YU ISSN 0015-3206
FZKAAA 19 (4) 387 (1987)

THEORETICAL STUDY OF THE EFFECTIVE MASS IN BISMUTH IN THE PRESENCE OF A QUANTIZING MAGNETIC FIELD

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Received 1 September 1986

Revised manuscript received 23 March 1987

UDC 538.955

Original scientific paper

An attempt is made to investigate theoretically the effective mass of the holes at the Fermi level in bismuth at low temperatures in the presence of a DC quantizing magnetic field along the trigonal axis by using the Abrikosov dispersion relation allowing various types of anisotropies in the energy spectrum. It is found that the dependence of the same mass on the Fermi energy and the magnetic quantum number is due solely to the effect of band non-parabolicity and is a characteristic feature of Abrikosov model. In addition, the corresponding well-known results of anisotropic parabolic energy bands are also obtained from the expressions derived.

1. Introduction

In recent years, there has been considerable interest in studying the different electronic properties of bismuth having nonparabolic and non-standard energy bands [1-4,8,9]. Nevertheless, there still remain scopes in the investigations made while the interest for further researches of the different other interesting features of bismuth is becoming increasingly important. One such important parameter is the

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effective mass of the carriers since it plays the most dominant role in carrier transport and has also been studied under various physical conditions[5-7]. It is worth remarking that the effective mass of the holes in bismuth has yet to be theoretically investigated magnetic quantization for the more difficult case which occurs from the use of Abrikosov dispersion relation of the carriers allowing various types of anisotropies in the energy spectrum[8]. The Abrikosov model explains the data for a large number of magnetooscillatory and resonance experiments[4].

In what follows we shall first derive an expression for the effective mass of the holes in Bi, in the presence of a quantizing magnetic field along the trigonal axis by using the above model. We shall study the effective mass at the Fermi level since at low temperatures where the quantum effects become prominent the carriers at the Fermi surface are the major participants in carrier transport. We shall investigate theoretically the doping and magnetic field variations of the same mass respectively by formulating the appropriate carrier statistics.

2. *Theoretical background*

The energy spectrum of the holes in bismuth can be expressed[9], following Abrikosov[8], as

$$[(\varepsilon/\varepsilon_g - p_2^2/2m_2\,\varepsilon_g)\,(1 + \varepsilon/\varepsilon_g + \mu\, p_2^2/2\,m_2\,\varepsilon_g)] = (p_1\,V_1)^2 + (p_3\,V_3)^2 \qquad (1)$$

where ε is the energy of the holes as measured from the edge of the valence band in the vertically downward direction, ε_g is the band gap, p_2 is the hole momentum along bisectrix axis, $\mu = \frac{m_2}{m_2'}$, $V_1^2 = \frac{\varepsilon_g}{2m_1}$, $V_3^2 = \frac{\varepsilon_g}{2m_3}$, the m_i ($i = 1,2$ and 3) are the effective hole masses at the botom of the valence band, m_2' is the longitudinal band-edge effective mass at the edge of the conduction band, p_1 and p_3 are the hole momenta along the binary and trigonal axes, respectively.

Thus the energy eigenvalue equation in the presence of a DC quantizing magnetic field B along the trigonal axis can be written as

$$[H_0\,(1 + a\,H_0)]\,\psi_B = H_B\,\psi_B = [E\,(1 + a\,E)]\,\psi_B \qquad (2)$$

where $a = 1/\varepsilon_g$, ψ_B is the eigenfunction under magnetic quantization,

$$H_B = \left[\frac{a\,(p_2 - |e|\,Bx)^2}{4\,m_1\,m_2'} + \frac{p_1^2}{2\,m_1} + \frac{p_3^2}{2\,m_3} + (p_2 - |e|\,Bx)^2 \left\{\frac{1}{2\,m_2}(1 + a\,\varepsilon) - \frac{a\,\varepsilon}{2m_2'}\right\}\right],$$

$|e|$ is carrier charge and E is the true energy of the system defined by $E\psi_B = H_0\psi_B$.

Therefore, the modified carrier energy spectrum under magnetic quantization, up to first order, can be expressed including spin effects as

$$E\,(1 + a\,E) = \left(n + \frac{1}{2}\right)\hbar\,\omega_0 + \frac{p_3^2}{2m_3} \pm \frac{1}{2}\,g_0\,\mu_0\,B + \beta\,(E, n) \qquad (3)$$

where n is magnetic quantum number, $\hbar = h/2\pi$, h is Planck's constant, $\omega_0 = e B (m_1 m_2)^{-1/2}$, g_0 is the magnitude of the spectroscopic splitting factor at the band edge, μ_0 is the Bohr magneton,

$$\beta(E, n) = \left[\left(n + \frac{1}{2}\right) \hbar \omega_0 \{A(E) - 1\} + \frac{3a}{8}\left(n^2 + n + \frac{1}{2}\right) \hbar^2 \omega_0^2 A^2(E)\right]$$

and

$$A(E) = [1 + a E(1 - \mu)]^{1/2}.$$

Therefore, the effective mass of the carriers at the Fermi level can be expressed as

$$m^*(n, E_F) = m_3 [1 + 2 a E_F - \Delta(E_F, n)] \tag{4}$$

where E_F is the Fermi energy in the presence of magnetic quantization as measured from the band egde in the absence of any quantization,

$$\Delta(E_F, n) = \left[\left(n + \frac{1}{2}\right) \hbar \omega_0 C(E_F) + \frac{3a}{4}\left(n^2 + n + \frac{1}{2}\right) \hbar^2 \omega_0^2 A(E_F) C(E_F)\right]$$

and

$$C(E_F) = a(1 - \mu)[2A(E_F)]^{-1}.$$

Thus, the determination of the effective hole mass at the Fermi level corresponding to a given magnetic sub-band would require the hole statistics which in turn is determined by the density of-states function. Using Eq. (3), the density-of-states function can be written by including spin and broadening effects as

$$N_B(E) = g_v e B (m_3)^{-1/2} h^{-2} \sum_{n=0}^{n_{max}} [\psi(E)]^{-1} [\{G^2(E) + H^2(E)\}^{-1/2}.$$

$$\{G(E) g(E) + H(E) \bar{h}(E)\} + g(E)] \tag{5}$$

where g_v is the valley degeneracy and the other functions are defined in Appendix.

Thus, combining Eq. (5) with the Fermi-Dirac occupation probability factor, the carrier statistics can be expressed as

$$n_0 = \frac{g_v e B \sqrt{m_3}}{2\pi \hbar^2} \sum_{n=0}^{n_{max}} [\psi(E_F) + U(E_F)] \tag{6}$$

where

$$U(E_F) = \sum_{r=1}^{s} 2 (k_B T)^{2r} (1 - 2^{1-2r}) \zeta(2r) \frac{d^{2r}}{d E_F^{2r}} [\psi(E_F)].$$

k_B is Boltzmann constant, T is temperature, $\zeta(2r)$ is the zeta function of order $2r$ and r is the set of real positive integers.

For $a \to 0$, as for parabolic energy bands, Eq. (1) gets simplified into the well-known form

$$\varepsilon = \frac{p_1^2}{2\,m_1} + \frac{p_2^2}{2\,m_2} + \frac{p_3^2}{2\,m_3}. \tag{7}$$

It is thus expected that under the above substitution the results derived in this paper should convert into simpler forms of parabolic energy bands under magnetic quantization. Thus using the above substitution, the Eqs. (3) to (6) assume the following forms

$$E = \left(n + \frac{1}{2}\right) \hbar\,\omega_0 \pm \frac{1}{2} g_0\,\mu_0\,B + (p_3^2/2\,m_3) \tag{8}$$

$$m^* (n, E_F) = m_3 \tag{9}$$

$$N_B(E) = g_v\,e\,B \sqrt{m_3}\,h^{-2} \sum_{n=0}^{n_{max}} [Y(E)/X(E)] \tag{10}$$

and

$$n_0 = \frac{2\,g_v\,e\,B \sqrt{m_3}}{h^2} \sum_{n=0}^{n_{max}} [Y(E_F) + Z(E_F)] \tag{11}$$

where the symbols are defined in Appendix.

It may be noted that in the absence of spin-splitting, Eq. (10) takes the form[10)]

$$N_B(E) = \frac{g_v\,e\,B \sqrt{m_3}}{h^2} \sum_{n=0}^{n_{max}} [E_Z + \sqrt{E_Z^2 + \Gamma^2}]\,[E_Z^2 + \Gamma^2]^{-1/2}. \tag{12}$$

It is worth mentioning that in the absence of broadening Eqs. (10) and (11) assume the following well-known forms[11)]:

$$N_B(E) = g_v\,\pi\,\hbar\,\omega_0 \left(\frac{2\,m_d}{h^2}\right)^{3/2} \sum_{n=0}^{n_{max}} [E - \left(n + \frac{1}{2}\right) \hbar\,\omega_0 \pm \frac{1}{2} g_0\,\mu_0\,B]^{-1/2} \tag{13}$$

and

$$n_0 = [g_v\,N_c\,\overline{\Theta}/2] \sum_{n=0}^{n_{max}} F_{-\frac{1}{2}}(\eta') \tag{14}$$

where

$$m_d = (m_1\,m_2\,m_3)^{1/3},$$

$$N_c = 2\,(2\,\pi\,m_d k_B\,T/h^2)^{3/2},$$

$$\overline{\Theta} = \hbar\,\omega_0/k_B T,$$

$$\eta' = (k_B\,T)^{-1}\,[E_F - \left(n + \frac{1}{2}\right) \hbar\,\omega_0 \mp \frac{1}{2} g_0\,\mu_0\,B]$$

and $F_j(\eta')$ is the one parameter Fermi-Dirac integral of order j[11)].

3. *Results and discussion*

Using Eqs. (4) and (6) together with the parameters[1,2,4] $m_1 = m_2 = m_2' = m_0/1.49$, $m_3 = m_0/1.41$, $g_v = 1$ (as applicable for holes) $E_g \doteq 0.0155$ eV, $T_D = 3$K, $g_0 = 55$ and $T = 4.2$ K we have plotted the normalized effective masses of the holes at the Fermi level of the first three magnetic sub-bands in bismuth as functions of the hole concentration for two given values of the quantizing magnetic field as shown in Fig. 1. In Fig. 2, using the same set of parameters, the normalized Fermi level masses of the holes of the first three magnetic sub-bands have been computed as functions of the reciprocal quantizing magnetic field corresponding to a given value of the hole concentration of 10^{22} m^{-3}. For these figures and the above discussion, the following features follow:

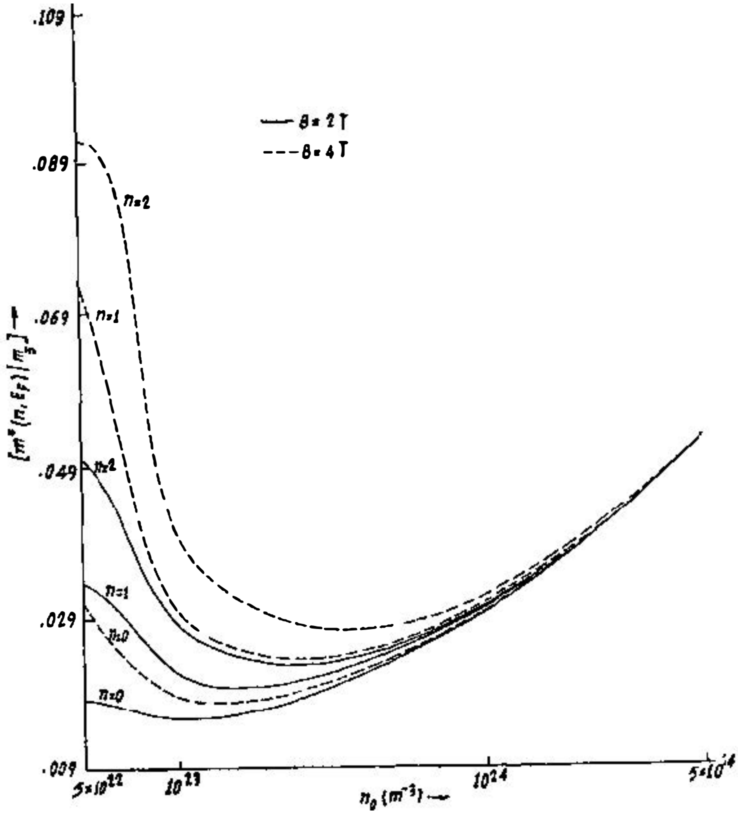

Fig. 1. Plot showing the dependence of the normalised effective mass at the Fermi level of the holes of the first three magnetic sub-bands in bismuth on hole concentration for two given values of quantizing magnetic field.

(i) The quantum number dependent behaviour of the effective mass of the carriers in Bi is solely due to band non-parabolicity which can be demonstrated by comparing Eqs. (4) and (9) and is a characteristic feature of the Abrikosov model. In

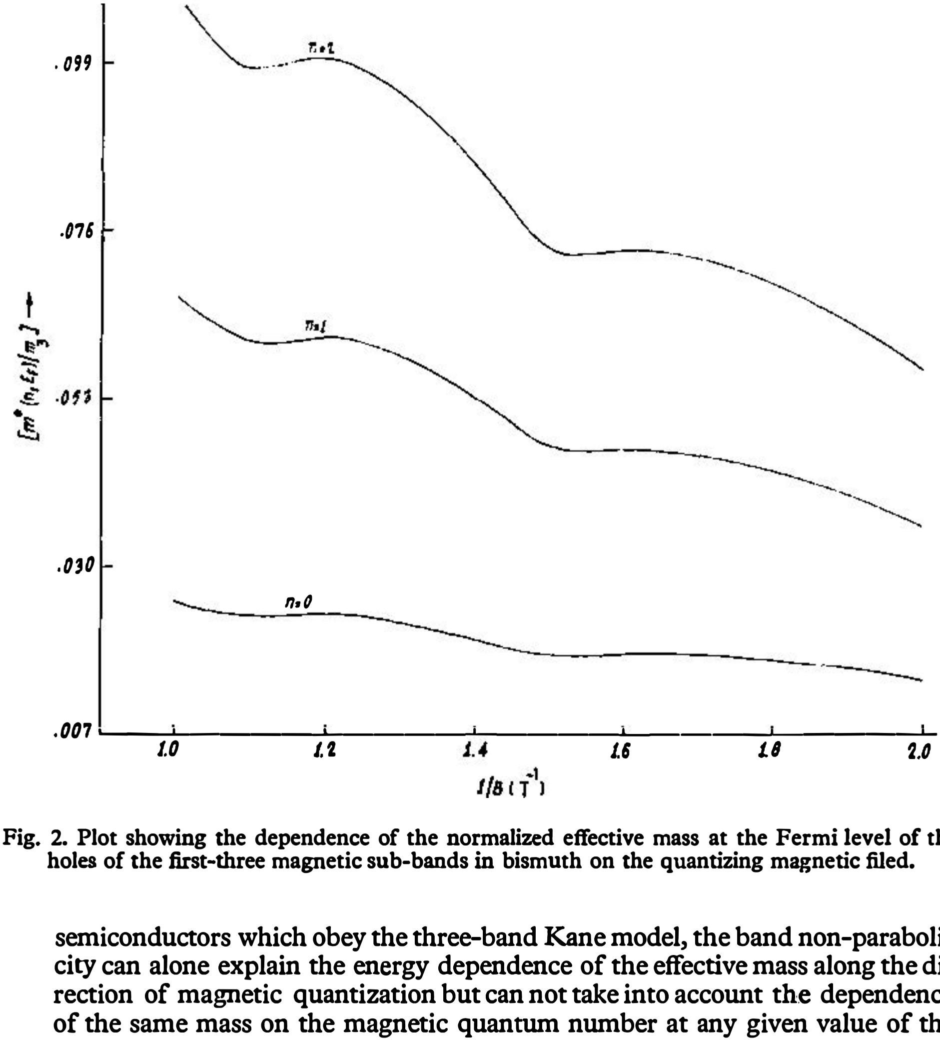

Fig. 2. Plot showing the dependence of the normalized effective mass at the Fermi level of the holes of the first-three magnetic sub-bands in bismuth on the quantizing magnetic filed.

semiconductors which obey the three-band Kane model, the band non-parabolicity can alone explain the energy dependence of the effective mass along the direction of magnetic quantization but can not take into account the dependence of the same mass on the magnetic quantum number at any given value of the electron energy. Incidentally the characteristic feature of the Abrikosov model is that the same band nonparabolicity also explains the dependence of the same mass on the magnetic quantum number.

(ii) The effective Fermi level masses increase with increasing carrier degeneracy in a continuous manner. This behaviour is expected since in non-parabolic bands the effective mass is a monotonic increasing function of Fermi energy.

(iii) The effective Fermi level masses corresponding to different magnetic quantum number differ widely with each other for relatively small values of n_0 while they converge to a single value for higher values of the carrier degeneracy in the whole range of concentrations considered. In the magnetic quantum limit, the effective mass at the Fermi level corresponding to the lowest magnetic sub-band will be the effective conductivity mass for hole transport in bismuth.

(iv) The same mass exhibits an oscillatory magnetic field dependence. 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. For each coincidence of a Landau level with the Fermi level, there would be a discontinuity in the density-of-states function resulting in a peak of large oscillations. Thus it may be noted that the origin of the oscillations in the effective mass in bismuth is the same as that of Shubnikov-de Hass oscillations. The appearance of the small oscillations in the figure is due to the redistribution of the holes among the quantized energy levels when the magnetic quantum number corresponding to the highest occupied level changes from one fixed value to the other.

It is worth noting that if the direction of application of the magnetic field is taken as an arbitrary one and not longitudinal direction as assumed in the present work, the effective mass of the carriers at the Fermi level corresponding to any given sub-band would be different analytically. Nevertheless, the arbitrary choice of the direction of application of the quantizing magnetic field would not result in a change of basic qualitative features of the index-dependent effective mass of the carriers in bismuth at the Fermi level corresponding to any particularly sub-band. The *SdH* oscillations which occur in degenerate semiconductors would further be influenced by the index-dependent oscillatory effective mass in bismuth and the contribution of the oscillatory effective mass to the oscillatory mobility would be important. Though the experimental verification of the basic content of our paper is not available to the best of our knowledge, the importance of the effective mass in the whole field of semiconductor physics is already well-known. Besides, though in a more rigorous treatment the many body effects and the dependence of the level width on the other physical parameters should be considered along with a self consistent procedure, this simplified analysis exhibits the basic qualitative features of the index dependent effective hole mass in bismuth. Finally, we remark that the basic aim of the present paper is not solely to demonstrate the effect of magnetic quantization on the effective hole mass at the Fermi level in bismuth by using the Abrikosov dispersion relation, but also to formulate the corresponding density-of-states function by including both the broadening and spin effects according to the said model since the various carrier transport and the derivation of the expressions of many important physical parameters are directly based on the density-of-states function in such materials.

Appendix

The functions $\bar{\psi}(E)$, $G(E)$, $H(E)$, $g(E)$, $\bar{h}(E)$, $Y(E)$, $X(E)$ and $Z(E_F)$ are defined as follows:

$$\psi(E) = [G(E) + \sqrt{G^2(E) + H^2(E)}]^{1/2} \tag{1.1}$$

$$G(E) = P(E) - t_0 \sqrt{\varrho(E)} \tag{1.2}$$

$$g(E) = [I(E) - (t_0/2)\, L(E)\, \varrho(E)^{-1/2}] \tag{1.3}$$

$$H(E) = \Theta(E) - t_0 \sqrt{\delta(E)} \tag{1.4}$$

$$\bar{h}(E) = [\Theta_0 - (t_0/2)\, d(E)\, \delta(E)^{-1/2}] \tag{1.5}$$

$$Y(E) = [\eta(E) + \sqrt{\eta^2(E) + \Gamma^2}]^{1/2} \tag{1.6}$$

$$X(E) = [\Gamma^2 + \eta^2(E)]^{1/2} \tag{1.7}$$

and

$$Z(E_F) = \sum_{r=1}^{s} 2(k_B T)^{2r} (1 - 2^{1-2r})\, \zeta(2r) \frac{d^{2r}}{d E_F^{2r}} [Y(E_F)] \tag{1.8}$$

where

$$P(E) = [a(E^2 - \Gamma^2) + Ea(n) \pm \frac{1}{2} g_0 \mu_0 B],$$

Γ is the level width and is given by[12] $\Gamma = \pi k_B T_D$ in which T_D is the Dingle temperature,

$$a(n) = \left[1 - \frac{3}{8} (a \hbar \omega_0)^2 \left(n^2 + n + \frac{1}{2}\right)\right],$$

$$t_0 = \left(n + \frac{1}{2}\right) \hbar \omega_0,$$

$$\varrho(E) = \left[\frac{1}{2} \{\varkappa(E) + \sqrt{\varkappa^2(E) + y^2}\}\right],$$

$$\varkappa(E) = [1 + a E (1 - \mu)],$$

$$y = a \Gamma (1 - \mu),$$

$$\Theta(E) = \Gamma [(a(n) + 2a E],$$

$$I(E) = [\Theta(E)/\Gamma],$$

$$\delta(E) = \frac{1}{2} [\sqrt{y^2 + \varkappa^2(E)} - \varkappa(E)],$$

$$L(E) = \left[\frac{a_0}{2} + a_0 \varkappa(E) \{y^2 + \varkappa^2(E)\}^{-1/2}\right],$$

$$a_0 = a(1 - \mu),$$

$$\Theta_0 = 2 a \Gamma,$$

$$d(E) = \left[a_0 \varkappa(E) \{\varkappa^2(E) + y^2\}^{-1/2} - \frac{a_0}{2} \right],$$

$$\eta(E) = [E_z \pm \frac{1}{2} \mu_0 g_0 B]$$

and

$$E_z = [E - \left(n + \frac{1}{2}\right) \hbar \omega_0].$$

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TEORIJSKO RAZMATRANJE EFEKTIVNE MASE U BIZMUTU U PRISUSTVU KVANTIZIRAJUĆEG MAGNETSKOG POLJA

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Originalni znanstveni rad

Pokušalo se teorijski istražiti efektivnu masu šupljina na Fermi nivou u bizmutu na niskim temperaturama u prisustvu kvantizirajućeg magnetskog polja istosmjerne struje duž trigonalne osi koristeći Abrikosovu disperzionu relaciju, dopuštajući različite tipove anizotropije u energetskom spektru. Pronađeno je da je ovisnost iste mase o Fermi energiji i magnetskom kvantnom broju isključivo efekt ne-paraboličnosti vrpce, što je karakteristično svojstvo Abrikosovog modela. Iz dobivenih relacija također su dobiveni dobro poznati rezultati za anizotropne parabolične energetske vrpce.