THEORETICAL ANALYSIS OF THE EINSTEIN RELATION IN NON-PARABOLIC MATERIALS

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Abstract In this paper an attempt is made to study the Einstein relation for the diffusivity mobility ratio (DMR) in non-parabolic materials having tetragonal band-structure by deriving the generalized electron energy spectrum incorporating the anisotropies of the energy band constants within the frame work of k.p. formalism. It is found, taking degenerate $n-CdGeAs_2$ as an example, that the above ratio oscillates in a periodic manner with the orientation of the magnetic field with respect to the c-axis. The ratio shows an oscillatory magnetic field dependence, as expected since the origin of the oscillations in the DMR is same as that of the Shuvnikov-de-Hass (SdH) oscillations and also increases with increasing electron concentration as expected in degenerate semiconductors. The corresponding well known results for isotropic two-band Kane model, both in the presence and absence of magnetic quantization, are also obtained from the expression derived. Also an experimental method of determining DMR in degenerate semiconductors is suggested for materials having arbitrary dispersion laws.

Keywords : Einstein Relation, Tetragonal Semiconductors.

INTRODUCTION

The Einstein relation for the diffusivity-mobility ratio of the carriers in semiconductors (DMR) is known to be very useful[1-2] , since the diffusion constant can be obtained from the ratio by knowing the values of the experimentally determined mobility. In addition, the DMR is more accurate than any of the individual relations for the diffusivity or the mobility which are considered to be the two most widely used properties of carrier transport in electronic devices. Since the performance of semiconductor devices at the device terminals and the speed of operation of modern switching devices are significantly influenced by the degree of carrier degeneracy, the simplest way of analyzing them would be to use the expression for the DMR which, in turn, enables us to express the above features of the devices made of degenerate materials in terms of carrier concentration[3-4]. The connection of the DMR with the velocity auto-correlation function[5] and the relation of the same ratio with the screening length[6] have been studied. The classical value of the DMR is equal to $\left(k_B T / |e|\right)$(where k_B, T and $|e|$ are the Boltzman constant, temperature and carrier charge respectively) and this relation is the well-known Einstein relation[8]. This relation is valid both for electrons and holes. In this conventional form, the relation holds only for non-degenerate materials although its validity has been suggested erroneously for degenerate compounds[2]. It is well-known from the fundamental work of Landsberg[7] that the Einstein relation, in electronic materials is essentially determined by the respective energy band structures. It has, therefore, different values in various degenerate materials and varies significantly with electron concentration, with the magnitude of the quantizing magnetic field, with quantizing electric field as in inversion layers, with size quantization as in ultrathin films, with quantum wires, etc. The nature of some of these variations have been studied in literature[6]. Nevertheless there still remain scopes in the investigations made while the interest for the further researches of the DMR in tetragonal semiconductors having other band structures under various physical conditions is becoming increasingly important. With a view to exploring some of these aspects, an attempt is made to study the DMR in non-parabolic materials having tetragonal band-structure under quantizing magnetic field.

It is worth remarking that the effects of a quantizing magnetic field on the band structures of non-parabolic materials are more striking than that of the parabolic one and are easily observed in experiments. Under magnetic quantization, the general characteristics of the band structure remain the same, but in each band the energy of the electron corresponding to the velocity transverse to the magnetic field becomes discrete due to quantization of the area of the k-space in the direction perpendicular to the direction of application of the quantizing magnetic field. This quantum nature of Landau levels leads to a host of interesting transport phenomena. Also the magneto DMR in the tetragonal semiconductors is discussed. We have suggested an experimental method of determining the DMR in degenerate materials having arbitrary dispersion laws. We have plotted the DMRs as functions of various physical variables taking nCd_3As_2 as an example.

THEORETICAL BACKGROUND

Formulation Of DMR In Bulk Specimens Of Tetragonal Semiconductors :

$A_3^{II}B_2^{v}$ and ternary chalcopyrite semiconductors are called tetragonal semiconductors since they have the tetragonal crystal structure[10]. These materials are being increasingly used as non-linear optical elements[11] and light emitting diodes[12]. Rowe and Shay[13] have demonstrated that the quasi-cubic model can[14] be used to explain the observed splitting and symmetry properties of the conduction and valence bands at the zone center of k-space of the aforementioned semiconductors. The s-like conduction band is singly degenerate and p-like valence band is triply degenerate. The latter splits into three subbands because of spin-orbit and crystal field interactions. The largest contribution of the crystal field parameter occurs from the presence of the non-cubic potential[15]. Incorporating the anisotropic crystal potential to the Hamiltonian, Bodnar[16] proposed a dispersion relation of the conduction electrons in the same semiconductor by using the assumption of an isotropic spin-orbit splitting parameter. It would, therefore, be of much interest to investigate the DMR in these materials by generalizing the above model within the framework of $\vec{k}.\vec{p}$ formalism. This is done, in what follows by taking $n-Cd_3As_2$ as an example of tetragonal semiconductors which is being increasing used in Hall pick-ups and thermal detectors.

The form of $\vec{k}.\vec{p}$ matrix for tetragonal semiconductors can be expressed as

$$H = \begin{bmatrix} H_1 & H_2 \\ H_2^+ & H_1 \end{bmatrix} \qquad \ldots\ldots(1)$$

$H_1 =$

$$\begin{bmatrix} E_g & P_{||}K_z & 0 & 0 \\ P_{||}K_z & -\left(\delta + (1/3)\Delta_{||}\right) & \left(\sqrt{2}/3\right)\Delta_\perp & 0 \\ 0 & \left(\sqrt{2}/3\right)\Delta_\perp & \left(-\sqrt{2}/3\right)\Delta_\perp & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$H_2 =$

$$\begin{bmatrix} 0 & 0 & \left(P_\perp/\sqrt{2}\right)\left(k_x - ik_y\right) & \left(k_x - ik_y\right)\left(P_{||}/\sqrt{2}\right) \\ 0 & 0 & 0 & 0 \\ -f_{,-} & 0 & 0 & 0 \\ f_{,+} & 0 & 0 & 0 \end{bmatrix}$$

in which E_g is the energy band gap, $P_{||}$ and $P_\perp$ the momentum matrix elements parallel and perpendicular to the crystal axis respectively. δ is the crystal field splitting parameter, $\Delta_{||}$ and $\Delta_\perp$ are the spin-orbit splitting parameters along and perpendicular to the C-axis respectively and $i = \sqrt{i}$. Thus, neglecting the contribution of the higher bands and the free electron energy, the diagonalisation of the above matrix leads to the dispersion relation of the conduction electron in bulk specimens of tetragonal semiconductors as

$$C(E) = A(E)k_s^2 + B(E)k_z^2 \qquad \ldots\ldots(2)$$

$$C(E) = E\left(E+E_g\right)\left[\left(E+E_g\right)\left(E+E_g+\Delta_{||}\right) + \right.$$
$$\left. +\delta\left(E+E_g+\frac{2}{3}\Delta_{||}\right) + \frac{2}{9}\left(\Delta_{||}^2 - \Delta_\perp^2\right)\right],$$

$$k_s^2 = k_x^2 + k_y^2$$

E is the energy as counted from the edge of the conduction band in the vertically upward direction in the absence of any quantization,

$$A(E) = \hbar^2 E_g\left(E_g+\Delta_\perp\right)\left[2m_\perp^*\left(E_g+\frac{2}{3}\Delta_\perp\right)\right]^{-1}$$
$$\left[\delta\left(E+E_g+\Delta_{||}\right) + \left(E+E_g\right)\left(E+E_g+\frac{2}{3}\Delta_{||}\right) + \right.$$
$$\left. +\frac{1}{9}\left(\Delta_{||}^2 - \Delta_\perp^2\right)\right]$$

and

$$B(E) = \hbar^2 E_g\left(E_g+\Delta_{||}\right)$$
$$\left[2m_{||}^*\left(E_g+\frac{2}{3}\Delta_{||}\right)\right]^{-1}\left[\left(E+E_g\right)\left(E+E_g+\frac{2}{3}\Delta_{||}\right)\right],$$

$\hbar^2 = h/2\pi$, h is the Planck's constant and $m_{||}$ and $m_\perp$ are the longitudinal and transverse effective electron masses at the edge of the conduction band, respectively. The use of equation (2) leads to the expression of the density-of-states function as

$$D_0(E) = 2/(2\pi)^3 (d/dE)[V(E)]$$
$$= \left(3\pi^2\right)^{-1} P(E) \qquad \ldots\ldots(3)$$

where V(E) is the volume of k-space as formed by equation (2),

$$P(E)=\left[\ 3/2\left(C_1(E)\sqrt{C}(E)\right)/\left(A(E)\sqrt{B}(E)\right)-\right.$$
$$-\left(A_1(E)[C(E)]^{3/2}/\left(A^2(E)\sqrt{B}(E)\right)-\left(C[E]^{3/2}B_1(E)\right)/\right.$$
$$\left./2A(E)[B(E)]^{3/2}\right)\Big],$$
$$C_1(E)=\left[\left(2E+E_g\right)\right]C(E)\left[E\left(E+E_g\right)\right]^{-1}+E\left(E+E_g\right)$$
$$\left(2E+2E_g+\delta+\Delta_{||}\right)\Big],$$
$$A_1(E)=\left[2m_\perp^*\left(E_g+\frac{2}{3}\Delta_\perp\right)\right]^{-1}\left[\hbar^2E_g\left(E_g+\Delta_\perp\right)\right]$$
$$\left[\delta+2E+2E_g+\frac{2}{3}\Delta_{||}\right],$$
$$B_1(E)=\left[2m_{||}^*\left(E_g+\frac{2}{3}\Delta_{||}\right)^{-1}\left[\hbar^2E_g\left(E_g+\Delta_{||}\right)\right]\right.$$
$$\left.\left[2E+2E_g+\frac{2}{3}\Delta_{||}\right]\right]$$

Combining equation (3) with the Fermi-Dirac occupation probability factor and using the generalized sommerfield's lemma[5], the electron concentration can be written as

$$n_0=\left(3\pi^2\right)^{-1}\left[M\left(E_F\right)+N\left(E_F\right)\right] \quad \ldots\ldots(4)$$

The DMR in the present case can, in general, be written as [7]

$$D/\mu=\left(\left(1/|e|\right)n_0\right)/\left(\partial n_0/\partial E_F\right) \quad \ldots\ldots(5)$$

Thus combining the equations (3) and (4) we get

$$D/\mu=\left(|e|\right)^{-1}\left[\left[M\left(E_F\right)+N\left(E_F\right)\right]\left[M'\left(E_F\right)+N'\left(E_F\right)\right]\right]^{-1} \quad \ldots\ldots(6)$$

where the primes indicate the differentiation with respect to E_F.

Formulation Of DMR In Tetragonal Semiconductors Under Magnetic Quatization

The modified electron energy spectrum in tetragonal semiconductors under arbitrary magnetic quatization can be written as

$$C(E)=Z_\pm(n,E,\theta)+a(E,\theta)\left(k_z'\right)^2 \quad \ldots\ldots(7)$$

where $Z_\pm(n,E,\theta)=\left(2|e|B/\hbar\right)\left(n+\frac{1}{2}\right)\left[\ A(E)\right.$

$$\left\{\ A(E)Cos^2\theta+B(E)Sin^2\theta\right\}\Big]^{1/2}\pm\left[\ \left(|e|B\hbar E_g/6\right)\right.$$
$$\left\{\ \left(E_g+\Delta_\perp\right)/\left(m_\perp^*\left(E_g+\frac{2}{3}\Delta_\perp\right)\right)\right\}^{1/2}\Big]\Big[\ E+E_g+\delta+$$
$$\left(\Delta_{||}^2-\Delta_\perp^2\right)\big)/\left(3\Delta_{||}\right)^2\left(\Delta_{||}^2Cos^2\theta\left(E_G+\Delta_\perp\right)\right)/$$
$$/\left(m_\perp^*\left(E_g+\frac{2}{3}\Delta_\perp\right)\right)+\left(E+E_g\right)^2\Delta_\perp^2Sin^2\theta\left(E_g+\Delta_{||}\right)\big)/$$
$$\left./\left(m_\perp^*\left(E_g+\frac{2}{3}\Delta_\perp\right)\right)\right]\Big]^{1/2},$$
$$a(E,\theta)=A(E)B(E)/A(E)Cos^2\theta+B(E)Sin^2\theta.$$

n(=0,1,2,…..) is the Landau quantum number, $k_z'\left(=k_zCos\theta+k_xSin\theta\right)$ is the direction of application of quantizing magnetic field B which makes an angle θ with k_x axis and lies in the k_xk_z plane.

Thus combining the appropriate equations using the generalized Sommerfield's lemma, the electron concentration in tetragonal semiconductors can be expressed as

$$n_0=\left(|e|B/\left(2\pi^2\hbar\sqrt{2}\right)\right)\sum_{n=0}^{n_{max}}\left[g_1\left(n,E_{FB},\theta\right)+g_2\left(n,E_{FB},\theta\right)\right] \quad \ldots\ldots(8)$$

where E_{FB} is the Fermi energy in the presence of magnetic quantization as measured from the edge of the conduction band in the absence of any quantization and the functions $g_1\left(n,E_{FB},\theta\right)$ and $g_2\left(n,E_{FB},\theta\right)$ are functions of n,E_{FB},θ. Combining equations (8) and (5), the magneto DMR in tetragonal semiconductors can be written as

$$(D/\mu)_B=\left(1/|e|\right)\left[\sum_{n=0}^{n_{max}}\left[g_1\left(n,E_{FB},\theta\right)+g_2\left(n,E_{FB},\theta\right)\right]\right]$$
$$\left[\sum_{n=0}^{n_{max}}\left[g_1'\left(n,E_{FB},\theta\right)+g_2'\left(n,E_{FB},\theta\right)\right]\right]^{-1} \quad \ldots\ldots(9)$$

where the primes denote the differentiation with respect to Fermi energy.

Special Cases

(a) under the substitution a $\delta=0$, $\Delta_{||}=\Delta_\perp=\Delta$ and $m_{||}^*=m_\perp^*=m^*$ equation (7) assumes the form,

$$\gamma(E)=\left(n+\frac{1}{2}\right)\hbar\omega_0+\hbar^2K_z^2/2m^*\pm$$
$$\left[eB\hbar\Delta/\left(6m^*\left(E+E_g+\frac{2}{3}\Delta\right)\right)\right] \quad \ldots\ldots(10)$$

where $\omega_0=|e|B/m^*$, the function $\gamma(E)$ has been defined as

$$\gamma(E)=E\left(E+E_g\right)\left(E+E_g+\Delta\right)\left(E_g+\frac{2}{3}\Delta\right)/$$

$\left(E_g\left(E_g+\Delta\right)\left(E+E_g+\frac{2}{3}\Delta\right)\right)$ and the equation (10) is the well-known magneto three band Kane model. For this model the equations (8) and (9) get simplified as

$$n_0=\left(|e|B\sqrt{m^*}/2\pi^2\hbar^2\right)\sum_{n=0}^{n_{max}}\left[G_1\left(n,E_{FB}\right)+G_2\left(n,E_{FB}\right)\right] \quad \ldots\ldots(11)$$

and

$$(D/\mu)_B = (1/|e|)\left[\sum_{n=0}^{n_{max}} [G_1(n,E_{FB}) + G_2(n,E_{FB})]\right]$$

$$\left[\sum_{n=0}^{n_{max}} [G_1'(n,E_{FB}) + G_2'(n,E_{FB})]\right]^{-1} \quad \ldots\ldots(12)$$

where $G_1(n,E_{FB})$ and $G_2(n,E_{FB})$ are functions of n, E_{FB}.

In the absence of spin and broadening, the expressions of n_0 and DMR for the two band Kane model can, respectively, be expressed under the assumption $\alpha E_{FB} << 1$ as

$$n_0 = N_c\theta\sum_{n=0}^{n_{max}}(t_0)^{-1/2}\left[\left(1+\frac{3}{2}\alpha b\right)F_{-1/2}(\eta'') + \left(\frac{3}{4}\alpha k_B T\right)F_{-1/2}(\eta')\right. \quad \ldots\ldots(13)$$

and

$$(D/\mu)_B = (k_B T/|e|)\left[\sum_{n=0}^{n_{max}}\left(1+\frac{3}{2}\alpha b\right)F_{1/2}(\eta') \left(\frac{3}{4}\alpha k_B T\right)F_{1/2}(\eta')\right](t_0)^{-1/2}$$

$$\left[\sum_{n=0}^{n_{max}} 1/\sqrt{t_0}\left(1+\frac{3}{2}\alpha b\right)F_{-3/2}(\eta') + \left(\frac{3}{4}\alpha k_B T\right)F_{-1/2}(\eta')\right]\Bigg]^{-1} \quad \ldots\ldots(14)$$

where $\theta = \hbar\omega_0/k_B T$, $t_0 = \left[1+\alpha\left(n+\frac{1}{2}\right)\hbar\varpi_0\right]$, $b = \left(n+\frac{1}{2}\right)\hbar\omega_0/t_0$ and $\eta' = [E_{FB} - b]/k_B T$. For parabolic energy bands $\alpha \to 0$ and the equations (13) and (14) get simplified as $n_0 = N_c\theta\sum_{n=0}^{n_{max}} F_{-1/2}(\eta')$;

$$\eta' = (k_B T)^{-1}\left[E_{FB} - \left(n+\frac{1}{2}\right)\hbar\omega_0\right] \quad \ldots\ldots(15)$$

and

$$(D/\mu)_B = (k_B T|e|)\left[\sum_{n=0}^{n_{max}} F_{-1/2}(\eta')\right]\left[\sum_{n=0}^{n_{max}} F_{-3/2}(\eta')\right]^{-1} \quad \ldots\ldots(16)$$

Suggestion For Experimental Determination Of DMR For Degenerate Semiconductors Having Arbitrary Dispersion Laws

The thermoelectric power of the electrons in semiconductors in the presence of a very large magnetic field is independent of scattering mechanism and can be written as[17]

$$G = (S_0/(|e|n_0)) \quad \ldots\ldots(17)$$

where S_0 is the entropy. The equation (17) can be written under the condition of carrier degeneracy as

$$G = (\pi^2 k_B{}^2 T)(3G(|e|)^2) \quad \ldots\ldots(18)$$

Thus we can determine the DMR by knowing G which is an experimentally measurable quantity[18,19].

RESULTS AND DISCUSSIONS

Using $n-Cd_3As_2$ as an example of tetragonal semiconductors together with the parameters[18]. $m_{||}^* = 3.03m_0$, $m_\perp^* = 0.04m_0$, $E_g = 0.095eV$, $\delta = 0.085eV$, $\Delta_{||} = 0.24eV$, $\Delta_\perp = 0.29eV$ and $T=4.2k$. Using the appropriate equations and together with $T_D = 3K$, $T = 4.2K$, B=1 Tesla and $n_0 = 2.2\times10^{22}m^{-3}$. The plots of the normalized DMR have been shown as function of 1/B and n_0 in figures 1 and 2 respectively.

It appears from figure 2 that the DMR oscillates with 1/B due to SdH effect. The band anisotropies enhance the numerical value of the DMR in $n-Cd_3As_2$ as compared to other types of band models. At extremely large values of the quantizing magnetic field, the condition for the quantum limit (n=0) will be reached when the DMR will be found to decrease with increasing magnetic field. The DMR increases in an oscillatory way with increasing electron concentration for all the models. Our calculation is only valid under the conditions of carrier degeneracy since under non-degenerate conditions, the DMR varies with only temperature in a liner manner. The DMR will in general, be anisotropic in the presence of magnetic quantization. It appears that for investigating the DMR under magnetic quantization, we have determined the magnetic field directional element of the corresponding tensor of DMR as a function B. Thus we note that the DMR as defined here refers to the direction of the application of the quantizing magnetic field.

The complicated variations of the DMR with respect to any physical variable is determined by the carrier statistics. The natures of variations are apparent from the figures. Since G decreases with increasing n_0 in an oscillatory way, therefore the DMR will increase with electron concentration in an increasing manner as apparent from equation (18). Finally we may note that this statement is the indirect test of our simplified theoretical analysis.

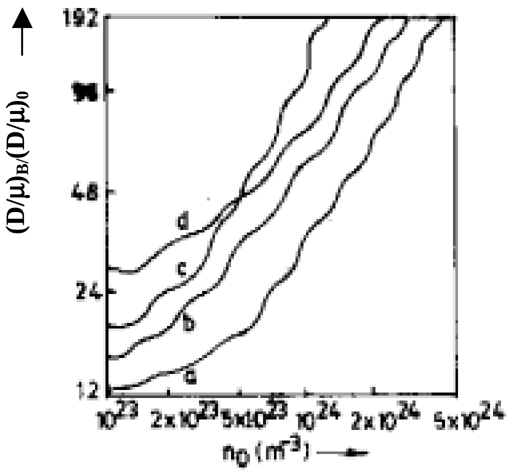

Fig 1 : Plot of the normalized magneto DMR versus n_0 **in** $n-Cd_3As_2$ **in accordance with (a) proposed dispersion law (b) three-band Kane model (c) two-band Kane model (d) parabolic energy band** $\left(\theta = 75^0, B = 1.5 Tesla\right)$**.**

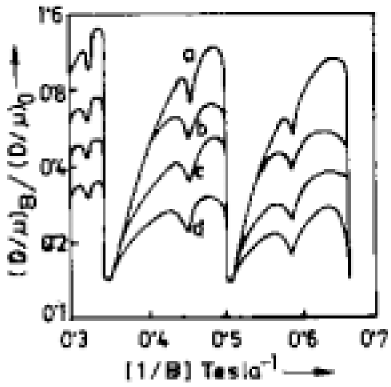

Fig 2 : Plot of the normalized magneto DMR versus 1/B in $n-Cd_3As_2$ **in accordance with (a) the generalized dispersion law (b) three-band Kane model (c) two-band Kane model and (d) parabolic model** $\theta = 75^0$ **,** $n_o = 10^{23} m^{-3}$ **.**

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