2.1 Investigation on Tetragonal Materials

2.1.1 Introduction

It is well known that the $A_{III}^2B_{II}^5$ and the ternary chalcopyrite compounds are called tetragonal materials due to their tetragonal crystal structures [1]. These materials find extensive use in non-linear optical elements [2], photodetectors [3] and light emitting diodes [4]. Rowe and Shay [5] showed that the quasi-cubic model [6] can be used to explain the observed splitting and symmetry properties of the band structure at the zone center of $k$ space of the aforementioned materials. The s-like conduction band is singly degenerate and the p-like valence bands are triply degenerate. The latter splits into three sub-bands because of the spin–orbit and the crystal field interactions. The largest contribution to the crystal field splitting is from the non-cubic potential [7]. The experimental results on the absorption constants, the effective mass, and the optical third order susceptibility indicate that the fact that the conduction band in the same materials corresponds to a single ellipsoidal revolution at the zone center in $k$-space [1, 8]. Introducing the crystal potential in the Hamiltonian, Bodnar [9] derived the electron dispersion relation in the same material under the assumption of an isotropic spin–orbit splitting constant. It would, therefore, be of much interest to investigate the DMR in these compounds by including the anisotropies of the spin–orbit splitting constant and, the effective electron mass together with the inclusion of crystal field splitting, within the framework of $k.p$ formalism since, these are the important physical features of such materials [1].

In what follows, in Sect. 2.1.2 on the theoretical background the expressions for the electron concentration and the DMR for tetragonal compounds have been derived on the basis of the generalized dispersion relation. In Sect. 2.1.3, it has been shown that the corresponding results for III–V, ternary and quaternary materials form special cases of our generalized analysis. The expressions for $n_0$ and DMR for semiconductors whose energy band structures are
defined by the two-band model of Kane and that of parabolic energy bands have further been formulated under certain constraints. For the purpose of numerical computations, n-Cd$_3$As$_2$ and n-CdGeAs$_2$ have been used as examples of $A_{III}B_{II}$ and the ternary chalcopyrite compounds, which are being extensively used in Hall pick-ups, thermal detectors, and non-linear optics [3]. In addition, the DMR has also been numerically investigated by taking n-InAs and n-InSb as examples of III–V semiconductors, n-Hg$_{1-x}$Cd$_x$Te as an example of ternary compounds and n-In$_{1-x}$Ga$_x$As$_y$P$_{1-y}$ lattice matched to InP as example of quaternary materials in accordance with the three and the two band models of Kane together with parabolic energy bands, respectively, for the purpose of relative comparison. The importance of the aforementioned materials in electronics has been discussed in Sect. 2.1.3. Section 2.1.4 contains the results and discussions.

2.1.2 Theoretical Background

The form of \( \mathbf{k.p} \) matrix for tetragonal semiconductors can be expressed, extending Bodnar’s [9] relation, as

\[
H = \begin{bmatrix}
H_{11} & H_{12} \\
H_{21} & H_{22}
\end{bmatrix},
\]

(2.1)

where

\[
H_1 = \begin{bmatrix}
E_g & 0 & P_{||} k_z & 0 \\
0 & (-2\Delta_{||}/3) & (\sqrt{2}\Delta_{\perp}/3) & 0 \\
0 & P_{||} k_z & (\sqrt{2}\Delta_{\perp}/3) - (\delta + \frac{1}{2}\Delta_{||}) & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

and

\[
H_2 = \begin{bmatrix}
0 & -f_+ & 0 & f_- \\
f_+ & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
f_+ & 0 & 0 & 0
\end{bmatrix},
\]

in which \( E_g \) is the band gap, \( P_{||} \) and \( P_{\perp} \) are the momentum matrix elements parallel and perpendicular to the direction of crystal axis respectively, \( \delta \) is the crystal field splitting constant, \( \Delta_{||} \) and \( \Delta_{\perp} \) are the spin–orbit splitting constants parallel and perpendicular to the \( C \)-axis respectively, \( f_{\pm} \equiv (P_{\perp}/\sqrt{2})(k_x \pm ik_y) \) and \( i = \sqrt{-1} \). Thus, neglecting the contribution of the higher bands and the free electron term, the diagonalization of the above matrix leads to the dispersion relation of the conduction electrons in bulk specimens of tetragonal compounds [1] as

\[
\psi_1(E) = \psi_2(E) k_x^2 + \psi_3(E) k_z^2,
\]

(2.2)

where

\[
\psi_1(E) \equiv E + E_g \left[ (E + E_g)(E + E_g + \Delta_{||}) + \delta \left( E + E_g + \frac{2}{3}\Delta_{||} \right) \right. \\
\left. + \frac{2}{9} \left( \Delta_{||}^2 - \Delta_{\perp}^2 \right) \right], \quad k_s^2 = k_x^2 + k_y^2,
\]
\varepsilon_2 (E) \equiv \frac{\hbar^2 E_g (E_g + \Delta_\perp)}{[2m^*_\perp (E_g + \frac{2}{3} \Delta_\perp)]} \left[ \delta \left( E + E_g + \frac{1}{3} \Delta_\parallel \right) + (E + E_g) \times \left( E + E_g + \frac{2}{3} \Delta_\parallel \right) + \frac{1}{9} \left( \Delta_\parallel^2 - \Delta_\parallel^2 \right) \right],

\psi_3 (E) \equiv \frac{\hbar^2 E_g (E_g + \Delta_\parallel)}{[2m^*_\parallel (E_g + \frac{2}{3} \Delta_\parallel)]} \left[ \left( \psi_1 (E) \right)^2 \left( \psi_2 (E) \right)^2 \right] + \left[ \left( \psi_3 (E) \right)^2 \left( \psi_4 (E) \right)^2 \right],

\psi_4 (E) \equiv \left[ \frac{3}{2} \frac{\psi_1 (E)}{\psi_2 (E)} \left( \psi_1 (E) \right)' \right] - \left[ \frac{\psi_2 (E)}{\psi_3 (E)} \left( \psi_2 (E) \right)' \right]^{3/2} \left[ \psi_3 (E) \right]^{3/2} \left[ \psi_4 (E) \right]^{3/2}

\left[ \left( \psi_1 (E) \right)' \right] \equiv \left[ \left( 2E + E_g \right) \psi_1 (E) \left( E + E_g \right)^{-1} \right] \times \left( 2E + 2E_g + \delta + \Delta_\parallel \right),

\left[ \left( \psi_2 (E) \right)' \right] \equiv \left[ 2m^*_\perp \left( E_g + \frac{2}{3} \Delta_\perp \right) \right]^{-1} \left[ \hbar^2 E_g (E_g + \Delta_\perp) \right] \times \left[ \delta + 2E + 2E_g + \frac{2}{3} \Delta_\parallel \right],

and \left[ \left( \psi_3 (E) \right)' \right] \equiv \left[ 2m^*_\parallel \left( E_g + \frac{2}{3} \Delta_\parallel \right) \right]^{-1} \left[ \hbar^2 E_g (E_g + \Delta_\parallel) \right] \left[ 2E + 2E_g + \frac{2}{3} \Delta_\parallel \right],

in which, the primes denote the differentiation of the differentiable functions with respect to \( E \).

Combining (2.3b) with the Fermi–Dirac occupation probability factor and using the generalized Sommerfeld’s lemma [10], the electron concentration can be written as

\[ n_0 = g_v (3\pi^2)^{-1} M (E_F) + N (E_F), \]

where \( M (E_F) \equiv \left[ \frac{\left( \psi_1 (E_F) \right)^2}{\psi_2 (E_F) \sqrt{\psi_3 (E_F)}} \right], \ E_F \) is the Fermi energy as measured from the edge of the conduction band in the vertically upward direction in the
The Einstein Relation in Bulk Specimens of Compound Semiconductors

absence of any quantization, \( N(E_F) \equiv \sum_{r=1}^{s} L(r)M(E_F) \), \( r \) is the set of real positive integers whose upper limit is \( s \), \( L(r) \equiv \left[ 2 (k_B T)^{2r} \left( 1 - 2^{1-2r} \right) \xi (2r) \right] \times \left[ \frac{\epsilon^{2r}}{\epsilon E_F} \right] \) and \( \zeta (2r) \) is the Zeta function of order \( 2r \) [11].

Thus the use of the (2.4) and (1.11) leads to the expression of DMR as

\[
\frac{D}{\mu} = \frac{1}{|e|} \frac{[M(E_F) + N(E_F)]}{\left[ \{M(E_F)\}' + \{N(E_F)\}' \right]}
\]

(2.5)

2.1.3 Special Cases for III–V Semiconductors

(a) Under the substitutions \( \delta = 0 \), \( \Delta || = \Delta \perp = \Delta \) (the isotropic spin–orbit splitting constant) and \( m^*_\parallel = m^*_\perp = m^* \) (the isotropic effective electron mass at the edge of the conduction band), (2.2) assumes the form [1]

\[
\frac{\hbar^2 k^2}{2m^*} = \gamma(E), \quad \gamma(E) \equiv \frac{E(E + E_g)(E + E_g + \Delta) \left( E_g + \frac{2}{3} \Delta \right)}{E_g(E_g + \Delta)(E + E_g + \frac{2}{3} \Delta)},
\]

(2.6)

which is the well-known three band model of Kane [1]. Equation (2.6) is the dispersion relation of the conduction electrons of III–V, ternary and quaternary materials and should be used as such for studying the electron transport in n-InAs where the spin orbit splitting constant is of the order of band gap.

The III–V compounds are used in integrated optoelectronics [12, 13], passive filter devices [14], distributed feedback lasers and Bragg reflectors [15]. Besides, we shall also use n-Hg\(_{1-x}\)Cd\(_x\)Te and n-In\(_{1-x}\)Ga\(_x\)As\(_y\)P\(_{1-y}\) lattice matched to InP as examples of ternary and quaternary materials respectively. The ternary alloy n-Hg\(_{1-x}\)Cd\(_x\)Te is a classic narrow-gap compound and is technologically an important optoelectronic semiconductor because its band gap can be varied to cover a spectral range from 0.8 to over 30\( \mu \)m by adjusting the alloy composition [16]. The n-Hg\(_{1-x}\)Cd\(_x\)Te finds applications in infrared detector materials [17] and photovoltaic detector [18] arrays in the 8-12\( \mu \)m wave bands. The above applications have spurred an Hg\(_{1-x}\)Cd\(_x\)Te technology for the production of high mobility single crystals, with specially prepared surface layers and the same material is suitable for narrow subband physics because the relevant material constants are within experimental reach [19]. The quaternary compounds are being extensively used in optoelectronics, infrared light emitting diodes, high electron mobility transistors, visible heterostructure lasers for fiber optic systems, semiconductor lasers, [20], tandem solar cells [21], avalanche photodetectors [22], long wavelength light sources, detectors in optical fiber communications, [23] and new types of optical devices, which are being prepared from the quaternary systems [24].

Under the aforementioned limiting conditions, the density-of-states function, the electron concentration, and the DMR in accordance with the three band model of Kane assume the following forms
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\[ D_0(E) = 4\pi g_\nu \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{\gamma(E) [\gamma_1(E)]}, \]  

(2.7)

\[ n_0 = \frac{g_\nu}{3\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \left[ M_1(E_F) + N_1(E_F) \right], \]  

(2.8)

and

\[ \frac{D}{\mu} = \frac{1}{|e|} \left[ M_2(E_F) + N_2(E_F) \right] \left[ \{M_2(E_F)\}' + \{N_2(E_F)\}' \right]^{-1}, \]  

(2.9)

where \( \gamma_1(E) \equiv \gamma(E) \left[ \frac{1}{E + E_g} + \frac{1}{E + E_g + \Delta} - \frac{1}{E + E_g + 2\Delta} \right], \) \( M_1(E_F) \equiv [\gamma(E_F)]^{3/2} \) and \( N_1(E_F) \equiv \sum_{r=1}^s L(r) M_1(E_F). \)

(b) Under the inequalities \( \Delta \gg E_g \) or \( \Delta \ll E_g \), (2.6) gets simplified as [1]

\[ \frac{\hbar^2 k^2}{2m^*} = E (1 + \alpha E), \quad \alpha \equiv 1/E_g, \]  

(2.10)

which is known as the two-band model of Kane [1]. Under the above constraints, the forms of the DOS, the electron statistics and the DMR can, respectively, be written as,

\[ D_0(E) = 4\pi g_\nu \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{I(E) [I_1(E)]}, \]  

(2.11)

\[ n_0 = \frac{g_\nu}{3\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \left[ M_2(E_F) + N_2(E_F) \right], \]  

(2.12)

and

\[ \frac{D}{\mu} = \frac{1}{|e|} \left[ M_2(E_F) + N_2(E_F) \right] \left[ \{M_2(E_F)\}' + \{N_2(E_F)\}' \right]^{-1}, \]  

(2.13)

where \( I(E) \equiv E (1 + \alpha E), \) \( I_1(E) \equiv (1 + 2\alpha E), \) \( M_2(E_F) \equiv [I(E_F)]^{3/2} \) and \( N_2(E_F) \equiv \sum_{r=1}^s L(r) M_2(E_F). \)

(c) Under the constraints \( \Delta \gg E_g \) or \( \Delta \ll E_g \) together with the inequality \( \alpha E_F \ll 1 \), we can write [1]

\[ n_0 = g_\nu N_c \left[ F_{1/2}(\eta) + \left( \frac{15\alpha k_B T}{4} \right) F_{3/2}(\eta) \right], \]  

(2.14)

and

\[ \frac{D}{\mu} = \left[ \frac{k_B T}{|e|} \right] \left[ \left( \frac{F_{1/2}(\eta) + \left( \frac{15\alpha k_B T}{4} \right) F_{3/2}(\eta)}{F_{-1/2}(\eta) + \left( \frac{15\alpha k_B T}{4} \right) F_{1/2}(\eta)} \right) \right], \]  

(2.15)
where \( N_C \equiv 2\left(\frac{2\pi m^* k_B T}{\hbar^2}\right)^{3/2} \eta \equiv \frac{E_F}{k_B T} \) and \( F_j(\eta) \) is the one parameter Fermi–Dirac integral of order \( j \) which can be written as \([25]\),

\[
F_j(\eta) = \left(\frac{1}{\Gamma(j+1)}\right) \int_0^\infty y^j (1 + \exp(y - \eta))^{-1} \, dy, \quad j > -1, \tag{2.16}
\]

where \( \Gamma(j+1) \) is the complete Gamma function or for all \( j \), analytically continued as a complex contour integral around the negative axis

\[
F_j(\eta) = A_j \int_{-\infty}^{(0+)} y^j (1 + \exp(-y - \eta))^{-1} \, dy, \tag{2.17}
\]

in which \( A_j \equiv \frac{\Gamma(-j)}{2\pi\sqrt{-1}} \).

(d) For relatively wide gap materials \( E_g \to \infty \) and (2.14) and (2.15) assume the forms

\[
n_0 = g_v N_c F_{1/2}(\eta) \tag{2.18}
\]

and

\[
\frac{D}{\mu} = \left(\frac{k_B T}{|e|}\right) \left[ \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)} \right]. \tag{2.19}
\]

Equation (2.19) was derived for the first time by Landsberg [1].

(e) Combining (2.18) and (2.19) and using the formula \( \frac{d}{d\eta} [F_j(\eta)] = F_j - F_{j-1}(\eta) \) \([25]\) as easily derived from (2.16) and (2.17) together with the fact that under the condition of extreme carrier degeneracy

\[
F_{1/2}(\eta) = \left[\frac{4}{3\sqrt{\pi}}\right] (\eta)^{3/2}, \tag{2.20}
\]

we can write

\[
n_0 = \frac{g_v}{3\pi^2} \left[ \frac{2m^* E_F (1 + \alpha E_F)}{\hbar^2} \right]^{3/2}, \tag{2.21}
\]

and

\[
\frac{D}{\mu} = \frac{1}{|e|} \left(\frac{2}{3}\right) E_F \left(\frac{1 + \alpha E_F}{1 + 2\alpha E_F}\right). \tag{2.22}
\]

For \( \alpha \to 0 \), (2.21) and (2.22) assume the forms

\[
n_0 = \frac{g_v}{3\pi^2} \left[ \frac{2m^* E_F}{\hbar^2} \right]^{3/2}, \tag{2.23}
\]

and

\[
\frac{D}{\mu} = \frac{2E_F}{3|e|}. \tag{2.24}
\]
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(f) Under the condition of non-degenerate electron concentration $\eta \ll 0$ and $F_j(\eta) \equiv \exp(\eta)$ for all $j$ [25]. Therefore (2.18) and (2.19) assume the well-known forms as [1]

$$n_0 = g_v N_c \exp(\eta), \quad (2.25)$$

and

$$\frac{D}{\mu} = k_B T / |e| \quad (2.26)$$

2.1.4 Result and Discussions

Using n-Cd$_3$As$_2$ as an example of A$_2$III-B$_5$II compounds for the purpose of numerical computations and using (2.4) and (2.5) together with the energy band constants at $T = 4.2$ K, as given in Table 2.1, the variation of the DMR as a function of electron concentration has been shown in curve (a) of Fig. 2.1. The circular points exhibit the same dependence and have been obtained by using (1.15) and taking the experimental values of the thermoelectric power in n–Cd$_3$As$_2$ in the presence of a classically large magnetic field [26]. The curve (b) corresponds to $\delta = 0$. The curve (c) shows the dependence of the DMR on $n_0$ in accordance with the three-band model of Kane using the energy band constants as $E_g = 0.095$ eV, $m^* = (m_{||}^* + m_{\perp}^*) / 2$ and $\Delta = (\Delta_{||} + \Delta_{\perp}) / 2$. The curves (d) and (e) correspond to the two-band model of Kane and that of the parabolic energy bands. By comparing the curves (a) and (b) of Fig. 2.1, one can easily assess the influence of crystal field splitting on the DMR in tetragonal compounds. Figure 2.2 represents all cases of Fig. 2.1 for n-CdGeAs$_2$ which has been used as an example of ternary chalcopyrite materials where the values of the energy band constants of the said compound are given in Table 2.1.

It appears from Fig. 2.1 that, the DMR in tetragonal compounds increases with increasing carrier degeneracy as expected for degenerate semiconductors and agrees well with the suggested experimental method of determining the same ratio for materials having arbitrary carrier energy spectra. It has been observed that the tetragonal crystal field affects the DMR of the electrons quite significantly in this case. The dependence of the DMR is directly determined by the band structure because of its immediate connection with the Fermi energy. The DMR increases non-linearly with the electron concentration in other limiting cases and the rates of increase are different from that in the generalized band model.

From Fig. 2.2, one can assess that the DMR in bulk specimens of n-CdGeAs$_2$ exhibits monotonic increasing dependence with increasing electron concentration. The cases (b), (c) and (d) of Fig. 2.2 for n-CdGeAs$_2$ exhibit the similar trends with change in the respective numerical values of the DMR. The influence of spectrum constants on the DMR for n-Cd$_3$As$_2$ and n-CdGeAs$_2$ can also be assessed by comparing the respective variations as drawn in Figs. 2.1 and 2.2 respectively.
### Table 2.1. The numerical values of the energy band constants of few materials

| Materials                  | $|E_g| = 0.095$ eV, $\Delta_{II} = 0.27$ eV, $\Delta_{I} = 0.25$ eV, $m^*_0 = 0.00697m_0$ ($m_0$ is the free electron mass). | n – Cd$_3$As$_2$ |
|----------------------------|-----------------------------------------------------------------------------------------------------------------|-----------------|
| $m^*_0 = 0.01393m_0$, $\delta = 0.085$eV, $g_v = 1$ [25, 73] and $\varepsilon_{sc} = 16\varepsilon_0$ ($\varepsilon_{sc}$ and $\varepsilon_0$ are the permittivity of the semiconductor and free space respectively) [74]. |                                                                                                                   |                 |
| n – CdGeAs$_2$             | $E_g = 0.57$ eV, $\Delta_{I} = 0.30$ eV, $\Delta_{II} = 0.36$ eV, $m^*_0 = 0.034m_0$, $m^*_0 = 0.039m_0$, $T = 4K$, $\delta = -0.21$ eV, $g_v = 1$ [1, 26] and $\varepsilon_{sc} = 18.4\varepsilon_0$ [75]. |                 |
| n–InAs                    | $E_g = 0.36$ eV, $\Delta = 0.43$ eV and $m^* = 0.026m_0$, $g_v = 1$, $\varepsilon_{sc} = 12.25\varepsilon_0$ [76]. |                 |
| n–InSb                    | $E_g = 0.2352$ eV, $\Delta = 0.81$ eV and $m^* = 0.01359m_0$, $g_v = 1$, $\varepsilon_{sc} = 15.56\varepsilon_0$ [76]. |                 |
| n– Ga$_{1-x}$Al$_x$As     | $E_g(x) = (1.424 + 1.266x + 0.26x^2)eV$, $\Delta(x) = (0.34 - 0.5x)eV$, $m^*(x) = [0.066 + 0.088x]m_0$, $g_v = 1$, $\varepsilon_{sc} = [13.18 - 3.12x] \varepsilon_0$ [77]. |                 |
| Hg$_{1-x}$Cd$_x$Te         | $E_g(x) = (-0.302 + 1.93x + 5.35 \times 10^{-4}(1 - 2x)T - 0.810x^2 + 0.832x^3) eV$, $\Delta(x) = (0.63 + 0.24x - 0.27x^2) eV$, $m^*_0 = 0.1m_0E_g(eV)^{-1}$, $g_v = 1$ and $\varepsilon_{sc} = [20.262 - 14.812x + 5.22795x^2] \varepsilon_0$ [78]. |                 |
| In$_{1-x}$Ga$_x$As$_y$P$_{1-y}$, lattice matched to InP | $E_g = (1.337 - 0.73y + 0.13y^2) eV$, $\Delta = (0.114 + 0.26y - 0.22y^2) eV$, $m^* = (0.08 - 0.039y) m_0$, $y = (0.1896 - 0.4052x)(0.1896 - 0.0123x)^{-1}$, $g_v = 1$ [79] and $\varepsilon_{sc} = [10.65 + 0.1320y] \varepsilon_0$ [80]. |                 |
| CdS                       | $m^*_0 = 0.7m_0$, $m^*_0 = 1.5m_0$ and $\lambda_0 = 1.4 \times 10^{-10} eVm$, $g_v = 1$ [76] and $\varepsilon_{sc} = 15.56\varepsilon_0$ [81]. |                 |
| n-PbTe                    | $m^*_0 = 0.070m_0$, $m^*_0 = 0.54m_0$, $m^*_0 = 0.010m_0$, $m^*_0 = 1.4m_0$, $P_l = 141$ meV nm, $P_\perp = 486$ meV nm, $E_g = 190$ meV, $g_v = 4$ [12] and $\varepsilon_{sc} = 33\varepsilon_0$ [76, 82]. |                 |
| n-PbSnTe                  | $m^*_0 = 0.063m_0$, $m^*_0 = 0.41m_0$, $m^*_0 = 0.089m_0$, $m^*_0 = 1.6m_0$, $P_l = 137$ meV nm, $P_\perp = 464$ meV nm, $E_g = 90$ meV, $g_v = 4$ [12] and $\varepsilon_{sc} = 60\varepsilon_0$ [76, 82]. |                 |
| n-Pb$_{1-x}$Sn$_x$Se      | $x = 0.31$, $g_v = 4$, $m^*_0 = 0.143m_0$, $m^*_0 = 2.0m_0$, $m^*_0 = 0.167m_0$, $m^*_0 = 0.286m_0$, $P_l = 3.2 \times 10^{-10}$ eVm, $P_\perp = 4.1 \times 10^{-10}$ eVm, $E_g = 0.137eV$, $g_v = 4$ [12] and $\varepsilon_{sc} = 31\varepsilon_0$ [76, 83]. |                 |
| Stressed n-InSb           | $m^*_0 = 0.048m_0$, $E_g = 0.081$ eV, $B_2 = 9 \times 10^{-10}$ eVm, $C_1 = 3$ eV, $C_2 = 2$ eV, $\alpha_0 = -10$ eV, $b_0 = -1.7$ eV, $d_0 = -4.4$ eV, $S_{xx} = 0.6 \times 10^{-3}$ (kbar)$^{-1}$, $S_{yy} = 0.42 \times 10^{-3}$ (kbar)$^{-1}$, $S_{zz} = 0.39 \times 10^{-3}$ (kbar)$^{-1}$ and $S_{xy} = 0.5 \times 10^{-3}$ (kbar)$^{-1}$, $\varepsilon_{sc} = \sigma S_{xx}$, $\varepsilon_{yy} = \sigma S_{yy}$, $\varepsilon_{xy} = \sigma S_{xy}$ and $\sigma$ is the stress in kilobar, $g_v = 1$ [44]. |

(Continued)
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Table 2.1. Continued

<table>
<thead>
<tr>
<th>Material</th>
<th>For conduction bands, along &lt;111&gt; direction,</th>
</tr>
</thead>
<tbody>
<tr>
<td>PtSb₂</td>
<td>$\lambda_1 = 0.33 \text{ eV}, ; l_1 = 1.09 \text{ eV}, ; \nu_1 = 0.17 \text{ eV}, ; n_1 = 0.22 \text{ eV}, ; a = 0.643 \text{ nm}, ; I_0 = 0.30 (\text{eV})^2, ; \delta_0 = 0.33 \text{ eV}, ; g_\nu = 8 ; [%56]\text{ and } \varepsilon_{\text{sc}} = 30 \varepsilon_0 ; [%56,84]$</td>
</tr>
<tr>
<td>n-GaSb</td>
<td>$E_g = 0.81 \text{ eV}, ; \Delta = 0.80 \text{ eV}, ; P = 9.48 \times 10^{-10} \text{ eVm}, ; \zeta_0 = -2.1, ; \nu_0 = -1.49, ; \varphi_0 = 0.42, ; g_\nu = 1 ; [%53]\text{ and } \varepsilon_{\text{sc}} = 15.85 \varepsilon_0 ; [%53,85]$</td>
</tr>
<tr>
<td>HgTe</td>
<td>$m^*<em>1 = 0.028 m_0, ; g</em>\nu = 1$ and $\varepsilon_\infty = 15.2 \varepsilon_0 ; [%52]$</td>
</tr>
<tr>
<td>Bismuth</td>
<td>$E_g = 0.0153 \text{ eV}, ; m_1 = 0.00194 m_0, ; m_2 = 0.313 m_0, ; m_3 = 0.00246 m_0, ; m'<em>2 = 0.36 m_0, ; g</em>\nu = 3$ and $g_\varepsilon = 2 ; [%42]$</td>
</tr>
</tbody>
</table>

Fig. 2.1. The plot of the DMR in the bulk specimens of n-Cd₃As₂ as a function of electron concentration in accordance with (a) the generalized band model; (b) $\delta = 0$; (c) the three band model of Kane; (d) the two band model of Kane and (e) the parabolic energy bands. The dotted circular points show the same dependence which have been obtained by using (1.15) and taking the experimental values of the thermoelectric power of the electrons in bulk n-Cd₃As₂ in the presence of a classically large magnetic field [26]

Using the appropriate equations, one can numerically evaluate the DMR as a function of electron concentration for n-InAs, whose energy band constants are presented in Table 2.1. This is shown in Fig. 2.3 by curves (a), (b) and (c) respectively, in accordance with the three and two band models of Kane together with the model of parabolic energy bands. Figure 2.4 exhibits all the cases of Fig. 2.3 for n-InSb whose energy band constants are given in Table 2.1.
Fig. 2.2. The plot of the DMR in the bulk specimens of n-CdGeAs$_2$ as a function of electron concentration in accordance with (a) the generalized band model; (b) $\delta = 0$; (c) the three band model of Kane; (d) the two band model of Kane and (e) the parabolic energy bands

From Figs. 2.3 and 2.4 one can observe that the numerical values of the DMR for n-InAs and n-InSb in accordance with the three band model of Kane are less than that of the corresponding parabolic energy bands for relatively large values of the electron concentration. Also, the numerical values of the DMR in accordance with two-band model of Kane also changes as compared with the corresponding three-band model of Kane for n-InAs. The influence of energy band constants on the DMR for n-InAs and n-InSb becomes apparent by comparing Figs. 2.3 and 2.4 respectively.

For n-Hg$_{1-x}$Cd$_x$Te together with the numerical values of the spectrum constants as given in Table 2.1, the DMR has been plotted at $T = 4.2$ K as a function of electron concentration as shown in Fig. 2.5 for all cases of Fig. 2.3. Figure 2.6 represents the variation of the DMR with respect to alloy composition $x$ in this case.

It appears from Fig. 2.5 that the DMR of ternary materials increases with increasing carrier degeneracy. From Fig. 2.6, it appears that the DMR in ternary materials decreases with increasing alloy composition. The plots of Figs. 2.5 and 2.6 are valid for $x > 0.17$, due to the fact that for $x < 0.17$, the band gap becomes negative in n-Hg$_{1-x}$Cd$_x$Te leading to a semimetallic state.

For n-In$_{1-x}$Ga$_x$As$_y$P$_{1-y}$ lattice matched to InP together with the values of the energy band constants as given in Table 2.1, the DMR has been plotted as a function of electron concentration as shown in Fig. 2.7 in accordance with the three and two band models of Kane together with the isotropic parabolic energy band. It appears that the DMR monotonically increases with increasing $n_0$. Figure 2.8 shows the dependence of the DMR in n-In$_{1-x}$Ga$_x$As$_y$P$_{1-y}$...
2.1 Investigation on Tetragonal Materials

Fig. 2.3. The plot of the DMR in bulk specimens of n-InAs as a function of electron concentration in accordance with (a) the three-band model of Kane, (b) the two-band model of Kane, and (c) the parabolic energy bands.

Fig. 2.4. The plot of the DMR in bulk specimens of n-InSb as a function of electron concentration in accordance with (a) the three-band model of Kane, (b) the two-band model of Kane, and (c) the parabolic energy bands.
Fig. 2.5. The plot of the DMR in bulk specimens of $n$-Hg$_{1-x}$Cd$_x$Te as a function of electron concentration in accordance with (a) the three band model of Kane; (b) the two band model of Kane and (c) the parabolic energy bands ($x = 0.3$).

Fig. 2.6. The plot of the DMR in bulk specimens of $n$-Hg$_{1-x}$Cd$_x$Te as a function of alloy composition ($x$) in accordance with (a) the three band model of Kane; (b) the two band model of Kane and (c) the parabolic energy bands ($n_0 = 10^{22}$ per cubic meter).
2.1 Investigation on Tetragonal Materials

Fig. 2.7. The plot of the DMR in bulk specimens of $n\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ lattice matched to InP as a function of electron concentration in accordance with (a) the three band model of Kane; (b) the two band model of Kane and (c) the parabolic energy bands ($y = 0.037$).

Fig. 2.8. The plot of the DMR in bulk specimens of $n\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ lattice matched to InP as a function of alloy composition ($x$) in accordance with (a) the three band model of Kane; (b) the two band model of Kane and (c) the parabolic energy bands ($y = 0.037$).
lattice matched to InP on the alloy composition of \( x \) for all cases of Fig. 2.6. The DMR decreases with increasing \( x \) for all types of band models in this case. From Figs. 2.5 up to 2.8, one can infer the influence of energy band constants on the DMR for ternary and quaternary compounds respectively.

It may be noted that in recent years, the electron mobility in compound semiconductors has been extensively investigated, but the diffusion constant (a very important device quantity which cannot be easily determined experimentally) of such materials has been relatively less investigated. Therefore, the theoretical results presented in this chapter will be useful in determining the diffusion constants for even relatively wide gap materials whose energy band structures can be approximated by the parabolic energy bands.

We wish to point out that in formulating the basic dispersion relation we have taken into account the combined influences of the crystal field-splitting constant, the anisotropies in the effective electron masses, and the spin–orbit splitting constants, respectively, since these are the significant physical features of the tetragonal compounds.

In the absence of crystal-field splitting together with the assumptions of isotropic effective electron mass and isotropic spin–orbit splitting constant respectively, our basic equation (2.2) converts to the well-known form of the three-band model of Kane as given by (2.6). Many technologically important compounds obey the inequalities \( \Delta \gg E_g \) or \( \Delta \ll E_g \). Under these constraints, (2.6) gets simplified into (2.10) and is known as the two-band model of Kane. Finally, for \( E_g \to \infty \), as for relatively wide gap materials the above equation transforms into the well-known form \( E = \frac{\hbar^2 k^2}{2m^*} \). In addition, the DMR in ternary and quaternary materials has also been investigated in accordance with the three and two band models of Kane together with the parabolic energy band for the purpose of relative assessment. Therefore, the influence of energy band constants on the DMR can also be studied from the present investigation and the basic equation (2.2) covers various materials having different energy band structures. Finally, one infers that, this simplified analysis exhibits the basic features of the DMR in bulk specimens of many technologically important compounds and for n-Cd\(_3\)As\(_2\), the theoretical result is in good agreement with the suggested experimental method of determining the same ratio.

### 2.2 Investigation for II–VI Semiconductors

#### 2.2.1 Introduction

The II–VI compounds are being extensively used in infrared detectors [27], ultra high speed bipolar transistors [28], optic fiber communications [29], and advanced microwave devices [30]. These materials possess the appropriate direct band gap to produce light emitting diodes and lasers from blue to red wavelengths [31]. The Hopfield model describes the energy spectra of both
the carriers of II–VI semiconductors where the splitting of the two-spin states by the spin orbit coupling and the crystalline field has been taken into account [32]. The DMR in II–VI compounds on the basis of the Hopfield model has been studied by formulating the expression of carrier concentration in Sect. 2.2.2. Section 2.2.3 contains the result and discussions for the numerical computation of the DMR taking p-CdS as an example.

2.2.2 Theoretical Background

The group theoretical analysis shows that, based on the symmetry properties of the conduction and valence band wave functions, both the energy bands of II–VI semiconductors can be written as

\[ E = a'_0 k^2 + b'_0 k_z^2 \pm \bar{\lambda}_0 k_s, \]  

(2.27)

where \( a'_0 \equiv \frac{\hbar^2}{2m^*_1} \), \( b'_0 \equiv \frac{\hbar^2}{2m^*_1} \) and \( \bar{\lambda}_0 \) represents the splitting of the two spin-states by the spin–orbit coupling and the crystalline field.

The volume in k-space enclosed by (2.27) can be expressed as

\[ V(E) = \frac{\pi}{2a'_0} \int_{-(E/b'_0)^{1/2}}^{(E/b'_0)^{1/2}} \left[ \bar{\lambda}_0^2 + 2a'_0 \sqrt{E} - 2a'_0 b'_0 k_z^2 - \bar{\lambda}_0 \left( \bar{\lambda}_0^2 - 4a'_0 b'_0 k_z^2 + 4a'_0 E \right) \right] \]  

(2.28)

From (2.28), one can write

\[ V(E) = \frac{\pi}{2a'_0} \left[ \frac{E^3/2}{3a'_0 \sqrt{b'_0}} + \frac{3 (\bar{\lambda}_0)^2 \sqrt{E}}{8 a'_0} - \frac{3 \bar{\lambda}_0}{4 a'_0} \left( E + \frac{\bar{\lambda}_0^2}{4a'_0} \right) \right] \]  

(2.29)

Hence, the density of states function can be written using (2.3a) and (2.29) as

\[ D_0(E) = \frac{g_v}{2\pi^2 a'_0 \sqrt{b'_0}} \left[ \sqrt{E} - \left( \frac{\bar{\lambda}_0}{2 \sqrt{a'_0}} \right) \sin^{-1} \left( \frac{\sqrt{E + (\bar{\lambda}_0)^2 / 4a'_0}}{\sqrt{E + (\bar{\lambda}_0)^2 / 4a'_0}} \right) \right] \]  

(2.30)

Combining (2.30) with the Fermi–Dirac occupation probability factor, the carrier concentration can be written as

\[ n_0 = \frac{4\pi g_v}{3a'_0 \sqrt{b'_0}} \left[ \tau_1(E_F) + \tau_2(E_F) \right], \]  

(2.31)
where \( \tau_1 (E_F) \equiv \left[ \frac{E_F^{3/2}}{\bar{\lambda}_0} + \frac{3}{8} \frac{(\bar{\lambda}_0)^2}{a_0} \sqrt{E_F} - \frac{3}{4} \frac{\lambda_0}{\sqrt{a_0}} \left( E_F + \frac{(\bar{\lambda}_0)^2}{4a_0} \right) \sin^{-1} \left( \frac{\sqrt{E_F}}{E_F + \frac{(\bar{\lambda}_0)^2}{4a_0}} \right) \right] \), and \( \tau_2 (E_F) \equiv \sum_{r=1}^{s} L(r) \tau_1 (E_F) \).

Combining (2.31) and (1.11), the DMR in bulk specimens of II–VI semiconductors assumes the form

\[
\frac{D}{\mu} = \frac{1}{|e|} \left[ \frac{\tau_1 (E_F) + \tau_2 (E_F)}{[\tau_1 (E_F)]' + [\tau_2 (E_F)]'} \right],
\]

(2.32)

Under the condition \( \bar{\lambda}_0 \to 0 \), (2.27) gets simplified as

\[
E = a_0' k_s^2 + b_0' k_z^2,
\]

(2.33)

Thus, under the condition \( \bar{\lambda}_0 \to 0 \), (2.32) reduces to the well-known form as given by (2.19).

### 2.2.3 Result and Discussions

Using (2.31) and (2.32) together with the spectrum constants as given in Table 2.1, for p-CdS, the DMR has been plotted as a function of hole concentration \( p_0 \) as shown by curve (a) of Fig. 2.9 in which the plot for \( \bar{\lambda}_0 = 0 \) (curve

![Fig. 2.9. The plot of the dependence of the DMR on hole concentration \( p_0 \) for bulk specimens of p-CdS for (a) \( \bar{\lambda}_0 \neq 0 \) and (b) \( \bar{\lambda}_0 = 0 \)](image_url)
2.3 McClure–Choi, the Cohen, the Lax, and the Parabolic Ellipsoidal Band

(b) has also been drawn for the purpose of assessing the influence of the splitting of the two spin states by the spin–orbit coupling and the crystalline field on DMR. From Fig. 2.8 it appears that the DMR increases with increasing hole concentration at a rate greater than that corresponding to the zero value of $\tilde{\lambda}_0$. For relatively low values of $p_0$, the effect of $\tilde{\lambda}_0$ increases whereas the same constant affects the DMR less significantly for relatively higher values of carrier degeneracy. The presence of $\tilde{\lambda}_0$ enhances the numerical values of DMR in II–VI compounds for the whole range of concentration considered as compared with that corresponding to $\tilde{\lambda}_0 = 0$.

2.3 Investigation for Bi in Accordance with the McClure–Choi, the Cohen, the Lax, and the Parabolic Ellipsoidal Band Models

2.3.1 Introduction

It is well-known that the carrier energy spectra in Bi differ considerably from the simple spherical energy wave vector dispersion relation of the degenerate electron gas and several models have been developed to describe the energy spectra of Bi. Earlier works [33, 34] demonstrated that the physical properties of Bi could be described by the ellipsoidal parabolic energy band model. Shoenberg [33] showed that the de Haas-Van Alphen and cyclotron resonance experiments supported the ellipsoidal parabolic model, though the latter work showed that Bi could be described by the two-band model due to the fact that the magnetic field dependence of many physical properties of Bi supports the above model [35]. The experimental results of the magneto-optical [35] and the ultrasonic quantum oscillations [36] favor the Lax ellipsoidal non-parabolic model [35]. Kao [37], Dinger and Lawson [38] and Koch and Jensen [39] observed that the Cohen model [40], is in better agreement with the experimental results. McClure and Choi [41] presented a new model of Bi, which was more accurate and general than those that were currently available. They showed that it can explain the data for a large number of magneto-oscillatory and resonance experiments. We shall study the influence of different energy band models on the DMR in bulk specimens of Bi which have been investigated by formulating the carrier concentration in Sect. 2.3.2. Section 2.3.3 contains the result and discussions in this context.

2.3.2 Theoretical Background

(a) The McClure and Choi model

The carrier energy spectra in Bi can be written, following McClure and Choi, [42] as
\[ E (1 + \alpha E) = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{p_z^2}{2m_3} + \frac{p_y^2}{2m_2} \alpha E \left\{ 1 - \left( \frac{m_2}{m'_2} \right) \right\} + \frac{p_z^2 \alpha}{4m_2m'_2} - \frac{\alpha p_x^2 p_y^2}{4m_1m_2} - \frac{\alpha p_y^2 p_z^2}{4m_1m_3} \]  

(2.34)

where \( m_1, m_2 \) and \( m_3 \) are the effective carrier masses at the band-edge along \( x, y \) and \( z \) directions respectively and \( m'_2 \) is the effective mass tensor component at the top of the valence band (for electrons) or at the bottom of the conduction band (for holes).

The area of the ellipse in the \( k_x - k_z \) plane can be expressed as

\[ A (E, k_y) = \tilde{T}_0 \left[ E (1 + \alpha E) - \theta_2 (E) k_y^2 - \theta_3 k_y^4 \right], \]

(2.35)

where \( \tilde{T}_0 \equiv \left( \frac{2\pi \sqrt{m_1 m_3}}{\hbar^2} \right) \), \( \theta_2 (E) \equiv \left( \frac{\alpha E k^2}{2m_2} \right) \left( 1 - \frac{m_2}{m'_2} \right) + \frac{\hbar^2}{2m_2} \), \( \theta_3 \equiv \left( \frac{\alpha \hbar^4}{4m_2 m'_2} \right) \) and \( \theta_4 \equiv \left( \frac{\alpha \hbar^2}{2m_2} \right) \).

The volume of k-space enclosed by (2.34) can be written as

\[ V (E) = \left( \frac{4\pi \sqrt{m_1 m_3}}{\hbar^2 \theta_4} \right) \int_0^{p_0 (E)} \left[ \frac{h_0 (E)}{\theta_5^2 - k_y^2} + \theta_2 (E) + \theta_3 (\theta_5^2 + k_y^2) \right] \, dk_y, \]

(2.36)

where \( p_0 (E) \equiv \left( \frac{\sqrt{2m_2 m'_2}}{\hbar \sqrt{\theta_4}} \right) \left[ -\theta_2 (E) + \sqrt{\theta_2^2 (E) + \theta_3 E (1 + \alpha E)} \right]^{1/2} \), \( \theta_5 \equiv (\theta_4)^{-1/2} \) and \( h_0 (E) \equiv \left[ E (1 + \alpha E) - \theta_2 (E) \theta_5^2 - \theta_3 \theta_5^4 \right] \).

From (2.36) one obtains

\[ V (E) = \frac{4\pi \sqrt{m_1 m_3}}{\hbar^2 \theta_4} \left[ \frac{h_0 (E)}{2\theta_5} \ln \left| \frac{\theta_5 + p_0 (E)}{\theta_5 - p_0 (E)} \right| + \theta_2 (E) + \theta_3 \theta_5^2 \right] p_0 (E) \]

\[ + \frac{\theta_3}{3} \left[ p_0 (E) \right]^3. \]

(2.37)

The density-of-states function in this case can be expressed using (2.3a) as

\[ D_0 (E) = \left( \frac{g_v \sqrt{m_1 m_3}}{\pi^2 \hbar^2 \theta_4} \right) \left[ \left\{ h_0 (E) \right\}' \ln \left| \frac{\theta_5 + p_0 (E)}{\theta_5 - p_0 (E)} \right| + h_0 (E) \left( p_0 (E) \right)' \right] \]

\[ + \left\{ \theta_2 (E) \right\}' \left( p_0 (E) \right)' + \left\{ \theta_3 \right\} \left\{ p_0 (E) \right\}' \left\{ \theta_3 \right\} \left( p_0 (E) \right)' \]  

(2.38)

where \( \left\{ h_0 (E) \right\}' \equiv \left[ 1 + 2\alpha E - \left( \frac{\alpha \hbar^2}{2m_2} \right) \left( 1 - \frac{m_2}{m'_2} \right) \right], \left\{ \theta_2 (E) \right\}' \equiv \left( \frac{\alpha \hbar^2}{2m_2} \right) \times \left( 1 - \frac{m_2}{m'_2} \right) \) and
\[
\{p_0(E)\}' = \left[ \frac{1}{2} \frac{\theta_2(E)}{p_0(E)} \right] - \frac{2\theta_2(E)}{2\theta_2(E)} \left[ \theta_2(E) + \theta_3(1 + 2\alpha E) \right] \left( 2\sqrt{\theta_2^2(E) + \theta_3 E (1 + \alpha E)} \right)^{-1}.
\]

Therefore the electron concentration is given by
\[
n_0 = \theta_6 \left[ M_2(E_F) + N_2(E_F) \right].
\]

(b) The Cohen model

In accordance with Cohen [40], the dispersion law of the carriers in Bi is given by
\[
E(1 + \alpha E) = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_3} + \frac{\alpha E p_y^2}{2m_2} + \frac{\alpha p_y^4}{4m_2m^2} + \frac{p_0^2}{2m_2} (1 + \alpha E),
\]

In this case the area of the ellipse in the \( k_x - k_z \) plane can be written as
\[
A(E, k_y) = \frac{2\pi \sqrt{m_1m_3}}{\hbar^2} \left[ E(1 + \alpha E) - \frac{\alpha p_y^4}{4m_2m_2} + \frac{\alpha E p_y^2}{2m_2} - \frac{\alpha E}{2m_2} (1 + \alpha E) \right].
\]

Therefore the volume enclosed by (2.41) is given by
\[
V(E) = \frac{4\pi \sqrt{m_1m_3}}{\hbar^2} \int_0^{\theta_0(E)} \left[ E(1 + \alpha E) - \frac{\alpha E p_y^2}{2m_2} - \frac{\alpha E}{2m_2} (1 + \alpha E) \right] dk_y.
\]
where \( \bar{p}_0(E) \equiv \frac{1}{\hbar} \left[ \frac{\alpha}{2m_1m_2} \right]^{-1/2} \left[ - \left[ \frac{1 + \alpha E}{2m_2} - \frac{\alpha E}{m_2} \right] + \left[ \frac{1 + \alpha E}{2m_1m_2} - \frac{\alpha E}{2m_2} \right]^2 \right]^{1/2} \). Thus, combining (2.44) and (1.11), we can write the expression of the DMR in bismuth in accordance with the Cohen model as

\[
D = \frac{1}{\mu} \frac{[M_3(E_F)] + N_3(E_F)}{[M_3(E_F)] + [N_3(E_F)]},
\]

(c) The Lax model

The carrier spectrum of Bi in accordance with the Lax model is given by [35]
\[ E (1 + \alpha E) = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{p_z^2}{2m_3}. \]  
(2.46)

For this model, under the condition \( \alpha E_F \ll 1 \), the expressions for \( n_0 \) and DMR in Bi, in accordance with the Lax non-parabolic and ellipsoidal model, get simplified to (2.14) and (2.15) where

\[ N_c \equiv 2 \left[ \frac{2\pi (m_1m_2m_3)^{\frac{1}{3}} k_B T}{\hbar^2} \right]^\frac{2}{3}. \]

(d) Ellipsoidal parabolic model

The carrier energy spectra for this type of band model of Bi can be written as [33]

\[ E = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{p_z^2}{2m_3}. \]  
(2.47)

For this model, the expressions of carrier concentration and DMR are respectively given by (2.18) and (2.19) where \( N_c \) has been defined as above.

2.3.3 Result and Discussions

Using (2.39) and (2.40) and taking the spectrum constants from Table 2.1, in curve (a) of Fig. 2.10, the DMR in Bi has been plotted as a function of electron concentration by using the McClure and Choi model. The curves (b),

![Fig. 2.10. The plot of the DMR in bulk specimens of bismuth as a function of electron concentration in accordance with the model of (a) the McClure Choi; (b) the Cohen; (c) the Lax and (d) the ellipsoidal parabolic energy bands.](image)
(c) and (d) exhibit the same dependence in accordance with the Cohen, the Lax, and the parabolic ellipsoidal models respectively.

From Fig. 2.10, it appears that the DMR increases with increasing \( n_0 \) for all the models of Bi. In accordance with the model of McClure and Choi, the DMR exhibits the least numerical values as compared to the other models of Bi. For various energy band models, the values of the DMR with respect to the electron concentration are different. The rates of variations of the DMR with respect to \( n_0 \) are also different for different types of energy band models. It should be noted that under the condition \( \alpha \rightarrow 0 \), the models of McClure and Choi, the Cohen and the Lax reduce to (2.47). Thus, under certain constraints, all the three energy models are reduced to the ellipsoidal parabolic energy bands and the expression for the DMR under the same condition gets simplified to the well-known equation (2.19) as given for the first time by Landsberg [1].

The Cohen model is often used to describe the dispersion relation of the carriers of IV–VI semiconductors. The model of Bi, by Lax, under the condition of the isotropic effective mass of the carriers of the band edge (i.e. \( m_1 = m_2 = m_3 = m^* \)) reduces to the two-band model of Kane, which is used to investigate the physical features of III–V compounds, in general, excluding n-InAs. Thus, the analysis is valid not only for bismuth, but also for all lead chalcogenides, III–V compounds excluding n-InAs, and wide-gap materials respectively. The influence of the energy band models on the DMR of Bi can also be assessed from the Fig. 2.10. It can be noted that the present analysis is valid for the holes of Bi with the appropriate values of the energy band constants.

2.4 Investigation for IV–VI Semiconductors

2.4.1 Introduction

The IV–VI compounds are being extensively used in thermoelectric devices, superlattices, and other quantum effect devices [43]. The dispersion relation of the carriers of the IV–VI compounds could be described by the Cohen model [40], which includes the band non-parabolicity and the anisotropies of the effective masses of the carriers. The DMR in bulk specimens of IV–VI materials has been studied, taking n-PbTe, n-PbSnTe, and n-Pb\(_{1-x}\)Sn\(_x\)Se as examples. Sections 2.4.2 and 2.4.3 contain the theoretical background and the result and discussions in this context.

2.4.2 Theoretical Background

The expressions of \( n_0 \) and the DMR in this case are given by (2.44) and (2.45) in which the energy band constants correspond to the IV–VI compounds.
2.4.3 Result and Discussions

Using (2.44) and (2.45) together with the spectrum constants as given in Table 2.1 for n-PbTe, n-PbSnTe, and n-Pb\(_{1-x}\)Sn\(_x\)Se, the DMR has been plotted as a function of electron concentration \(n_0\) as shown in Fig. 2.11 where the plots (a), (b) and (c) correspond to the said materials respectively in accordance with the Cohen model. From Fig. 2.11, it appears that the DMR for a fixed \(n_0\) is maximum for n-PbTe and minimum for n-Pb\(_{1-x}\)Sn\(_x\)Se. For relatively low values of \(n_0\), the values of the DMR for the three materials exhibit convergence behavior whereas for relatively large values of \(n_0\), the numerical values differ from each other. Besides, our present analysis is also valid for p-type IV–VI materials with the proper change in the energy band constants.

2.5 Investigation for Stressed Kane Type Semiconductors

2.5.1 Introduction

In recent years there has been a considerable interest in studying the various electronic properties of stressed materials because of their important physical characteristics [44]. In this section we shall study the DMR in stressed...
semiconductors, taking stressed n-InSb as an example for numerical computations. Sections 2.5.2 and 2.5.3 contains the theoretical background and the result and discussions in this context.

2.5.2 Theoretical Background

The electron energy spectrum in stressed Kane type semiconductors can be written \[44\] as

\[
\left( \frac{k_x}{a_0 (E)} \right)^2 + \left( \frac{k_y}{b_0 (E)} \right)^2 + \left( \frac{k_z}{c_0 (E)} \right)^2 = 1, \tag{2.48}
\]

where

\[
[a_0 (E)]^2 \equiv \frac{\bar{K}_0 (E)}{A_0 (E) + \frac{1}{2} D_0 (E)}, \quad \bar{K}_0 (E) \equiv \left[ E - C_1 \varepsilon - \frac{2C_2 \varepsilon^2}{3E_g} \right] \left( \frac{3E_g'}{2B_2^2} \right),
\]

\[
C_1 \quad \text{is the conduction band deformation potential,} \quad \varepsilon \quad \text{is the trace of the strain tensor } \hat{\varepsilon} \text{ which can be written as } \hat{\varepsilon} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{xy} & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix}, \quad C_2 \quad \text{is a constant which describes the strain interaction between the conduction and valance bands}, \quad E_g' \equiv E_g + E - C_1 \varepsilon, \quad B_2 \quad \text{is the momentum matrix element},
\]

\[
\bar{A}_0 (E) \equiv \left[ 1 - \frac{(\bar{a}_0 + C_1)}{E_g'} + \frac{3\bar{b}_0 \varepsilon_{xx}}{2E_g'} - \frac{\bar{b}_0 \varepsilon}{2E_g'} \right], \quad \bar{a}_0 \equiv -\frac{1}{3} \left( \bar{b}_0 + 2\bar{m} \right), \quad \bar{b}_0 \equiv \frac{1}{3} (\bar{l} - \bar{m}), \quad \bar{a}_0 \equiv \frac{2\bar{n}}{\sqrt{3}},
\]

\[
\bar{l}, \bar{m}, \bar{n} \quad \text{are the matrix elements of the strain perturbation operator}, \quad \bar{D}_0 (E) \equiv (d_0 \sqrt{3}) \frac{\bar{A}_0 }{E_g'}, \quad \bar{b}_0 (E) \equiv \left( \frac{\bar{b}_0 (E)}{E_g'} \right), \quad \bar{c}_0 (E) \equiv \left( \frac{\bar{c}_0 (E)}{E_g'} \right), \quad \bar{l}_0 (E) \equiv \left( \frac{\bar{l}_0 (E)}{E_g'} \right), \quad \bar{m}_0 (E) \equiv \left( \frac{\bar{m}_0 (E)}{E_g'} \right), \quad \bar{n}_0 (E) \equiv \left( \frac{\bar{n}_0 (E)}{E_g'} \right),
\]

\[
[a_0 (E)]^2 \equiv \frac{\bar{K}_0 (E)}{A_0 (E) - \frac{1}{2} D_0 (E)}, \quad [\bar{c}_0 (E)]^2 \equiv \frac{\bar{K}_0 (E)}{L_0 (E)} \quad \text{and} \quad L_0 (E) \equiv \left[ 1 - \frac{(\bar{a}_0 + C_1)}{E_g'} + \frac{3\bar{b}_0 \varepsilon_{xx}}{2E_g'} - \frac{\bar{b}_0 \varepsilon}{2E_g'} \right].
\]

The density-of-states function in this case can be written using (2.3a) and (2.48) as

\[
D_0 (E) = g_v \left( 3\pi^2 \right)^{-1} \left[ a_0 (E) \bar{b}_0 (E) [\bar{c}_0 (E)]' + \bar{a}_0 (E) \left[ \bar{b}_0 (E) \right]' \bar{c}_0 (E) + [\bar{a}_0 (E)]' \bar{b}_0 (E) \bar{c}_0 (E) \right], \tag{2.49}
\]
Combining (2.49) with the Fermi–Dirac occupation probability factor and using the generalized Sommerfelds lemma [10], the electron concentration in this case can be expressed as

\[ n_0 = g_v \left( \frac{3\pi^2}{2} \right)^{-1} [M_4 (E_F) + N_4 (E_F)], \]  

(2.50)

where \( M_4 (E_F) \equiv \left[ \bar{a}_0 (E_F) \bar{b}_0 (E_F) \bar{c}_0 (E_F) \right] \) and \( N_4 (E_F) \equiv \sum_{r=1}^{s} L (r) M_4 (E_F). \)

Thus using (2.50) and (1.11) we get

\[ D \mu = \frac{1}{|e|} \frac{[M_4 (E_F) + N_4 (E_F)]}{\left[ \left\{ M_4 (E_F) \right\} + \left\{ N_4 (E_F) \right\} \right]}, \]

(2.51)

In the absence of stress together with the substitution \( B^2_2 \equiv \frac{3\hbar^2 E_g}{4m^*} \), (2.51) gets simplified to (2.13).

### 2.5.3 Result and Discussions

Using (2.50) and (2.51) together with the energy band constants as given in Table 2.1 at \( T = 4.2 \text{ K} \), the DMR has been plotted as a function of electron concentration \( n_0 \) in stressed n-InSb as shown in Fig. 2.12 where the curves (a), and (b) correspond to the presence and absence of stress respectively.

![Fig. 2.12. The plot of the DMR in bulk specimens of stressed n-InSb as a function of the electron concentration both in the presence and absence of stress as shown by the curves (a) and (b) respectively](image-url)
It appears that stress enhances the numerical values of the DMR to a large extent as compared to that of the stress free condition. The rates of increase of DMR for both the cases are different as concentration increases.

2.6 Summary

In Chap. 2, an attempt is made to present the DMR in tetragonal compounds on the basis of a generalized electron dispersion law by considering the anisotropies of the effective electron masses and the spin–orbit splitting constants together with the inclusion of crystal field splitting constant within the framework of $k.p$ formalism. The theoretical result is in agreement with the suggested experimental method of determining the DMR for materials having arbitrary dispersion laws. Under certain limiting conditions, the results for III–V materials as defined by the three and two band models of Kane have been obtained as special cases of the generalized analysis. The concentration dependence of the DMR has also been numerically computed for $n$-Cd$_3$As$_2$, n-CdGeAs$_2$, n-InAs, n-InSb, n-Hg$_{1-x}$Cd$_x$Te, and n-In$_{1-x}$Ga$_x$As$_y$P$_{1-y}$ lattice matched to InP respectively. The II–VI compounds obey the Hopfield model and p-type CdS has been used for numerical computation. The DMR has also been investigated for Bi in accordance with the models of the McClure and Choi, the Cohen, the Lax, and the parabolic ellipsoidal energy bands respectively. The IV–VI materials obey the Cohen model and n-PbTe, n-PbSnTe, and n-Pb$_{1-x}$Sn$_x$Se have been used for investigations. The chapter ends with the study of the DMR in stressed Kane type semiconductors taking stressed n-InSb as an example, which obey the dispersion relation as suggested by Seiler et al. [44].

Thus, a wide class of technologically important materials has been covered in this chapter whose energy band structures are defined by the appropriate carrier energy spectra. Under certain limiting conditions, all the results of the DMRs for different materials having various band structures lead to the well-known expression of the DMR for degenerate semiconductors having parabolic energy bands as obtained for the first time by Landsberg. For the purpose of condensed presentation, the specific electron statistics related to a particular energy dispersion law for a specific material and the Einstein relation have been presented in Table 2.2.

2.7 Open Research Problems

The problems under these sections of this book are by far the most important part for the readers. Few open and allied research problems are presented from this chapter onward to the end. The numerical values of the energy band constants for various materials are given in Table 2.1 for the related computer simulations.
The carrier statistics and the Einstein relation in bulk specimens of tetragonal, III–V, ternary, quaternary, II–VI, all the models of Bismuth, IV–VI and stressed materials

<table>
<thead>
<tr>
<th>Type of materials</th>
<th>The carrier statistics</th>
<th>The Einstein relation for the diffusivity mobility ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Tetragonal compounds</td>
<td>In accordance with the generalized dispersion relation as formulated in this chapter $n_0 = g_\nu \left( \frac{3\pi^2}{2k^2 M} \right)^{-1}</td>
<td>M(\varepsilon_F) + N(\varepsilon_F)</td>
</tr>
<tr>
<td>2. III–V, ternary and quaternary compounds</td>
<td>In accordance with the three band model of Kane which is a special case of our generalized analysis $n_0 = \frac{g_\nu}{8\pi} \left( \frac{2m^*}{h^2} \right)^{3/2} [M_1(\varepsilon_F) + N_1(\varepsilon_F)]$ (2.8)</td>
<td>$\frac{D}{\mu} = \frac{1}{[M(\varepsilon_F)]^{1/2}} \frac{</td>
</tr>
<tr>
<td></td>
<td>Equation (2.8) is a special case of (2.4) Under the conditions $\Delta \gg E_K$ or $\Delta \ll E_K$, $n_0 = \frac{g_\nu}{8\pi} \left( \frac{2m^*}{h^2} \right)^{3/2} [M_2(\varepsilon_F) + N_2(\varepsilon_F)]$ (2.12)</td>
<td>Equation (2.9) is a special case of (2.5) Under the conditions $\Delta \gg E_K$ or $\Delta \ll E_K$, $\frac{D}{\mu} = \frac{1}{[M_2(\varepsilon_F)]^{1/2}} \frac{</td>
</tr>
<tr>
<td></td>
<td>Equation (2.12) is a special case of (2.8) and is valid for the two band model of Kane Under the conditions $\Delta \gg E_K$ or $\Delta \ll E_K$ together with the condition $\alpha \varepsilon_F &lt; 1$ $n_0 = g_\nu N_e \left[ F_{1/2}(\eta) + \left( \frac{15\alpha k_B T}{2} \right) F_{3/2}(\eta) \right]$ (2.14)</td>
<td>Equation (2.13) is a special case of (2.9) and is valid for the two band model of Kane Under the conditions $\Delta \gg E_K$ or $\Delta \ll E_K$ together with the condition $\alpha \varepsilon_F &lt; 1$ $\frac{D}{\mu} = \left[ \frac{F_{1/2}(\eta)}{F_{1/2}(\eta)} + \frac{15\alpha k_B T}{2} \right] F_{3/2}(\eta)$ (2.15)</td>
</tr>
<tr>
<td></td>
<td>For $E_K \to \infty$, $n_0 = g_\nu N_e F_{1/2}(\eta)$ (2.18)</td>
<td>For $E_K \to \infty$, $\frac{D}{\mu} = \left[ \frac{F_{1/2}(\eta)}{F_{1/2}(\eta)} + \frac{15\alpha k_B T}{2} \right] F_{3/2}(\eta)$ (2.19)</td>
</tr>
<tr>
<td></td>
<td>Equation (2.18) is a special case of (2.14) and is valid for parabolic energy bands Under the condition of extreme carrier degeneracy $n_0 = \frac{g_\nu}{8\pi} \left( \frac{2m^*}{h^2} \right)^{3/2} E_F(1 + \alpha E_F)$ (2.21)</td>
<td>Equation (2.19) is a special case of (2.15) Under the condition of extreme carrier degeneracy $\frac{D}{\mu} = \frac{1}{[M_2(\varepsilon_F)]^{1/2}} \frac{</td>
</tr>
</tbody>
</table>

(Continued)
Table 2.2. Continued

<table>
<thead>
<tr>
<th>Type of materials</th>
<th>The carrier statistics</th>
<th>The Einstein relation for the diffusivity mobility ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>For $\alpha \to 0$, $n_0 = g_v N_c \exp(\eta)$ (2.25)</td>
<td>For $\alpha \to 0$, $n_0 = \frac{\alpha m^* E_F}{k_B T} \left( \frac{\eta}{2} \right)^3 \sqrt{\frac{2m^* E_F}{\hbar^2}}$ (2.23)</td>
<td>$D_\mu = \frac{2E_F}{</td>
</tr>
<tr>
<td>Under the condition of non-degenerate electron concentration</td>
<td>Under the condition of non-degenerate electron concentration</td>
<td>$D_\mu = \frac{k_B T}{</td>
</tr>
<tr>
<td>3. II–VI compounds</td>
<td>4. Bismuth</td>
<td>5. IV–VI compounds</td>
</tr>
<tr>
<td>(a) The McClure and Choi model:</td>
<td>(a) The McClure and Choi model:</td>
<td>The expressions of $n_0$ in this case are given by (2.44) in which the constants of the energy band spectrum correspond to the carriers of the IV–VI semiconductors</td>
</tr>
<tr>
<td>$n_0 = g_v N_c \left[ \frac{\eta}{2} \left( \frac{M_3 (E_F)}{N_3 (E_F)} \right) \right]$ (2.39)</td>
<td>$n_0 = g_v N_c \left( \tau_1 (E_F) + \tau_2 (E_F) \right)$ (2.31)</td>
<td>The DMR in this case are given by (2.15)</td>
</tr>
<tr>
<td>(b) The Cohen model:</td>
<td>(b) The Cohen model:</td>
<td>The DMR in this case are given by (2.19)</td>
</tr>
<tr>
<td>$n_0 = \frac{\alpha m^* E_F}{k_B T} \left( \frac{\eta}{2} \right)^3 \sqrt{\frac{2m^* E_F}{\hbar^2}}$ (2.44)</td>
<td>$n_0 = g_v N_c \left( \tau_1 (E_F) + \tau_2 (E_F) \right)$ (2.31)</td>
<td></td>
</tr>
<tr>
<td>(c) The Lax model:</td>
<td>(c) The Lax model:</td>
<td></td>
</tr>
<tr>
<td>$n_0 = \frac{\alpha m^* E_F}{k_B T} \left( \frac{\eta}{2} \right)^3 \sqrt{\frac{2m^* E_F}{\hbar^2}}$ (2.44)</td>
<td>$n_0 = \frac{\alpha m^* E_F}{k_B T} \left( \frac{\eta}{2} \right)^3 \sqrt{\frac{2m^* E_F}{\hbar^2}}$ (2.44)</td>
<td></td>
</tr>
<tr>
<td>where $N_c \equiv 2 \left( m_1 m_2 n_3 \right)^{1/3} \frac{2k_B T}{\hbar^2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(d) The parabolic ellipsoidal model:</td>
<td>(d) The parabolic ellipsoidal model:</td>
<td></td>
</tr>
<tr>
<td>The electron statistics in this case are given by (2.18), with $N_c$ as defined above</td>
<td>The DMR in this case are given by (2.15)</td>
<td></td>
</tr>
<tr>
<td>6. Stressed compounds</td>
<td>6. Stressed compounds</td>
<td>The DMR in this case are given by (2.19)</td>
</tr>
<tr>
<td>$n_0 = g_v \left( \frac{3\pi^2}{2} \right)^{-1} \left[ M_4 (E_F) + N_4 (E_F) \right]$ (2.50)</td>
<td>$n_0 = g_v \left( \frac{3\pi^2}{2} \right)^{-1} \left[ M_4 (E_F) + N_4 (E_F) \right]$ (2.50)</td>
<td>$n_0 = g_v \left( \frac{3\pi^2}{2} \right)^{-1} \left[ M_4 (E_F) + N_4 (E_F) \right]$ (2.50)</td>
</tr>
</tbody>
</table>
(R2.1) Investigate the Einstein relation for the materials having the respective dispersion relations as given below:

(A) The conduction electrons of n-GaP obey two different dispersion laws as given in the literature [45, 46]. In accordance with Rees [45], the electron energy spectrum is given by

\[ E = \frac{\hbar^2 k_x^2}{2m_{\perp}} + \frac{\hbar^2 k_y^2}{2m_{\parallel}} + \frac{\hbar^2 k_z^2}{2m_{\perp}^*} - \left( \frac{\hbar^4 k_0^2}{m_{\parallel}^2} (k_x^2 + k_y^2) + |V_G|^2 \right)^{1/2} - |V_G|, \quad (R2.1a) \]

where \( k_0 \) and \(|V_G|\) are constants of the energy spectrum with \( m_{\parallel}^* = 0.92m_0, m_{\perp}^* = 0.25m_0, k_0 = 1.7 \times 10^{19} \text{m}^{-1}, |V_G| = 0.21 \text{eV}, g_v = 6, g_s = 2 \) and \( \varphi = 1 \).

(1) In accordance with Ivchenko and Pikus [46], the electron dispersion law can be written as

\[ E = \frac{\hbar^2 k_x^2}{2m_{\perp}} + \frac{\hbar^2 k_y^2}{2m_{\perp}^*} \pm \frac{\Delta}{2} \pm \left( \frac{\Delta}{2} \right)^2 + P_k k_z^2 + D_s k_x^2 k_y^2 \right)^{1/2}, \quad (R2.1b) \]

where \( \Delta = 335 \text{meV}, P_1 = 2 \times 10^{-10} \text{eVm}, D_1 = P_1 a_1 \) and \( a_1 = 5.4 \times 10^{-10} \text{m} \).

(B) In addition to the Cohen model, the dispersion relation for the conduction electrons for IV–VI compounds can also be described by the models of Dimmock [47], Bangert et al. [48], and Foley et al. [49] respectively.

(1) In accordance with the Dimmock model [47], the carrier energy spectrum of IV–VI materials assumes the form

\[ E = \frac{\hbar^2 k_x^2}{2m_{\perp}} + \frac{\hbar^2 k_y^2}{2m_{\perp}^*} + \frac{\Delta}{2} \pm \left( \frac{\Delta}{2} \right)^2 + P_k k_z^2 + D_s k_x^2 k_y^2 \right)^{1/2}, \quad (R2.2) \]

where \( \epsilon \) is the energy as measured from the center of the band gap \( E_g, m_{\perp}^x \) and \( m_{\parallel}^x \) represent the contribution of the transverse and longitudinal effective masses of the external \( L_x^\perp \) and \( L_x^\parallel \) bands arising from the \( k.p \) perturbations with the other bands taken to the second order and \( g_v = 4 \).

(2) In accordance with Bangert et al. [48] the dispersion relation is given by

\[ \Gamma (E) = F_1 (E) k_x^2 + F_2 (E) k_z^2, \quad (R2.3) \]

where \( \Gamma (E) \equiv 2E, F_1 (E) \equiv \frac{R_1^2}{E + E_s} + \frac{S_1^2}{E + \Delta s} + \frac{Q_1^2}{E + E_s}, F_2 (E) \equiv \frac{2C_2^2}{E + E_s} + \frac{(S_1 + Q_1)^2}{E + \Delta s}, \]

\[ R_1^2 = 2.3 \times 10^{-19} \text{ (eVm)}^2, C_2^2 = 0.83 \times 10^{-19} \text{ (eVm)}^2, Q_1^2 = 1.3 R_1^2, \]

\[ S_1^2 = 4.6 R_1^2, \Delta s = 3.07 \text{eV}, \Delta s' = 3.28 \text{eV} \text{ and } g_v = 4. \text{ It may be noted that under the substitutions } S_1 = 0, Q_1 = 0, R_1^2 \equiv \frac{\hbar^2 E_s}{m_{\perp}^x}, C_2^2 \equiv \frac{\hbar^2 E_s}{m_{\parallel}^x}, (R2.3) \text{ assumes the form } E (1 + \alpha E) = \frac{\hbar^2 k_x^2}{2m_{\perp}^x} + \frac{\hbar^2 k_z^2}{2m_{\parallel}^x} \text{ which is the simplified Lax model.} \]
(3) The carrier energy spectrum of IV–VI semiconductors in accordance with Foley et al. [49] can be written as

\[ E + \frac{E_g}{2} = E_-(k) + \left[ \left( E_+(k) + \frac{E_g}{2} \right)^2 + P^2_{\perp} k^2_z + P^2_{\parallel} k^2_z \right]^{1/2}, \]  

(R2.4)

where \( E_+(k) = \frac{\hbar^2 k^2}{2m^*_\perp} + \frac{\hbar^2 k^2}{2m^*_\parallel} \), \( E_-(k) = \frac{\hbar^2 k^2}{2m^*_\perp} + \frac{\hbar^2 k^2}{2m^*_\parallel} \) represents the contribution from the interaction of the conduction and the valance band edge states with the more distant bands and the free electron term,

\[ \frac{1}{m^*_\perp} = \frac{1}{2} \left[ \frac{1}{m_{tc}} \pm \frac{1}{m_{tv}} \right], \]

\[ \frac{1}{m^*_\parallel} = \frac{1}{2} \left[ \frac{1}{m_{tc}} \pm \frac{1}{m_{tv}} \right], \]

For n-PbTe, \( P_\perp = 4.61 \times 10^{-10} \text{eV m}, P_\parallel = 1.48 \times 10^{-10} \text{eV m}, \frac{m_0}{m_{\parallel}} = 10.36, \frac{m_0}{m_{\perp}} = 0.75, \frac{m_0}{m_{tv}} = 11.36, \frac{m_0}{m_{tc}} = 1.20 \) and \( g_v = 4 \).

(C) The importance of Germanium is well known since the inception of semiconductor physics. The conduction electrons of n-Ge obey two different dispersion laws since band non-parabolicity has been included in two different ways as given literature [50,51]. In accordance with Cardona et al. [50] and Wang et al. [51] the electron dispersion laws in Ge can respectively, be expressed as

\[ E = -E_g \frac{2}{2} + \frac{\hbar^2 k^2}{2m^*_\parallel} \left[ \frac{E_g^2}{4} + E_g k^2_z \left( \frac{\hbar^2}{2m^*_\perp} \right) \right]^{1/2}, \]  

(R2.5)

and

\[ E = a_9 k^2_z + b_9 k^2_z - c_9 k^4_z - d_9 k^2_z k^2_z - e_9 k^4_z, \]  

(R2.6)

where \( a_9 = \left( \frac{\hbar^2}{2m^*_\parallel} \right), m^*_\parallel = 1.588 m_0, b_9 = \left( \frac{\hbar^2}{2m^*_\perp} \right), m^*_\perp = 0.0815 m_0, \]

\( c_9 = 1.4A_9, \)

\[ A_9 = \frac{1}{4} \left( \frac{\hbar^4}{E_g m^*_\perp} \right) \left[ 1 - \frac{m^*_\perp}{m_0} \right], \]

\( E_g = 2.2 \text{ eV}, \)

\( d_9 = 0.8A_9, \)

\( e_9 = 0.005A_9, \)

\( g_v = 4 \) and \( g_s = 2. \)

(D) The dispersion relation of the conduction electrons of zero-gap materials (e.g. HgTe) is given by [52]

\[ E = \frac{\hbar^2 k^2}{2m^*} + \frac{3e^2}{128 \varepsilon_\infty} k - \left( \frac{2E_B}{\pi} \right) \ln \left| \frac{k}{k_0} \right|, \]  

(R2.7)

where \( \varepsilon_\infty \) is the semiconductor permittivity in the high frequency limit, \( E_B \equiv \frac{m_0 e^2}{2m^*_\infty} \) and \( k_0 \equiv \frac{m_0 e^2}{2\pi \varepsilon_\infty}. \)
(E) The conduction electrons of n-GaSb obey the following three dispersion relations:

1. In accordance with the model of Seiler et al. [53]

\[
E = \left[ -\frac{E_g}{2} + \frac{E_k}{2} \left[ 1 + \alpha_4 k^2 \right]^{1/2} + \frac{\bar{\delta}_0 h^2 k^2}{2m_0} + \frac{\bar{\tilde{\omega}}_0 f_1(k) \hbar^2}{2m_0} + \frac{\bar{\delta}_0 f_2(k) \hbar^2}{2m_0} \right],
\]

(R2.8)

where \(\alpha_4 \equiv 4P^2 (E_g + \frac{2}{\pi^2 \Delta}) [E_g^2 (E_g + \Delta)]^{-1}\), \(P\) is the isotropic momentum matrix element, \(f_1(k) \equiv k^{-2} \left[ k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2 \right]\) represents the warping of the Fermi surface, \(f_2(k) \equiv \left[ \{k^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2) - 9k_x^2 k_y^2 k_z^2 \}^{1/2} \right]^{-1}\) represents the inversion asymmetry splitting of the conduction band and \(\bar{\delta}_0, \bar{\tilde{\omega}}_0\) and \(\bar{\omega}_0\) represent the constants of the electron spectrum in this case.

It should be noted that under the substitutions, \(\bar{\delta}_0 = 0, \bar{\omega}_0 = 0\) and \(P^2 \equiv \frac{h^2}{2m^*} E_g (E_g + \Delta)\), (R2.8) assumes the form of (2.10), which represents the well known two band model of Kane.

2. In accordance with the model of Mathur et al. [54],

\[
E = \frac{\hbar^2 k^2}{2m_0} + \frac{E_{\pi^*} \bar{\pi}_1}{2} \left[ \left( 1 + \frac{2\hbar^2 k^2}{E_{\pi^*}} \left\{ \frac{1}{m^*} - \frac{1}{m_0} \right\} \right)^{1/2} - 1 \right],
\]

(R2.9)

where \(E_{\pi^*} = \left\{ E_g + \left[ (5 \times 10^{-5} T^2) \left( 2 (112 + T)^{-1} \right) \right] \right\} \text{eV} \).

3. In accordance with the model of Zhang et al. [55]

\[
E = \left[ E_2^{(1)} + E_2^{(2)} K_{4,1} \right] k^2 + \left[ E_4^{(1)} + E_4^{(2)} K_{4,1} \right] k^4 + k^6 \left[ E_6^{(1)} + E_6^{(2)} K_{4,1} + E_6^{(3)} K_{6,1} \right].
\]

(R2.10)

where \(K_{4,1} \equiv \frac{8}{1134024} \left[ \frac{k^4}{k^2} - \frac{3}{2} \right], K_{6,1} \equiv \sqrt{0.0067275} \left[ \frac{k^4}{k^2} + \frac{1}{2 \pi^2} \left( \frac{k^4}{k^2} - \frac{3}{2} \right) \right] \right\} \text{eV} \), the coefficients are in eV, the values of \(k\) are 10 \((\frac{a}{2\pi})\) times those of \(k\) in atomic units (\(a\) is the lattice constant), \(E_2^{(1)} = 1.0239620, E_2^{(2)} = 0, E_4^{(1)} = -1.1320772, E_4^{(2)} = 0.05658, E_6^{(1)} = 1.1072073, E_6^{(2)} = -0.1134024\) and \(E_6^{(3)} = -0.0072275\).

(F) The dispersion relation of the carriers in p-type Platinum antimonide (PtSb2) following Entage [56] can be written as

\[
\left( E + \lambda_1 \frac{a^2}{4} k^2 - l_1 k_3^2 \frac{a^2}{4} \right) \left( E + \delta_0' - \nu_1 \frac{a^2}{4} k^2 - n_1 \frac{a^2}{4} k_3^2 \right) = I_0 \frac{a^4}{16} k^4,
\]

(R2.11)

where \(\lambda_1, l_1, \delta_0', \nu_1, n_1, I_0\) and \(a\) are the energy band constants and \(a\) is the lattice constant.
In addition to the well known three band model of Kane, the conduction electrons of n-GaAs obey the following three dispersion relations:

1. In accordance with the model of Stillman et al. [57]
   \[ E = \frac{\hbar^2 k^2}{2m^*} - \left( 1 - \frac{m^*}{m_0} \right)^2 \left( \frac{\hbar^2 k^2}{2m^*} \right)^2 \left[ \frac{3E_g + 4\Delta + \left( \frac{2\Delta^2}{E_g} \right)}{(E_g + \Delta)(2\Delta + 3E_g)} \right], \tag{R2.12} \]

2. In accordance with the model of Newson et al. [58]
   \[ E = \alpha_0 k^4 + \left( \frac{\hbar^2}{2m^*} + (2\alpha_0 + \beta_0) k_s^2 \right) k_x^2 + \frac{\hbar^2}{2m^*} k_y^2 + (2\alpha_0 + \beta_0) k_x^2 k_y^2 + \alpha_0 (k_x^4 + k_y^4), \tag{R2.13} \]
   where \( \alpha_0 = -1.97 \times 10^{-37} \text{ eV m}^4 \) is the non-parabolicity constant and \( \beta_0 = -2.3 \times 10^{-37} \text{ eV m}^4 \) is the wrapping constant.

3. In accordance with the model of Rossler [59]
   \[ E = \frac{\hbar^2 k^2}{2m^*} + \bar{\alpha}_{10} k^4 + \beta_{10} \left( k_x^2 k_y^2 + k_z^2 k_y^2 + k_x^2 k_z^2 \right) \pm \gamma_{10} \left( k^2 \left( k_x^2 k_y^2 + k_z^2 k_y^2 + k_x^2 k_z^2 \right) - 9k_x^2 k_y^2 k_z^2 \right)^{1/2}, \tag{R2.14} \]
   where \( \bar{\alpha}_{10} = \alpha_{11} + \alpha_{12} k, \beta_{10} = \beta_{11} + \beta_{12} k \) and \( \gamma_{10} = \gamma_{11} + \gamma_{12} k \), in which,
   \[ \alpha_{11} = -2132 \times 10^{-40} \text{ eV m}^4, \alpha_{12} = 9030 \times 10^{-50} \text{ eV m}^5, \]
   \[ \beta_{11} = -2493 \times 10^{-40} \text{ eV m}^4, \beta_{12} = 12594 \times 10^{-50} \text{ eV m}^5, \]
   \[ \gamma_{11} = 30 \times 10^{-30} \text{ eV m}^3 \text{ and } \gamma_{12} = -154 \times 10^{-42} \text{ eV m}^4. \]

In addition to the well known three band model of Kane, the conduction electrons of n-InSb obey the following three dispersion relations:

1. To the fourth order effective mass theory, and taking into account the interactions of the conduction, the heavy hole, the light hole, and the split-off bands, the electron energy spectrum in n-InSb is given by [60]
   \[ E = \frac{\hbar^2 k^2}{2m^*} + \beta_1 k^4, \tag{R2.15} \]
   where \( \beta_1 \equiv \frac{K_kh^4}{4E_g(m^*)}, K_2 \equiv -\left[ \frac{1 + y_1 x_1}{1 + y_1 x_1} \right] (1 - y_1)^2, x_1 \equiv \left[ 1 + \left( \frac{\Delta}{E_g} \right) \right]^{-1} \text{ and } y_1 \equiv \frac{m^*}{m}. \]

2. In accordance with Johnson and Dickey [61], the electron energy spectrum assumes the form
   \[ E = -\frac{E_g}{2} + \frac{\hbar^2 k^2}{2} \left[ \frac{1}{m_0} + \frac{1}{m_{\gamma_b}} \right] + \frac{E_g}{2} \left[ 1 + 4\frac{\hbar^2 k^2}{2m_c} \bar{f}_1(E) \right]^{1/2}, \tag{R2.16} \]
where $\frac{m_e}{m_\gamma} \equiv P_0^2 \left[ \frac{(E_e + \frac{\Delta}{m})}{E_e + \frac{\Delta}{m}} \right]$, $P_0^2$ is the energy band constant, $f_1(E) \equiv \frac{(E_g + \frac{\Delta}{m})}{(E_e + \frac{\Delta}{m})}$, $m'_e = 0.139 m_0$ and $m_{\gamma b} = \left[ \frac{1}{m'_e} - \frac{2}{m_0} \right]^{-1}$.

In accordance with Agafonov et al. [62], the electron energy spectrum can be written as

$$E = \frac{\eta - E_g}{2} \left[ 1 - \frac{\hbar^2 k^2}{2\eta m^*} \left\{ \frac{D\sqrt{3} - 3\tilde{B}}{2} \left( \frac{k^2}{2m^*} \right) \right\} \left[ k_x^2 + k_y^2 + k_z^2 \right] \right],$$

(R2.17)

where $\eta \equiv (E_g^2 + \frac{8}{3} D^2 k^2)^{1/2}$, $\tilde{B} \equiv -21 \frac{\hbar^2}{m^*}$ and $D \equiv -40 \left( \frac{\hbar^2}{m^*} \right)$.

(1) The dispersion relation of the carriers in n-type Pb$_{1-x}$Ga$_x$Te with $x = 0.01$ following Vassilev [63] can be written as

$$E = E_g - 0.606k_x^2 - 0.0722k_y^2 \left[ E + E_g + 0.411k_x^2 + 0.0377k_y^2 \right]$$

$$= 0.23k_x^2 + 0.02k_y^2 \pm \left[ 0.06E_g + 0.061k_x^2 + 0.0066k_y^2 \right] k_z,$$

(R2.18)

where $E_g (= 0.21$ eV) is the energy gap for the transition point, the zero of the energy $E$ is at the edge of the conduction band of the $\Gamma$ point of the Brillouin zone and is measured positively upwards, $k_x$, $k_y$ and $k_z$ are in the units of $10^9$ m$^{-1}$.

(2) The charge carriers of Tellurium obey two different dispersion laws as given in the literature [64,65].

(1) The dispersion relation of the conduction electrons in Tellurium, following Bouat [64] can be written as

$$E = A_0 k_x^2 + B_0 k_y^2 \pm [\bar{\eta} k_x^2 + \bar{\eta} k_y^2]^{1/2},$$

(R2.19a)

where $A_0 = (6.7 \times 10^{-16}$ meV$^2$), $B_0 = (4.2 \times 10^{-16}$ meV$^2$), $\bar{\eta} = (6 \times 10^{-8}$ meV$^2$) and $\bar{\eta} = (3.8 \times 10^{-8}$ meV$^2$) are the band constants.

(2) The energy spectrum of the carriers in the two higher valence bands and the single lower valence band of Te can respectively be expressed as [65]

$$E = A_{10} k_x^2 + B_{10} k_y^2 \pm \left[ \Delta_{10}^2 + (\beta_{10} k_z)^2 \right]^{1/2},$$

and

$$E = \Delta_{||} + A_{10} k_x^2 + B_{10} k_y^2 \pm \beta_{10} k_z,$$

(R2.19b)

where $E$ is the energy measured within the valence bands, $A_{10} = 3.77 \times 10^{-11}$ eV m$^2$, $B_{10} = 3.57 \times 10^{-11}$ eV m$^2$, $\Delta_{10} = 0.628$ eV, $\beta_{10} = 6 \times 10^{-20}$ (eV m$^2$) and $\Delta_{||} = 1004 \times 10^{-5}$ eV are the spectrum constants.

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(K) The dispersion relation for the electrons in graphite can be written following Brandt [66] as

$$E = \frac{1}{2} [E_2 + E_3] \pm \left[ \frac{1}{4} (E_2 - E_3)^2 + \gamma k^2 \right]^{1/2},$$

(R2.20)
where \( E_2 \equiv \Delta - 2\gamma_1 \cos \phi_0 + 2\gamma_5 \cos^2 \phi_0, \phi_0 \equiv \frac{\alpha k_0}{2}, E_3 \equiv 2\gamma_2 \cos^2 \phi_0, \)
\( \eta_2 \equiv \left( \frac{\gamma_7}{2} \right) a_6 (\gamma_0 + 2\gamma_4 \cos \phi_0), \)
in which the band constants are \( \Delta = -0.0002 \text{ eV}, \gamma_0 = 3 \text{ eV}, \gamma_1 = 0.392 \text{ eV}, \gamma_2 = -0.019 \text{ eV}, \gamma_4 = 0.193 \text{ eV}, \gamma_5 = 0.194 \text{ eV}, a_6 = 2.46 \text{ Å} \) and \( c_0 = 6.74 \text{ Å}. \)

(L) The dispersion relation of the conduction electrons in Antimony (Sb) in accordance with Ketterson [67] can be written as

\[
2m_0E = \alpha_{11}p_x^2 + \alpha_{22}p_y^2 + \alpha_{33}p_z^2 + 2\alpha_{23}p_y p_z,
\]

(R2.21)

and

\[
2m_0E = a_1 p_x^2 + a_2 p_y^2 + a_3 p_z^2 + a_4 p_y p_z \pm a_5 p_x p_z \pm a_6 p_y p_y,
\]

(R2.22)

where \( a_1 = \frac{1}{4} (\alpha_{11} + 3\alpha_{22}), a_2 = \frac{1}{2} (\alpha_{22} + 3\alpha_{11}), a_3 = 0, a_4 = a_{33}, a_5 = \sqrt{3} \) and \( a_6 = \sqrt{3} (\alpha_{22} - \alpha_{11}) \) in which \( \alpha_{11} = 16.7, \alpha_{22} = 5.98, \alpha_{33} = 11.61 \) and \( \alpha_{23} = 7.54 \) are the system constants.

(M) The dispersion relation of the holes in \( p - \text{Bi}_2\text{Te}_3 \) can be written [68] as

\[
E \left( 1 + \frac{E}{E_g} \right) = \frac{h^2}{2m_0} \left[ \alpha_{11} k_x^2 + \alpha_{22} k_y^2 + \alpha_{33} k_z^2 + 2\alpha_{23} k_y k_z \right],
\]

(R2.23)

where \( x, y \) and \( z \) are parallel to binary, bisectrix and trigonal axes respectively, \( E_g = 0.145 \text{ eV}, \alpha_{11} = 32.5, \alpha_{22} = 4.81, \alpha_{33} = 9.02, \alpha_{23} = 4.15, g_z = 2 \) and \( g_v = 6 \).

(N) The dispersion relation of the holes in \( p-\text{InSb} \) in accordance with Cunningham [69] can be written as

\[
E = c_4 \left( 1 + \gamma_4 f_4 \right) k^2 \pm \frac{1}{2} \left[ 2\sqrt{2} \sqrt{c_4} \sqrt{16 + 5\gamma_4} \sqrt{E_4} g_4 \right],
\]

(R2.24)

where \( E \) is the energy of the hole as measured from the top of the valance and within it, \( c_4 \equiv \frac{h^2}{2m_0}, \theta_4 = 4.7 \text{ eV}, \gamma_4 = 5\gamma_4 \text{ eV}, b_4 = \frac{h^2}{c_4}, b_4 = \frac{3}{2} b_5 + 2 \theta_4, b_5 = 2.4 \text{ eV}, f_4 = \frac{1}{4} \left[ \sin^2 \theta + \sin^4 \theta \sin^2 \phi \right], \theta \) is measured from the positive \( z \)-axis, \( \phi \) is measured from positive \( x \)-axis, \( g_4 \equiv \sin \theta \left[ \cos^2 \theta + \frac{1}{4} \sin^4 \theta \sin^2 \phi \right] \) and \( E_4 = 5 \times 10^{-4} \text{ eV}. \)

(O) The dispersion relation of the valance bands of II–V compounds in accordance with Yamada [70] can be written as

\[
E = \frac{1}{2} \left( \ell_1 + \ell_2 \right) k_x^2 + \frac{1}{2} \left( \ell_3 + \ell_4 \right) k_y^2 + \frac{1}{2} \left( \ell_5 + \ell_6 \right) k_z^2 + \frac{1}{2} \left( \ell_7 + \ell_8 \right) k_x \\
\pm \sqrt{\left[ \frac{1}{2} \left( \ell_1 - \ell_2 \right) k_x^2 + \frac{1}{2} \left( \ell_3 - \ell_4 \right) k_y^2 + \frac{1}{2} \left( \ell_5 - \ell_6 \right) k_z^2 + \frac{1}{2} \left( \ell_7 - \ell_8 \right) k_x \right]^2 + t_{10}^2 k_y^2 + t_{10}^2}^{1/2},
\]

(R2.25)

where \( \ell_i (i = 1 \text{to} 8), t_9 \) and \( t_{10} \) are the constants of the energy spectra.
For $p-$CdSb, $\bar{t}_1 = -32.3 \times 10^{-20} \text{eVm}^2, \bar{t}_2 = -60.7 \times 10^{-20} \text{eVm}^2, \bar{t}_3 = -1.63 \times 10^{-19} \text{eVm}^2, \bar{t}_4 = -2.44 \times 10^{-19} \text{eVm}^2, \bar{t}_5 = -9.19 \times 10^{-19} \text{eVm}^2, \bar{t}_6 = -10.5 \times 10^{-19} \text{eVm}^2, \bar{t}_7 = 2.97 \times 10^{-19} \text{eVm}, \bar{t}_8 = -3.47 \times 10^{-19} \text{eVm}, \bar{t}_9 = 1.3 \times 10^{-19} \text{eVm}$ and $t_{10} = 0.070 \text{eV}.$

(P) The energy spectrum of the valance bands of CuCl in accordance with Yekimov et al. [71] can be written as

$$E_h = (\gamma_6 - 2\gamma_7) \frac{\hbar^2 k^2}{2m_0},$$

and

$$E_{l,s} = (\gamma_6 + \gamma_7) \frac{\hbar^2 k^2}{2m_0} - \frac{\Delta_1}{2} \pm \left[ \frac{\Delta_2^2}{4} + \gamma_7 \Delta_1 \frac{\hbar^2 k^2}{2m_0} + 9 \left( \frac{\gamma_7 \hbar^2 k^2}{2m_0} \right)^2 \right]^{1/2},$$

where $\gamma_6 = 0.53, \gamma_7 = 0.07, \Delta_1 = 70 \text{meV}.$

(Q) In the presence of stress, $\chi_6$ along $<001>$ and $<111>$ directions, the energy spectra of the holes in semiconductors having diamond structure valance bands can be respectively expressed following Roman [72] et al. as

$$E = A_6 k^2 \pm \left[ B_7^2 k^4 + \delta_6^2 + B_7 \delta_6 \left( 2k_z^2 - k_s^2 \right) \right]^{1/2},$$

and

$$E = A_6 k^2 \pm \left[ B_7^2 k^4 + \delta_7^2 + D_6 \frac{\sqrt{3}}{3} \delta_7 \left( 2k_z^2 - k_s^2 \right) \right]^{1/2},$$

where $A_6, B_7, D_6$ and $C_6$ are inverse mass band parameters in which

$\delta_6 \equiv l_7 \left( \bar{S}_{11} - \bar{S}_{12} \right) \chi_6, \bar{S}_{ij}$ are the usual elastic compliance constants, $B_7 \equiv \left( B_7^2 + \frac{\delta_6^2}{\gamma_7} \right)$ and $\delta_7 \equiv \left( \frac{D_6}{3} \frac{\bar{S}_{ij}}{\gamma_7} \right) \chi_6.$ For gray tin, $d_8 = -4.1 \text{eV}, l_7 = -2.3 \text{eV},$

$A_6 = 19.2 \frac{\hbar^2}{2m_0}, B_7 = 26.3 \frac{\hbar^2}{2m_0}, D_6 = 31 \frac{\hbar^2}{2m_0}$ and $c_6^2 = -1112 \frac{\hbar^2}{2m_0}.$

R2.2 Investigate the Einstein relation for all materials of problem (R2.1), in the presence of an arbitrarily oriented non-quantizing and (a) non-uniform electric field (b) alternating electric field respectively.

**Allied Research Problems**

R2.3 Investigate the Debye screening length, the carrier contribution to the elastic constants, the heat capacity, the activity coefficient, and the plasma frequency for all the materials of problem (R2.1).

R2.4 Investigate in detail, the mobility for elastic and inelastic scattering mechanisms for all the materials of problem (R2.1).

R2.5 Investigate the various transport coefficients in detail for all the materials of problem (R2.1).
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