E(E + E_g)(E + E_g + \Delta)\left(E_g + \frac{2}{3}\Delta\right)}{E_g(E_g + \Delta)\left(E + E_g + \frac{2}{3}\Delta\right)} = \frac{\hbar^2 k_z^2}{2m^*} + \left(n + \frac{1}{2}\right)\frac{\hbar eH}{m^*} \pm \frac{eB\hbar\Delta}{6m^*}\left(E + E_g + \frac{2}{3}\Delta\right)^{-1} \tag{8}$$

which is the well-known three-band Kane model under magnetic quantization[23]. The general forms of equations (4) to (7) will be unaltered for three-band Kane model where

$$\frac{\varepsilon'(\varepsilon' + E_g)(\varepsilon' + E_g + \Delta)\left(E_g + \frac{2}{3}\Delta\right)}{(\varepsilon' + E_g + \Delta)E_g(E_g + \Delta)} = \frac{\hbar^2}{2m^*}\left(\frac{l\pi}{d_0}\right)^2 + \left(n + \frac{1}{2}\right)\frac{\hbar eH}{m^*} \pm (eB\hbar\Delta/6m^*)\left(\varepsilon' + E_g + \frac{2}{3}\Delta\right)^{-1}.$$

Under the condition $\Delta \to \infty$, equation (8) assumes the form of well-known two-band Kane model as[24]

$$E(1 + \alpha E) = \left(n + \frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2 k_z^2}{2m^*} \pm \frac{1}{2} g^* \mu H \tag{9}$$

where

$$\alpha = 1/E_g, \qquad \omega_0 = eH/m^*, \qquad g^* = m_0/m^*, \qquad \mu = e\hbar/2m_0$$

and m_0 is the free electron mass. The general forms of equations (4) to (7) will not change for two Kane model where

$$\varepsilon'(1 + \alpha\varepsilon') = \left(n + \frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2}{2m^*}\left(\frac{l\pi}{d_0}\right)^2 \pm \frac{1}{2}g^*\mu H. \tag{10}$$

For $\alpha \to 0$ as for relatively wide band gap semiconductors, equations (9) and (10) get simplified as[24-25]

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2 k_z^2}{2m^*} \pm \frac{1}{2}g^*\mu H \tag{11a}$$

and

$$\varepsilon' = \left(n + \frac{1}{2}\right)\hbar\omega_0 \pm \frac{1}{2}g^*\mu H + \frac{\hbar^2}{2m^*}\left(\frac{l\pi}{d_0}\right)^2. \tag{11b}$$

3. *Results and discussion*

Using equations (4) and (5) and taking the parameters[18]

$$E_g = 0.58\ \text{eV}, \qquad \Delta_{\|} = 0.23\ \text{eV}, \qquad \Delta_{\perp} = 0.25\ \text{eV},$$

$$\delta = 0.08\ \text{eV}, \qquad m_{\|}^* = 0.03\ m_0, \qquad m_{\perp}^* = 0.05\ m_0,$$

$$\Gamma = 10^{-4}\ \text{eV}, \qquad T = 4.2\ \text{K}, \qquad H = 2\ \text{T}, \qquad n_0 = 10^{15}\ \text{m}^{-2}$$

as appropriate for ultrathin films of n-Cd_3P_2 we have plotted $S(H)/S(0)$ versus d_0 as shown in graph a of Fig. 1 in which the dotted plots e exhibits the same dependence for $\delta = 0$ for the purpose of assessing the influence of the crystal field splitting on the TPM. In addition in Fig. 1, plot b corresponds to ultrathin films of degenerate three-band Kane model of n-Cd_3P_2 (taking $m = 0.04\,m_0$ and $\Delta = 0.24$ eV for the purpose of comparison). We also plotted the normalized TPM in accordance with two-band Kane model and isotropic parabolic energy bands in the same figure. In Fig. 2, we present the computed normalized TPM as a function of surface electron concentration together with the same dependence for $\delta = 0$ such that the effect of crystal field splitting on the TPM is immediately apparent. In addition, plots corresponding to the simplified cases of ultrathin films in the degenerate three-band Kane model, two-band Kane model and in parabolic model of n-Cd_3P_2 are also presented in the figure. In Fig. 3 we have plotted the normalized TPM as a function of magnetic field in which the several simplified limiting cases have further been considered to study the influence of band structure on the TPM in ultrathin films of n-Cd_3P_2.

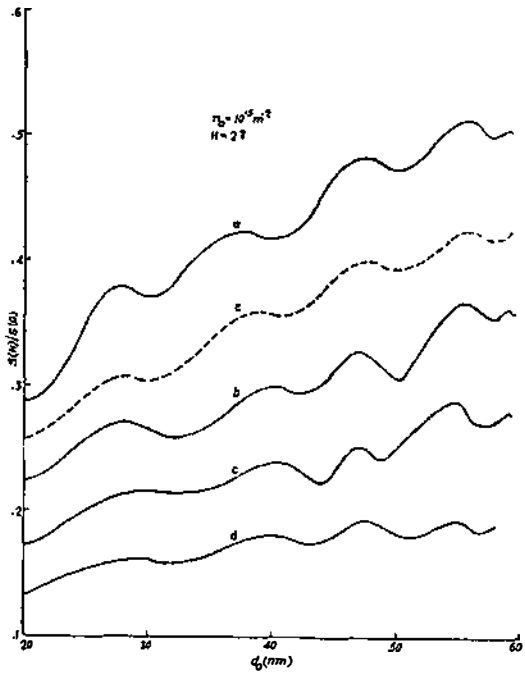

Fig. 1. Plot of the normalized TPM at 4.2K as a function of the thickness of ultrathin films: Curve a: degenerate n-Cd_3P_2 in accordance with our proposed band model; Curve b, the degenerate three-band Kane model; Curve c, the degenerate two-band Kane model; Curve d, the degenerate parabolic energy bands corresponding to $n_0 = 10^{15}\,m^{-2}$ and $H = 2$ T; the dashed curve e corresponds to $\delta = 0$.

The effect of size quantization is immediately apparent from Fig. 1 since the TPM depends strongly on the thickness of the ultrathin films, which is also a direct consequence of the effect of size quantization. The TPM oscillates with d_0 and the crystal field splitting parameter enhances the numerical magnitude of the TPM as compared with that corresponding to $\delta = 0$ at a given value of film thickness in the whole range of thickness considered. The TPM decreases with increasing electron concentration, as seen from Fig. 2, and the oscillatory dependence of the same power on n_0 will be less and less prominent with increasing film thickness. Ultimately, for thicker films or bulk specimens of the same semiconductor, the TPM will be found to increase continuously with increasing electron concentration in an non-oscillatory manner. It appears from Fig. 3 that the normalized TPM increases with increasing magnetic field in an oscillatory manner.

It may be noted that if we use equations (6) and (7) instead of equations (4) and (5) for the purpose of studying the TPM, the sharpness in the oscillatory dependence in all three figures will be greater for all types of band model. With varying magnetic field, each time a Landau level will cross the Fermi level, and a change will be reflected in the TPM through the distribution of the carriers among the Landau levels. It is worth remarking to note that the $3D$ quantization in the absence of broadening leads to discrete energy levels some what like atomic energy levels which in step produces very sharp changes. Under $3D$ quantization, there

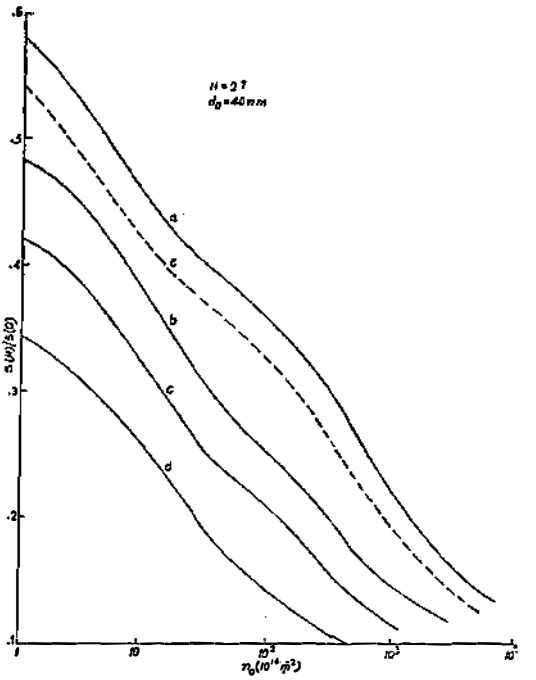

Fig. 2. Plot of the normalized TPM at 4.2K as a function of the surface electron concentration of ultrathin films of degenerate n-Cd_3P_2: Curve a, our proposed band model; Curve b, three-band Kane model; Curve c, two-band Kane model, Curve d, the parabolic energy bands corresponding to $d_0 = 40$ nm and $H = 2$ T; the dashed curve e corresponds to $\delta = 0$.

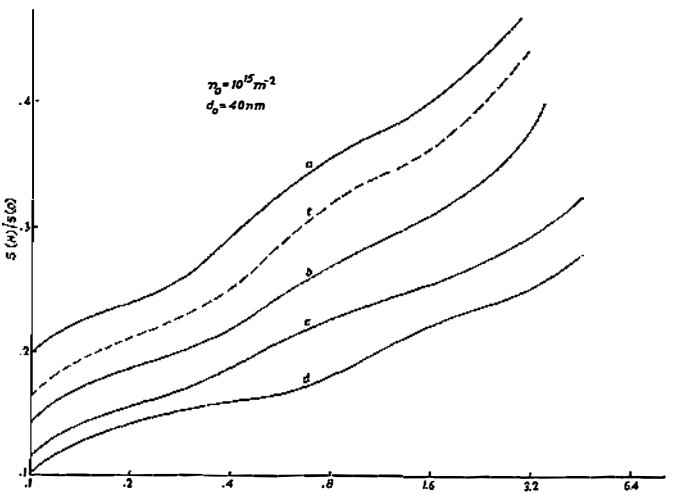

Fig. 3. Plot of the normalized TPM at 4.2K as a function of the quantizing magnetic field of ultrathin films of degenerate n-Cd_3P_2: Curve a, our proposed band model; Curve b, three-band Kane model; Curve c, two-band Kane model, Curve d, the parabolic energy bands corresponding to $d_0 = 40$ nm and $n_0 = 10^{15}$ m^{-2}; the dashed curve e corresponds to $\delta = 0$.

remains no free electron state in between any two Landau levels unlike that found for electron gases in semiconductors under 2*D* quantization. Consequently, the crossing of the Fermi level by the Landau level under 3*D* quantization would have much greater impact on the redistribution of the electrons amongst the available states, as compared to that found for 2*D* quantization. In the presence of broadening of Landau levels, the basic physics behind the 3*D* quantization is not applicable. Electron motion becomes possible in the broadened subbands and this the broadening parameter changes the expressions of the electron statistics and the TPM, respectively.

We wish to note that although the many-body effects, the hot electron effects, the arbitrary orientation of the quantizing magnetic fields, the formation of band tails and the influences of surface states and charges have been neglected in the present work, the general features of the effect of size quantization on the TPM as discussed here would also be valid for most of the narrow gap semiconductors since these semiconductors have non-parabolic energy bands obeying Kane's dispersion relation whereas our analysis is based on the generalization of the Kane's theory within the framework of $\vec{k} \cdot \vec{p}$ formalism and this simplified theory exhibits the basic features of the magneto TPM in ultrathin semiconducting films. Though the experimental verification of the basic content of this paper is not available in the literature to the best of our knowledge, but it may be noted that as far as the determination of the effective mass under degenerate electron distribution at the surface is concerned, measurement of magneto TPM as compared to the conductivity or cyclotron resonance would not be less advantageous regarding the experimental facilities required or accuracies achieved.

It must be mentioned that a direct research application of WSE in ultrathin films is the area of band structure[26]. By mapping the discrete quantum state energies as a function of film thickness, informations about the dispersion relations may be derived[26]. Finally it may be noted that the basic aim of the present paper is not solely to investigate the influence of size quantization on the thermoelectric power of the electrons under quantizating magnetic field in ultrathin films of $A_3{}^{II}B_2^{V}$ semiconductors by formulating the dispersion relation under magneto-size quantization but also to derive the appropriate electron statistics in its most generalized form by including spin and broadening, respectively, since the transport and the other phenomena in semiconductors and the study of different electronic properties of 2*D* semiconductor devices are based on the temperature dependent electron statistics in such materials.

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TEORIJSKO RAZMATRANJE TERMOELEKTROMOTORNE SILE U VEOMA TANKIM SLOJEVIMA POLUVODIČA $A_3^{II}B_2^{V}$ U PRISUSTVU KVANTIZIRAJUĆEG MAGNETSKOG POLJA

KAMAKHYA PRASAD GHATAK, ARDHENDU GHOSHAL i BHASWATI MITRA

Faculty of Engineering and Technology, University of Jadavpur, Calcutta-700 032, India

UDK 538.93

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Učinjen je pokušaj teorijskog razmatranja termoelektromotorne sile u veoma tankim slojevima poluvodiča $A_3^{II}B_2^{V}$ u prisustvu kvantizirajućeg magnetskog polja formuliranjem novog magneto-disperzionog pravila koristeći $\vec{k} \cdot \vec{p}$ formalizam u koji su uključene anizotropije parametara vrpce.