ISSN 1330–0008
CODEN FIZAE4

ON THE ELECTRIC SUSCEPTIBILITY MASS IN $A_3^{II}B_2^V$ SEMICONDUCTORS IN THE PRESENCE OF AN ARBITRARILY ORIENTED QUANTIZING MAGNETIC FIELD

KAMAKHYA PRASAD GHATAK

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

Received 23 January 1992
UDC 538.915

Original scientific paper

An attempt is made to investigate the electric susceptibility mass of electrons in $A_3^{II}B_2^V$ materials under arbitrary magnetic quantization by including the influence of spin and broadening of Landau levels. It is found, taking n-Cd_3P_2 as an example, that the same mass oscillates with inverse quantizing magnetic field and also with the angle of orientation of the same field. Besides, the same mass increases with increasing carrier degeneracy and the crystal field splitting parameter enhances the numerical magnitudes in all three variations. The corresponding results for the three-band Kane model, the two-band Kane model and that of parabolic energy bands have also been obtained as special cases of our generalized derivation.

1. Introduction

In recent years there has been considerable interest in studying the electric susceptibility mass (ESM) of the carriers in semiconductors because of their importance in investigations of carrier scattering mechanism in semiconductors[1–3]. Besides, the ESM can be determined from measurement in the infrared region of frequency dependence of the spectral reflectivity at normal incidence and provides useful information about very specialized band models[2]. The fact that ESM changes drastically in narrow-gap materials due to energy dependence of the effective mass of the carriers in non-parabolic bands has been well discussed[3]. Nevertheless, it appears from the literature that the ESM in $A_3^{II}B_2^V$ semiconductors has yet to be investigated under arbitrary magnetic quantization for the more interesting case which occurs from the presence of spin and broadening of Landau levels. This will make our analysis a generalized one since we can obtain the corresponding well known results for even isotropic energy bands under certain limiting conditions. It may also be noted that the above class of materials is being increasingly used as non-linear optical materials[4)] and light emitting diodes[5)]. Shay and Rowe[6)] have demonstrated that quasi-cubic model can be used to explain the observed symmetry and splitting of both bands at the zone centre of $A_3^{II}B_2^{V}$ semiconductors. Incorporating the anisotropic crystal potential to the Hamiltonian, Kildal[7,8)] proposed an E-$\vec{k}$ dispersion relation of the conduction electrons using the simplified assumptions of isotropic momentum-matrix elements and isotropic spin-orbit splitting parameters, respectively, through the anisotropics in the two aforementioned band parameters are significant physical features of $A_3^{II}B_2^{V}$ materials[9)].

In what follows, we shall formulate the ESM by including spin and broadening together with the use of generalized electron dispersion law as given elsewhere[10)]. We shall study the concentration and magnetic field dependences of the ESM, taking n-Cd_3P_2 as an example.

2. *Theoretical background*

The ESM of the electrons in semiconductors under magnetic quantization (m^*_{SB}) can be expressed, extending the method of Spitzer and Fan[1)], as

$$m^*_{SB} = 3\hbar^2 n_0 \left[\sum_{n=0}^{n_{\max}} N_B(E) \left(\frac{\partial E}{\partial k'_z} \right) f_0(E) \mathrm{d}E \right]^{-1} \varepsilon_0 \,, \tag{1}$$

where $\hbar = h/2\pi$, h is the Planck's constant, n_0 is the electron concentration, $n(= 0,\ 1,\ 2\ ...)$ is the Landau quantum number, k'_z is the arbitrary direction of application of the quantizing magnetic field B, $N_B(E)$ is the magneto-density-of-states function, E is the electron energy under magnetic quantization as measured from the edge of the conduction band in the absence of any field and $f_0(E)$ is the Fermi-Dirac occupation probability factor.

It appears, then, that the evaluation of ESM using Eq. (1) requires an expression for $N_B(E)$ which, in turn, is determined by the magneto-dispersion relation. The generalized dispersion relation of the conduction electrons in bulk specimens of $A_3^{II}B_2^{V}$ semiconductors can be written as[10)]

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

where the notations are defined in the above reference. The modified electron energy spectrum of $A_3^{II}B_2^{V}$ materials under arbitrary magnetic quantization can be expressed as

$$\gamma(E) = A_{\pm}(n, E, \Theta) + a(E, \Theta)(k'_z)^2, \tag{2b}$$

where

$$A_{\pm}(n,E,\Theta) = 2eB\hbar^{-1}\left(n+\frac{1}{2}\right)\left[f_1(E)\left\{f_1(E)\cos^2\Theta + f_2(E)\sin^2\Theta\right\}\right]$$

$$\pm\frac{eB\hbar E_g}{6}\left[\frac{E_g+\Delta_\perp}{m_\perp^*\left(E_g+(2/3)\Delta_\perp\right)}\right]^{1/2}\left[\left(E+E_g+\delta+\frac{\Delta_\parallel^2-\Delta_\perp^2}{3\Delta_\parallel}\right)^2\right.$$

$$\left.\times\frac{\Delta_\parallel^2\cos^2\Theta(E_g+\Delta_\perp)}{m_\perp^*\left(E_g+(2/3)\Delta_\perp\right)} + (E+E_g)^2\Delta_\perp^2\sin^2\Theta(E_g+\Delta_\parallel)\left\{m_\parallel^*\left(E_g+\frac{2}{3}\Delta_\parallel\right)\right\}^{-1}\right]^{1/2},$$

$$a(E,\Theta) = f_1(E)f_2(E)\left[f_1(E)\cos^2\Theta + f_2(E)\sin^2\Theta\right]^{1/2},$$

and $k_z' = k_z\cos\theta + k_x\sin\theta$ is the direction of application of B which makes an angle θ with k_z direction and lies in the k_x–k_z plane.

Using Eqs. (1) and (2) we get

$$m_{SB}^* = \frac{12\hbar^3\pi^2 n_0\varepsilon_0}{eBk_BT}\left[\sum_{n=0}^{n_{\max}}\ln\left|x^2(n)+y^2(n)\right|\right]^{-1}, \tag{3}$$

where $x(n) = [1 + (cos\lambda_0)\exp(\eta)]$, $\lambda_0 = \Gamma/k_BT$, Γ is broadening parameter[11)], $\eta = (E_F - E)/k_BT$, E_F is the Fermi energy in the presence of quantizing magnetic field as measured from the edge of the conduction band in the absence of any quantization, E is the root of Eq. (2b) when $k_z' = 0$, k_B is the Boltzmann constant, T is temperature and $y(n) = (\sin\lambda_0)\exp(\eta)$.

It appears, then, that the determination of ESM from Eq. (3) as a function of electron concentration n_0 requires an expression of electron statistics which can in turn, be expressed, using Eq. (2b), as

$$n_0 = \frac{eB}{2\pi^2\hbar}\sum_{n=0}^{n_{\max}}[\alpha_1+\alpha_2]\,, \tag{4}$$

where

$$\alpha_1 = \mathrm{Re}\left\{\left[a^{-1}(E_F^*,\Theta)\{\gamma(E_F^*) - A_{\pm}(n,E_F^*,\Theta)\}\right]^{1/2}\right\},$$

$$E_F^* = E_F + \mathrm{i}\Gamma,\quad i=\sqrt{-1},\quad \alpha_2 = \sum_{r=1}^{S}\nabla_r[\alpha_1]\,,$$

$$\nabla_r = 2(k_BT)^{2r}(1-2^{1-2r})\zeta(2r) - \frac{\mathrm{d}^{2r}}{\mathrm{d}E_F^{2r}}\,.$$

r is the set of positive integers and $\zeta(2r)$ is the zeta function[12] of order $2r$.

Special cases:

(1) Under the special conditions $\delta = 0$, $\Delta_\parallel = \Delta_\perp = \Delta$ (the isotropic spin-orbit splitting parameter) and $m^*_\parallel = m^*_\perp = m^*$ (the isotropic electron mass at the edge of the conduction band), Eq. (2b) assumes the form

$$\left[E(E+E_g)(E+E_g+\Delta)\left(E_g+\frac{2}{3}\Delta\right)\right]\left[E_g(E_g+\Delta)\left(E+E_g+\frac{2}{3}\Delta\right)\right]^{-1}$$

$$= \left(n-\frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2 k_z^2}{2m^*} + \frac{eB\hbar\Delta}{m^*}\left(E+E_g+\frac{2}{3}\Delta\right)^{-1}, \tag{5}$$

where $\omega_0 = eB/m^*$. Equation (5) is the well-known magneto-dispersion relation for the three-band Kane model[13].

Under the above substitutions the basic forms of Eqs. (3) and (4) the remain same, where

$$\alpha_1 = \mathrm{Re}\Bigg[\Bigg[\frac{2m^*}{\hbar^2}\Bigg\{E^*_F(E^*_F+E_g)(E^*_F+E_g+\Delta)\left(E_g+\frac{2}{3}\Delta\right)E_g^{-1}(E_g+\Delta)^{-1}$$

$$\times\left(E^*_F-E_g+\frac{1}{2}\Delta\right)^{-1} - \left(n+\frac{1}{2}\right)\hbar\omega_0 \pm \frac{eB\hbar\Delta}{5m^*}$$

$$\times\left(E^*_F+E_g+\frac{1}{2}\Delta\right)^{-1}\Bigg\}\Bigg]\Bigg].$$

(2) Under the condition $\Delta \to \infty$, Eq. (5) takes the form[14]

$$E(1+\alpha E) = \left(n+\frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2 k_z^2}{2m^*} \pm \frac{1}{2}g^*\mu B\,, \quad \alpha = 1/E_g\,, \tag{6a}$$

where $g^* = m_0/m^*$, m_0 is the free-electron mass and μ is the Bohr magneton. Thus for the two-band Kane model, the basic results Eqs. (3) and (4) will be unaltered, where

$$\alpha_1 = \mathrm{Re}\left\{\left[\frac{2m^*}{\hbar^2}\left\{E^*_F(1+\alpha E^*_F) - \left(n+\frac{1}{2}\right)\hbar\omega_0 \pm \frac{1}{2}g^*\mu B\right\}\right]^{1/2}\right\}.$$

We wish to note that neglecting spin and broadening, together with the condition $E_F/E_g \ll 1$, the expression of electron concentration in accordance with the two-band Kane model assumes the form[14)]

$$n_0 = N_c\Theta \sum_{n=0}^{n_{\max}} a^{-1/2} \left[\left(1 + \frac{3\alpha b}{2}\right) F_{-1/2}(\eta') + \frac{3}{4}\alpha_n F_{1/2}(\eta') \right], \tag{6b}$$

where the notations are defined in the above reference.

(3) Under the condition $a \to 0$, (6a) simplifies to the well known form[14)] as

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2 k_z^2}{2m^*} \pm g^* \mu B\,. \tag{7}$$

Thus for parabolic energy bands, the forms of Eqs. (3) and (4) will be unaltered where

$$\alpha_1 = \mathrm{Re}\left\{ \left[\frac{2m^*}{\hbar^2} \left\{ E_F^* - \left(n + \frac{1}{2}\right)\hbar\omega_0 \pm g^*\mu B \right\} \right]^{1/2} \right\}.$$

(4) Finally, neglecting spin and broadening, the expressions for ESM and n_0 for isotropic parabolic energy bands can be written as

$$m_{SB}^* = \frac{3\pi^2\hbar^3 n_0 \varepsilon_0}{eBk_BT} \left[\sum_{n=0}^{n_{\max}} F_0(\eta) \right]^{-1} \tag{8}$$

and

$$n_o = N_c\Theta \left[\sum_{n=0}^{n_{\max}} F_{-1/2}(\eta) \right], \tag{9}$$

where

$$\eta = \frac{1}{k_BT} \left[E_F - \left(1 + \frac{1}{2}\right)\hbar\omega_0 \right].$$

3. Results and discussion

Using Eqs. (3) and (4) and taking the paramerets[9)]

$$\Delta_\parallel = 0.25\mathrm{eV}, \quad \Delta_\perp = 0.28\mathrm{eV}, \quad \delta = 0.08\mathrm{eV}, \quad m_\parallel^* = 0.03m_0,$$

$$m_\perp^* = 0.05m_0, \quad n_0 = 2.28 \times 10^{22}\,\mathrm{m}^{-3}, \quad \Gamma = 2 \times 10^{-4}\mathrm{eV}, \quad \Theta = 60^\circ,$$

and $T = 4.2$ K, we have plotted the ESM in degenerate n-Cd_3P_2 as a function of quantizing magnetic field as shown in Fig. 1. In the same figure the curves

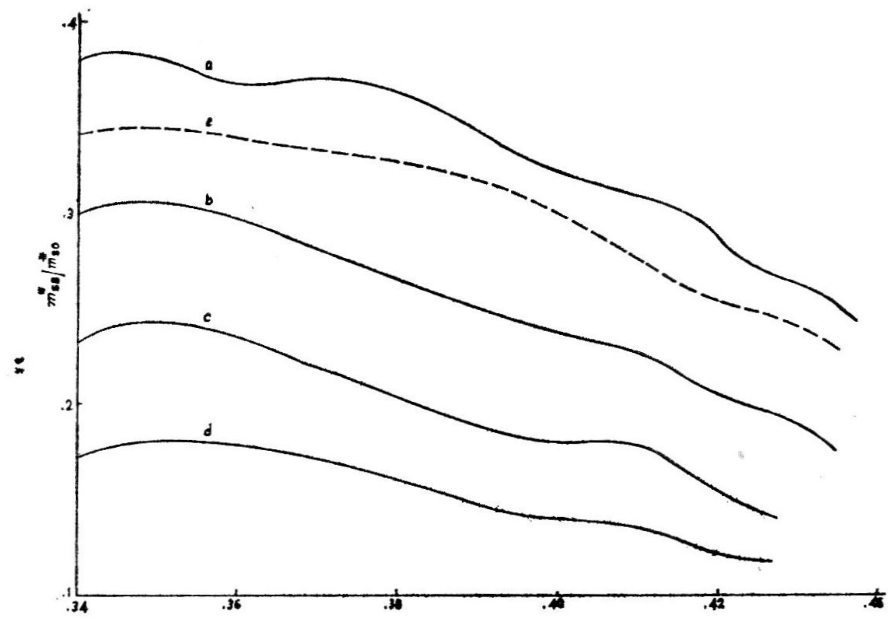

Fig. 1. Plot of the normalized ESM as a function of $1/B$ *at 4.2* K *by using (a) our proposed dispersion relation, (b) the isotropic three-band Kane model, (c) the isotropic two-band Kane model and (d) the parabolic energy bands. The dashed curve e corresponds to* $\delta = 0$.

correspond to the isotropic three-band Kane model (taking $\Delta = 0.3$ eV and $m^* = 0.04m_0$ for the purpose of numerical computation), the two-band Kane model and that of parabolic energy bands are also shown. Using the same parameters as used in obtaining Fig. 1, we have plotted the normalized ESM as functions of n_0 and θ as shown in Figs. 2 and 3 in which all simplified cases have further been shown. In all figures the dotted curves correspond to $\delta = 0$. From these figures and the above discussion the following features follow:

(i) As can be seen in Fig. 1 the ESM oscillates with $1/B$. The oscillatory dependence is due to the crossing over of the Fermi level by the sub-bands in steps, resulting in a successive reduction in the number of occupied Landau levels as the magnetic field is increased. The origin of the oscillations in ESM is the same as that of SdH oscillations. Besides, the ESM computed by using our proposed dispersion relation, exhibits greater numerical values as compared to all other limiting cases.

(ii) As can be seen in Fig. 2 the ESM increases with increasing surface electron concentration and the tetragonal crystal field affects the ESM quite significantly in $A_3^{II}B_2^{V}$ materials. Furthermore, for a fixed value of the electron concentration, the ESM is greater as compared to that in the absence of δ for the whole range of concentrations considered. Though ESM also increases nonlinearly with n_0 for all limiting cases, the rates of increases are totally band structure dependent.

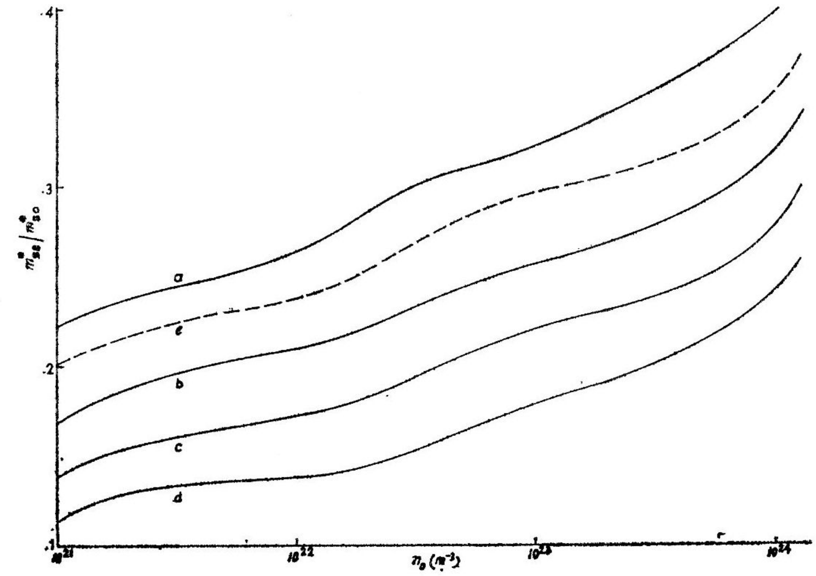

Fig. 2. Plot of the normalized ESM as a function of n_0 at 4.2 K *by using (a) our proposed dispersion law, (b) the isotropic three-band Kane model, (c) the isotropic two-band Kane model and (d) the parabolic energy bands. The dashed plot (e) corresponds to $\delta = 0$ ($B = 2$* T *and $\theta = 60°$).*

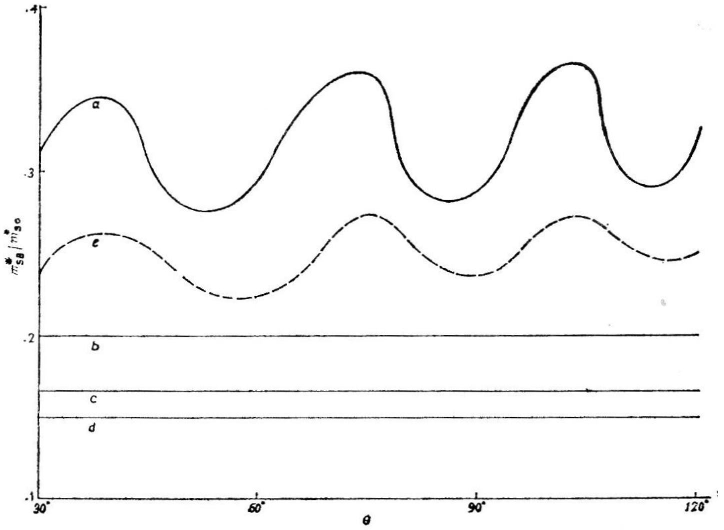

Fig. 3. Plot of the normalized ESM as a function of θ at 4.2 K *by using (a) our proposed model, (b) the isotropic three-band Kane model, (c) the isotropic two-band Kane model and (d) the parabolic energy bands. The dashed curve e corresponds to $\delta = 0$ ($B = 2$* T *and $n_0 = 2.28\ 10^{22}$* m^{-3}.

(iii) As can be seen in Fig. 3, the ESM also exhibits oscillatory dependence with θ. In the absence of anisotropics, the ESM turns out to be independent of θ for all other cases excluding $\delta = 0$ since the basic dispersion relation becomes spherical instead of being ellipsoidal. Thus the ESM for the three-band Kane model, the two-band Kane model and that of parabolic energy bands becomes independent of θ.

We must note that the many-body effects should be taken into account for a more complete treatment. However the basic qualitative features of our simplified analysis will not be altered even after the above modification. Though the experimental verification of the basic content of our paper is not available in the literature (to the best of our knowledge), the importance of ESM is already well-known. The basic aim of the present work is to formulate a simplified expression of the ESM in the $A_3^{II}B_2^{V}$ semiconductors under arbitrary magnetic quantization by including spin and broadening, respectively.

We wish to note that we have taken $A_3^{II}B_2^{V}$ semiconductors as an example of narrow-gap compounds having non-parabolic and non-standard energy bands. By incorporating the anisotropic crystal potential to the Hamiltonian together with anisotropic spin-orbit splitting parameters and the anisotropic effective electron masses, we have formulated the magneto dispersion relation of conduction electrons in the bulk specimen of the same semiconductor within the framework of $\vec{k}\cdot\vec{p}$ theory. In the absence of crystal field splitting and with the assumptions of isotropic effective electron mass and isotropic spin-orbit splitting parameter, Eq. (2b) converts into Eq. (5) which is the result of the magneto three-band Kane model[13]. The three-band Kane model is the best model for III-V semiconductors but must be used as such for studying the magneto-transport of n-InAs where the spin-orbit splitting parameter (Δ) is of the order of band gap (E_g). For many important semiconductors $\Delta \gg E_g$ (i.e. n-InSb, $Hg_{1-x}Cd_xTe$ etc.). Under this condition, Eq. (5) gets simplified into Eq. (6a) which is the result of the well known two-band Kane model[14]. Finally under the condition $E_g \to a$, Eq. (6a) assumes the form of Eq. (7), which is widely used to study the electronic properties of relatively wide band gap semiconductors. Thus we can conclude that our study of ESM covers various semiconductors having different band structures.

References

1) W. G. Spitzer and H. Y. Fan, Phys. Rev. **106** (1957) 882;

2) J. R. Dixon and H. R. Raidl, Phys. Rev. **138** (1965) 873;

3) G. Dinne and J. C. Wolley, Phys. Rev. **6B** (1972) 3898;

4) D. S. Chemla, P. J. Kupeck, D. S. Robertson and R. C. Smith, Opt. Commun. **3** (1971) 29;

5) J. L. Shay, K. J. Beckmann, E. Buchler and J. H. Wernick, Appl. Phys. Letts. **23** (1973) 226;

6) J. W. Rowe and J. L. Shay, Phys. Rev. **3B** (1971) 451;

7) H. Kildal, Phys. Rev. **10B** (1971) 451;

8) J. L. Shay and J. H. Wernick, *Ternary Chalcopyrite Semiconductors*, Pergamon press (1975);

9) S. L. Radautson, E. A. Arushanov, A. N. Mateprov and G. P. Chuiks, *Cadmium Arsenide and Phosphide*, Kishinov, USSR (1976);

10) K. P. Ghatak and M. Mondal, Fizika **18** (1986) 345;

11) A. I. Ponomarov, G. A. Potapov, G. E. Kharus and I. M. Tsidilkovskii, Soviet Phys. Semicond. **13** (1979) 502;

12) I. A. Ivic, *The Riemann Zeta-Function*, Wiley Interscience, New York (1986).

13) R. Dornhaus and G. Nimtz, Springer Tracts in Modern Physics **78** (1976) 1;

14) B. R. Nag. *Electron Transport in Compound Semiconductors*, Springer-Verlag, Berlin (1980).

O ELEKTRIČNOJ SUSCEPTIBILNOJ MASI U $A_3^{II}B_2^{V}$ POLUVODIČIMA PRI PROIZVOLJNOJ ORIJENTACIJI KVANTIZIRAJUĆEG MAGNETSKOG POLJA

KAMAKHYA PRASAD GHATAK

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

Received 23 January 1992

Original scientific paper

Razmatrana je električna susceptibilna masa elektrona u $A_3^{II}B_2^{V}$ materijalima uz proizvoljnu magnetsku kvantizaciju ukjučujući utjecaj spina i širenja Landauovih nivoa. Nađeno je, koristeći n-Cd_3P_2 kao primjer, da masa oscilira s inverzom magnetskog polja te također s kutom orijentacije polja. Pored toga, masa raste porastom degeneracije nosilaca naboja. Parametar cijepanja kristalnog polja povećava brojčanu vrijednost u sve tri varijacije. Kao posebni slučajevi općenitog razmatranja rezultati su primijenjeni na Kaneov model s dvije i tri vrpce, te na model paraboličnih energetskih vrpci.