11.1. Introduction:

It is well known that the effective mass of the carriers in semiconductors, which is strongly connected with the carrier mobility, is a very significant controlling factor of the physical properties of the solid devices [11.1-11.13]. It must be mentioned that among the various definitions of the effective mass of the carriers [11.4], it is effective momentum mass that should be regarded as the basic quantity [11.5]. This is due to the fact that it is the effective momentum mass that appears in the description of transport phenomena and all the other properties of the electron gas in a band with arbitrary band non-parabolicity [11.5]. It can be shown that it is the effective mass which enters in the formulation of different transport coefficients and plays the most dominant role in explaining the experimental results of various scattering mechanism [11.6]. The carrier degeneracy in semiconductors affects the effective mass when it is energy dependent. Under degenerate conditions only the carriers at the Fermi surface participate in the conduction process and hence the effective momentum mass of the carriers at the Fermi level (hereafter referred to as EMM) would be interest in the carrier transport under such conditions. The Fermi energy is again determined by the carrier energy spectrum.

Recently, various dispersion relations for materials under different physical conditions have been proposed which have created the interest of studying the EMM in such materials [11.7-11.16].
Nevertheless it appears from the literature that the EMM in ultrathin films of non-parabolic compound has yet to be investigated under arbitrary oriented magnetic field on the basis of a new electron dispersion law. In section 11.2 of this chapter the EMM under the aforementioned case has been investigated. Then an expression of the surface electron concentration per unit area has been formulated for the purpose of studying the doping dependence of the EMM. The various dimension dependent transport in different compounds and the derivation of the expressions of many important physical parameters are based on the temperature dependent electron statistics in such materials. The result of the corresponding EMM in the absence of the magnetic field is given in section 11.2.2 from which the simplified results of ultrathin films of wide-gap materials have also been derived as a special case.

It may be stated that, for the purpose of numerical computations, ultrathin films of $n-Hg_{1-x}Cd_xTe$ and $In_{x}Ga_{x}As_{y}P_{1-y}$ lattice matched to InP have been used as examples. In this context, it is worth remarking that the ternary compound $Hg_{1-x}Cd_xTe$ is a classic narrow-gap semiconductor and is an important optoelectronic material. Its band gap can be varied to cover the spectral range from $0.8\mu m$ to over $30\mu m$ by adjusting the alloy composition [11.17]. $Hg_{1-x}Cd_xTe$ finds extensive use in infrared detector materials and the photovoltaic detector arrays [11.18] in the 8 to 10 $\mu m$ wave bands. The above uses have spurred a $Hg_{1-x}Cd_xTe$ technology for the production of high-mobility single crystal with specially prepared surface layers and the same material is ideally suitable for narrow sub-band physics because the relevant material constants are within easy experimental reach [11.19]. Besides, quaternary materials, $In_{x}Ga_{x}As_{y}P_{1-y}$ lattice matches to InP, find extensive applications in the fabrication of photo detectors [11.20], heterojunction layers [11.21], light-emitting diodes [11.22], avalanche photodiodes [11.23], field-effect transistors, detectors [11.24] and other devices. In addition, new types of integrated optical devices such as switches, modulators, solar cells and filters are made from the quaternary systems [11.21]. The Kane type dispersion law has been used since the above model is valid for the description of electron properties of such small-gap materials [11.26]. An attempt is made to study the doping, thickness and alloy composition dependence of the EMM in the presence of an arbitrary oriented magnetic field taking $n-Hg_{1-x}Cd_xTe$ and $In_{x}Ga_{x}As_{y}P_{1-y}$ lattice matched to InP as examples.
11.2. Theoretical Background:

11.2.1 Formulation of the EMM in Ultrathin Films of Small-gap Semiconductors in the presence of an Arbitrary Oriented Magnetic Field

The dispersion relation of the conduction electrons in bulk specimens of small-gap materials can be expressed [11.27] as

\[ E = \left( \frac{\hbar^2 k^2}{2m^*} \right) - A \left( \frac{\hbar^2 k^2}{2m^*} \right)^2 \]  

(11.1)

where \( E \) is the total energy of the electron as measured from the edge of the conduction band in the vertically upward direction in the absence of any field, \( \hbar = h/2\pi \), \( h \) is the Planck constant, \( \vec{k} \) is the electron wave vector, \( m^* \) is the effective electron mass at the edge of the conduction band.

\[ A = \frac{1}{m^*} \left[ \frac{d_0 (3 + 4d_0 + 2\Delta^2 d_0^2)}{(1 + d_0 \Delta^2) (3 + 2d_0 \Delta)} \right] \]

in which \( m_0 \) is the free electron mass, \( d_0 = 1/E_g \), \( E_g \) is the band gap and \( \Delta \) is the spin orbit splitting constant.

In ultrathin films, in the presence of an arbitrary oriented magnetic field \( \vec{B} \), the Hamiltonian operator assumes the form

\[ \hat{H} = \frac{\left(-i\hbar \vec{\nabla} + e\vec{A}_0\right)^2}{2m^*} - \left(\frac{A}{4m^*} \right) \left(-i\hbar \vec{\nabla} + e\vec{A}_0\right)^4 \]  

(11.2)
where \( i = \sqrt{-1} \), \( \nabla = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z} \), \( i, j, k \) are the orthogonal triads along \( x, y \) and \( z \) directions respectively. \( \vec{A}_0 \) is the vector potential which can be written as \( \vec{A}_0 = \hat{i}zB_y + \hat{j}xB_x + \hat{k}yB_z \). \( \overrightarrow{B} = \hat{i}B_x + \hat{j}B_y + \hat{k}B_z \), \( B_x, B_y \) and \( B_z \) are the components of \( \overrightarrow{B} \) along \( x, y \) and \( z \) directions respectively. For the present problem, the 0th order wave function and the energy eigen value can, respectively, be written as

\[
\psi_0 = \left( \frac{2}{aL_xL_y} \right) \sin \left( \frac{n\pi}{a} \right) \exp \left( ik_x x + j y y \right)
\]

(11.3)

and

\[
E_n^0 = \frac{\hbar^2}{2m} \left( \frac{n\pi}{a} \right)^2 + \frac{\hbar^2 k_y^2}{2m} - \left[ \frac{\hbar^2}{2m} \left( \frac{n\pi}{a} \right)^2 + \frac{\hbar^2 k_x^2}{2m} \right]^{1/2}
\]

(11.4)

where \( n (=1,2,3,\ldots) \) is the size quantum number, \( a \) is the width of the ultrathin film along \( z \)-direction, \( k_x^2 = k_x^2 + k_y^2 \) and \( L_x \) and \( L_y \) are the sample dimensions along \( x \) and \( y \) direction respectively. Thus the modified electron energy spectrum up to the first order in ultrathin films of non-parabolic semiconductors in the presence of any arbitrarily oriented magnetic field \( \overrightarrow{B} \) can be written, neglecting spin, as

\[
P_1(n)k_x^2 + Q_k k_y^2 + R(n)k_y k_y + P_1(E,n)k_x + Q_1(E,n)k_y + C(E,n) = 0
\]

(11.5)

where the notations have been defined in Appendix 11.4.1.

The use of equation (11.5) leads to the expressions of the EMMs along \( x \) and \( y \) directions as

\[
m_x^*(n,E_F) = \left[ \frac{\hbar^2}{4P_1^2(n)} \right] \left( P_1^2(E_F,n) - 4P_1(n)C(E_F,n) - P_1(E_F,n) \right) T_1(E_F,n)
\]

(11.6)

and

\[
m_y^*(n,E_F) = \left[ \frac{\hbar^2}{4Q_1(n)} \right] \left( Q_1^2(E_F,n) - 4Q_1C(E_F,n) - P_1(E_F,n) \right) T_1(E_F,n)
\]

(11.7)
where $E_f$ is the Fermi energy and the functions $T_1(E_f,n)$ and $T_2(E_f,n)$ have been defined in the Appendix 11.4.2.

It appears, then, that the investigation of the EMM from equations (11.6) and (11.7) as function of doping requires an expression of the electron statistics, which in turn is determined by the density-of-states function. Thus, using equation (11.5), the density-of-states function can be expressed as

$$N(E) = \frac{1}{4\pi} \sum_{\nu=1}^{\infty} \left[ 2H'(E,n) - A'(E,n)D(E,n) - D'(E,n)A(E,n) \right] \left\{ A(E,n)D(E,n) - H^2(E,n) \right\}^{\frac{3}{2}} \theta(E - E_n)$$

(11.8)

where the notations have been defined in Appendix 11.4.3.

Combining equation (11.6) with the Fermi-Dirac occupation probability factor, the surface electron concentration per unit area can be written as

$$n_s = \frac{1}{2\pi} \sum_{\nu=1}^{\infty} \left[ L_1(n,E_f) + L_2(n,E_f) \right]$$

(11.9)

where the symbols have been defined in Appendix 11.4.3.

11.2.2 Special Cases

(a) In the absence of magnetic field, $B \to 0$ and under this condition the expressions of the dispersion relation, the EMM, density-of-states function and the surface electron concentration in ultrathin films of non-parabolic semiconductors can, respectively, be expressed as

$$k^2 = \left( \frac{m^*}{\hbar^2} \right) \left[ 1 - \sqrt{1 - 4AE} \right] - \left( \frac{n\pi}{a} \right)^2$$

(11.10)

$$m^*_z(n,E_f) = \frac{m^*}{\sqrt{1 - 4AE_f}}$$

(11.11)
\[ m^*(n, E_F) = \frac{m^*}{\sqrt{(1 - 4AE_F)}} \]  \hspace{1cm} (11.12)

\[ N(E) = \left( \frac{m^*}{\pi \hbar^2} \right) \sum_{n=1}^{\infty} \frac{1}{\sqrt{(1 - 4AE)}} H(E - E_F) \]  \hspace{1cm} (11.13)

and

\[ n_b = \frac{1}{2\pi} \sum_{m=1}^{\infty} \left[ L_2(n, E_F) + L_4(n, E_F) \right] \]  \hspace{1cm} (11.14)

where the notations have been defined in Appendix 11.4.5.

(b) For relatively wide gap materials \( E_g \to \infty \). Therefore the equations (11.10) to (11.13) get simplified as

\[ k_s^2 = \left( \frac{2m^* E}{\hbar^2} \right) \left( \frac{n\pi}{a} \right)^2 \]  \hspace{1cm} (11.15)

\[ m^*(n, E_F) = m^*(n, E_F) = m^* \]  \hspace{1cm} (11.16)

\[ N(E) = \left( \frac{m^*}{\pi \hbar^2} \right) \sum_{n=1}^{\infty} \frac{1}{2m^*} \left( \frac{n\pi}{a} \right)^2 \]  \hspace{1cm} (11.17)

and

\[ n_b = \left( \frac{m^* k_s T}{\pi \hbar^2} \right) \sum_{n=1}^{\infty} \ln \left[ 1 + \exp \left( \frac{k_BT}{h^2} \right) \right] \]  \hspace{1cm} (11.18)

where \( n_n = \frac{1}{k_s T} \left( E_F - \frac{\hbar^2}{2m^*} \left( \frac{n\pi}{a} \right)^2 \right) \) and \( F_j(n_n) \) is the one-parameter Fermi-Dirac integral of order j as defined in [11.27].

Thus the whole mathematical background can be summarized in the following way. The expressions of the EMM and \( n_n \) in ultrathin films of non-parabolic materials in the presence of an arbitrarily oriented magnetic field have been first formulated on the basis of a new electron dispersion law. The well-known results of EMM and \( n_n \) for ultrathin films of relatively wide-gap materials under certain limiting conditions have also been obtained in the absence of the magnetic field. The above fact is the indirect theoretical test of the analysis.
11.3. Results and Discussions:

Using equations (11.9) and (11.8) together with the parameters [11.28, 11.29]

\[ E_g = [-0.302 + 1.093x + 5.35 \left(10^{-4}T(1-2x)\right) - 0.810x^2 + 0.832x^3]eV, \]

\[ m^* = \frac{3\hbar^2E_g}{4p^2}, \quad p^2 = \left(\frac{\hbar^2}{2m_0}\right)(18 + 3x), \quad B_x = B_y = B_z = 1T, \quad \alpha = 40nm, \quad T = 4.2K, \]

\[ \Delta = (0.63 + 0.24x - 0.27x^2)kV \text{ for } Hg_{x}Cd_{1-x}Te \quad \text{and} \quad \gamma = 0.3, \quad m^* = (0.080 - 0.039\gamma)m_0 \]

\[ \Delta = (0.114 + 0.26\gamma - 0.22\gamma^2)kV \text{ for band constants of } In_{1-x}Ga_xAs, P_{1-x} \text{ lattice matched to InP}, \]

the normalized \( m^*_x(n, E_p) \) and \( m^*_y(n, E_p) \) versus \( n_0 \) have been plotted for both the materials as shown in figure 11.1 and 11.2 in the presence of an arbitrarily oriented magnetic field for the first three sub-bands in which the same dependence has also been plotted in the absence of magnetic field for the purpose of relative comparison. In figure 11.3 to 11.6 the normalized \( m^*_x(n, E_p) \) and \( m^*_y(n, E_p) \) have been plotted as functions of film thickness and alloy composition respectively for both the materials in which simplified limiting cases have further been considered. From the figures and the theoretical background the following features follow:

(i) The dependence of the EMM on the size quantum number is an intrinsic property of the arbitrarily oriented magnetic field for the 2D systems of non-parabolic materials. This dependence is due to the magnetic field, as can be demonstrated by comparing equation (11.6) with equation (11.11) and equation (11.7) with equation (11.12), respectively. The band non-parabolicity along can explain the energy dependence of the effective mass, but cannot take into account its functional dependence on size quantum number in small gap 2D systems as evident from equations (11.8) and (11.9) respectively.

(ii) The EMM corresponding to \( n=1 \) exhibits the highest numerical values for all cases. The EMM increases with increasing \( n_0 \) and decreases with increasing film thickness and alloy composition respectively in various manners as evident from all the figures.
Figure 11.1 Plots of $m_x(n, E_F)/m_0$ versus $n_0$ in ultrathin films of $Hg_{1-x}Cd_xTe$ in the presence of an arbitrarily oriented magnetic field corresponding to (a) $n=1$, (b) $n=2$ and (c) $n=3$. The curves ‘d’, ‘e’ and ‘f’ exhibit the same dependence for $In_xGa_{1-x}As$, $P_{1-y}$ lattice matched to InP for the first three sub-bands respectively. The plots of ‘g’ and ‘h’ exhibit the same dependence under the condition $B=0$ for $Hg_{1-x}Cd_xTe$ and $In_xGa_{1-x}As$, $P_{1-y}$ lattice matched to InP respectively.
Figure 11.2 Plots of $m^*(n, E_F)/m_0$ versus $n_0$ for all the plots of figure 11.1
Figure 11.3  Plots of \( m^*_X(n, E_F)/m_0 \) versus \( a \) (film thickness) for all the cases of figure 11.1 \( \bar{n}_0 = 10^{14} m^{-2}, B_X = B_Z = 1 \text{Tesla}, x = 0.5, y = 0.43 \) and \( T = 2.9K \).
Figure 11.4 Plots of $n(y,n,E,F)/m_0$ versus $a$ (film thickness) for all the cases of figure 11.1
Figure 11.5 Plots of $m^*_X(n, E_F)/m_0$ versus alloy composition for all the cases of figure 11.4 ($n_0 = 10^{16} \text{ m}^{-2}, B_X = 1.1 \text{ Tesla}, B_y = 0.9 \text{ Tesla}, B_z = 1.4 \text{ Tesla}, T = 5K \text{ and } a = 40nm$)
Figure 11.6 Plots of $m_y(n, E_F)/m_0$ versus alloy composition for all the cases of figure 11.1
(iii) The numerical values of the EMM in quaternary alloys are smaller than that of the same for ternary materials. Thus the influence of the material constant on the effective mass is also evident from figures. The presence of the arbitrarily oriented magnetic field in 2D isotropic small-gap systems introduces the mass anisotropy, which, in turn, depends on the quantum number and the Fermi energy as evident from equations (11.6) and (11.7) respectively.

(iv) From the differences in the numerical values of the EMM with respect to the type of dispersion relation evident from the figures, their influence on the Boltzmann transport in different materials under different physical conditions can be easily assessed.

(v) The oscillations in various transport co-efficient which occurs in 2D systems would further be influenced by the index dependent EMM in ultrathin films in the presence of an arbitrarily oriented magnetic field and the contributions of the EMM to the oscillatory mobility would be important.

11.4. Appendix:

11.4.1. The notations as given in equation (11.5) are defined as follows:

\[
P_i(n) = \left[ b_1 - Aa_1^2 + Aa_1a_2 - Aa_1 \right],
\]

\[
b_1 = b_2 = \frac{\hbar^2}{2m},
\]

\[
a_1 = \left( \frac{\hbar e B_z}{m^2} \right) < Z >, \quad < Z > = \frac{a}{2},
\]

\[
a_2 = \left( \frac{\hbar e B_z}{m^2} \right) < Z^2 >, \quad < Z^2 > = \left[ \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2} \right],
\]

\[
a_3 = \left( \frac{\hbar e B_z}{m^2} \right)^2 < Z^2 >,
\]

\[
Q_i = \left[ b_2 - Aa_1^2 + Aa_1a_3 - Aa_1 \right],
\]
\begin{align*}
a_4 &= \left( \frac{\hbar e B_y}{m^*} \right) L_z, \\
a_5 &= \left( \frac{\hbar e L_x B_z}{2m^*} \right), \\
a_6 &= \frac{1}{3} \left( \frac{\hbar e L_x B_z}{m^*} \right)^2, \\
R(n) &= A[a_1 a_1 - a_2 a_4 - 2a_3 a_4 - a_7], \\
a_{11} &= \left( \frac{\hbar^2 e^2 B^3_y}{m^*} \right) \langle Z \rangle, \\
P_2(E,n) &= [a_1 - A(a_5 + a_6) - Aa_2(E - a_{10}) + Aa_1(a_{11} + a_1 + a_1)] + 2Aa_4(E - a_{10})] \\
a_7 &= \left( \frac{\hbar e^3 B_y}{m^*} \right) < Z >, \\
a_8 &= \frac{1}{3} \left( \frac{\hbar^2 e L_x B_z B_y}{m^*} \right) < Z >, \\
a_9 &= a_8, \\
a_{10} &= \left( \frac{e^2}{2m^*} \right) \left[ B^2_y < Z > + \frac{1}{3} B^2_x L^2_x + \frac{1}{3} B^2_y L^2_y \right], \\
a_{11} &= \left( \frac{e^2 B^2_y}{2m^*} \right) \langle Z^2 \rangle, \\
a_{12} &= \frac{2}{3} \left( \frac{e L_x B_z}{2m^*} \right)^2, \\
a_{13} &= \frac{2}{3} \left( \frac{e L_x B_z}{2m^*} \right)^2, \\
Q(E,n) &= [a_4 - A(a_4 + a_5 + a_6) - Aa_3(E - a_{10}) + A(a_{11} + a_1 + a_1)a_4 + 2Aa_4(E - a_{10})], \\
a_{14} &= \left( \frac{\hbar e^3 L_x B^3_x}{4m^*} \right) \langle Z >, \\
a_{15} &= \left( \frac{\hbar e^3 L_x^2 B^3_y B^3_z}{2m^*} \right) \langle Z^2 >,
\end{align*}
11.4.2. The functions $T_1(E_F, n)$ and $T_2(E_F, n)$ have been defined as follows:

$$T_1(E_F, n) = \left[ \frac{P_2(E_F, n)P_1(E_F, n) - 2P_1(n)C(E_F, n)}{\sqrt{P_2^2(E_F, n) - 4P_1(n)C(E_F, n)}} - P_2'(E_F, n) \right],$$

$$T_2(E_F, n) = \left[ -Q_2(E_F, n) + \frac{Q_2(E_F, n)Q_1'(E_F, n) - 2Q_1(n)C'(E_F, n)}{\sqrt{Q_2^2(E_F, n) - 4Q_1(n)C(E_F, n)}} \right]$$

and the primes denote the differentiation with respect to $E_F$.

11.4.3. The notations as given in equation (11.8) are defined as follows:

$$H'(E, n) = -H(E, n)C'_1(E, n),$$

$$H(E, n) = \left[ \frac{R(n)}{2C_1(n)} \right],$$

$$C_1(E, n) = \left[ C(E, n) - P_1(n)I^1(E, n) - Q_1J^1(E, n) + R(n)I(E, n) + P_2(E, n)J(E, n) - Q_2(E, n)J(E, n) \right]$$

$$I(E, n) = \left[ \frac{2Q_2(E, n) - R(n)Q_2(E, n)}{R^2(n) - 4Q_1P_1(n)} \right],$$

$$J(E, n) = \left[ \frac{2P_2(E, n)Q_2(E, n) - R(n)P_2(E, n)}{R^2(n) - 4Q_1P_1(n)} \right].$$
\[
C'(E,n) = \left[ C'(E,n) - 2P(n \gamma(E,n)) - 2Q_1(n \gamma(E,n)) + R(n \gamma(E,n)) \right] + R(n \gamma(E,n)) \gamma(E,n)_1 - Q_2(E,n) \gamma(E,n)_1 - Q_{1}(E,n) \gamma(E,n)_1,
\]

\[
C'(E,n) = -[1 + 2A(E - a_{i0})],
\]

\[
I'(E,n) = \frac{2P_1(E,n) - R(n)Q_1(E,n)}{R^2(n) - 4Q_2P_1(n)},
\]

\[
P_1(E,n) = A(2a_1 - a_1),
\]

\[
Q_1(E,n) = A(2a_2 - a_2),
\]

\[
J'(E,n) = \frac{2P_2(E,n) - R(n)P_2(E,n)}{R^2(n) - 4Q_2P_1(n)},
\]

\[
A'(E,n) = -A(E,n)C_1(E,n),
\]

\[
A(E,n) = \frac{R(n)}{C_1(E,n)},
\]

\[
D(E,n) = \frac{Q_2}{C_1(E,n)}, \quad D'(E,n) = -D(E,n)C_1(E,n),
\]

\[\theta \] is the Heaviside step function and \( E_n \) is the size quantized energy of the \( i-th \) sub-band which can, in turn, be determined from the equation \( C(E_n, n) = 0 \).

### 11.4.4

The notation as given in equation (11.9) are defined as follows:

\[
L_1(n, E_F) = \frac{1}{\sqrt{\text{Area}(n, E_F) D(n, E_F) - H^2(n, E_F)}},
\]

\[
L_1(n, E_F) = \sum_{r=1}^{S} \nabla_r \left[ L_1(n, E_F) \right],
\]

\[r\] is the set of real positive integer whose upper limit is \( S \).

\[
\nabla_r = 2(k_B T)^{r} \left( 1 - 2^{2r} \right) \zeta(2r) \frac{d^{2r}}{dE_F^{2r}}, \quad \zeta(2r) \] is the Zeta function of order \( 2r \) and \( E_F \) is the Fermi energy in the present case.
11.4.5. The functions $E_n, L_3(n, E_F)$ and $L_3(n, E_F)$ are defined as follows:

\[
E_n = \frac{\hbar^2}{2m^*} \left( \frac{n\pi}{a} \right)^2 - A \left( \frac{\hbar^2}{2m^*} \left( \frac{n\pi}{a} \right)^2 \right)^2,
\]

\[
L_3(n, E_F) = \left[ \frac{m^*}{4\hbar^2} \left( 1 - \sqrt{1 - 4aE_F} \right) \right] \left( \frac{n\pi}{a} \right)^2,
\]

\[
L_4(n, E_F) = \sum_{r=1}^{s} \nu_r [L_3(n, E_F)].
\]