YU ISSN 0015—3206
FZKAAA 18 (1) 35 (1986)

EFFECT OF SIZE QUANTIZATION ON THE EFFECTIVE ELECTRON MASS IN ULTRATHIN FILMS OF BISMUTH

MANABENDRA MONDAL and KAMAKHYA P. GHATAK*

Department of Pure Physics,

University College of Science and Technology,

92, Acharya P. C. Road, Calcutta — 700 009, India

Received 5 September 1984

Revised manuscript received 23 December 1985

UDC 538.915

Original scientific paper

An attempt is made to investigate the effect of size quantization on the effective electron mass in ultrathin films of bismuth. It is found, on the basis of the Cohen model, that the effective electron mass at the Fermi level depends on the size quantum number and is strongly influenced bv the thickness of the film.

1. Introduction

It is well-known that the effective mass of the carriers in semiconductors is a very important parameter since it is this mass which plays the most dominant role in all types of carrier transport in semiconductors and has also been investigated in the literature[1-4] under various physical conditions. Nevertheless, the effective electron mass in ultrathin Bi-film having non-parabolic and non-standard energy bands has yet to be worked out for the more diffcult case which occurs from the use of the Cohen dispersion relation of the conduction electrons allowing anisotropies in the energy spectrum[5,6]. It may be mentioned in this

* Institute of Radio Physics and Electronics, University College of Science and Technology, 92, Acharya P. C. Road, Calcutta-700 009, *India.*

context that, in such ultrathin films where the film dimension is comparable to the de-Broglie wave length of the carriers, the restriction of the motion of the carriers along the direction normal to the film (say, the trigonal axis) may be viewed as carrier confinement in a one-dimensional potential well leading to the quantization (known as *quantum size effect*) of the wave vector of the carriers along the direction of trigonal axis which produces a discrete energy spectrum. In what follows, we shall first derive an expression of the effective mass of the electrons at the Fermi level in ultrathin films of bismuth. Besides, we shall derive the electron statistics for the purpose of investigation of the doping and the film-thickness dependence of the same mass under size quantization. It may be stated in this context that the various transport and other phenomena in semiconductors and the derivations of the expressions for many important physical parameters under the above physical condition are based on the electron statistics in such materials. Furthermore, it may be noted that we shall consider the effective mass of the electrons only at the Fermi level since in Bi, particularly in the range of very low temperatures, the electrons at Fermi surface are the major participants in electron transport.

2. *Mathematical background*

The electron energy spectrum in Bi can be expressed, according to Cohen[5,6], as

$$\left(E - \frac{p_2^2}{2m_2}\right)\left(E + E_g + \frac{p_2^2}{2m_2'}\right) = E_g\left[\frac{p_1^2}{2m_1} + \frac{p_3^2}{2m_3}\right] \ldots \qquad (1)$$

where 1, 2, 3 refer to the principal axes system of the quasi-ellipsoid, the m_i ($i =$ $= 1, 2$ and 3) are the effective masses of the electrons at the edge of the conduction band, E_g is the band gap, E is the energy as measured from the edge of the conduction band and m_2' is the longitudinal band edge effective mass for the valence band. The modified dispersion relation in the presence of size quantization can be written, assuming the plane of the ultrathin Bi film is normal to the direction of trigonal axis, as

$$\left(E - \frac{p_2^2}{2m_2}\right)\left(E + E_g + \frac{p_2^2}{2m_2'}\right) = E_g\left[\frac{p_1^2}{2m_1} + \frac{\hbar^2}{2m_3}\left(\frac{n\pi}{d_0}\right)^2\right] \ldots \qquad (2)$$

where $\hbar \equiv h/2\pi$, h is the Planck's constant, $n\,(= 1, 2, 3 \ldots)$ is the size quantum number and d_0 is the thickness of the ultrathin film. Therefore the effective mass of the electrons at the Fermi level E_F, which is measured from the edge of the conduction band in the absence of any quantization, can be expressed from (2) as

$$m_n^*(E_F) = m_n^*(E)\Big|_{E=E_F} = \frac{1}{2\pi}\left[\frac{\partial}{\partial E}\Phi(E)\right]\Big|_{E=E_F} \qquad (3)$$

where $\Phi(E)$ is the area enclosed by equation (2). Incidentally, following Dinger et al.[7], the enclosed area can be written as

$$\Phi(E) = 8\{[(A/C)\{H(E) + G(E)\}]^{1/2} \cdot [G(E)\gamma(\varkappa_E) + 2\{H(E) - G(E)\}\beta(\varkappa_E)\}/_{E=E_F}$$

where

$$A \equiv (\mu/4m_2^2),\ \mu \equiv m_2/m_2',\ c \equiv E_g/2m_1,\ H(E) \equiv [\delta(E) + (2A)^{-1}B(E)],$$

$$\delta(E) \equiv \frac{1}{2}[A^{-2}B^2(E) + 4F(E)A^{-1}],\ \ B(E) \equiv [E + E_g - \mu E]/2m_2,$$

$$F(E) \equiv \left[E(E + E_g) - \frac{E_g}{2m_3}\left(\frac{\hbar n\pi}{d_0}\right)^2\right],\ G(E) \equiv [\delta(E) - B(E)(2A)^{-1}], \tag{4}$$

$\gamma(\varkappa_E)$ and $\beta(\varkappa_E)$ are the complete elliptic integrals of first and second kind, respectively, and

$$\varkappa_E \equiv [H(E)/\{G(E) + H(E)\}]^{1/2}.$$

Thus, using (3) and (4), we get

$$m_n^*(E_F) = \frac{1}{2\pi}[T_1(E) + T_2(E)]/_{E=E_F} \tag{5}$$

where

$$T_1(E) \equiv 4(A/C)^{1/2}[G(E) + H(E)]^{-1/2} \cdot [2\{H(E) - G(E)\}\beta(\varkappa_E) + H(E)\gamma(\varkappa_E)] \cdot [H'(E) + G'(E)],$$

$$T_2(E) \equiv 8[(A/C)\{G(E) + H(E)\}^{1/2}][H'(E)\gamma(\varkappa_E) + 2\{H'(E) - G'(E)\}\beta(\varkappa_E) + 2\{H(E) - G(E)\}\Theta_1(\varkappa_E)L(E) - H(E)\Theta_3(\varkappa_E)L(E)],$$

$$H'(E) \equiv [\delta'(E) + (2A)^{-1}B'(E)],$$

$$\delta'(E) \equiv [A^{-2}B^2(E) + 4A^{-1}F(E)]^{-1/2} \cdot [(4m_2)^{-1}(1-\mu)B(E) + A^{-1}(E_g + 2E)],\ B'(E) \equiv \left(\frac{1-\mu}{2m_2}\right),$$

$$G'(E) \equiv [\delta'(E) - (2A)^{-1}B'(E)],\ \ \Theta_J(\varkappa_E) \equiv \int_0^{\pi/2} \varkappa_E[1 - \varkappa_E^2\sin^2 y]\sin y\, dy,$$

J is the set of real numbers and

$$L(E) \equiv [\varkappa_E/2][H'(E)\{H(E)\}^{-1} - \{G(E) + H(E)\}^{-1}\{G'(E) + H'(E)\}].$$

Thus, it appears that the effective mass at the Fermi level will be different for the carriers of different sub-bands in Bi having non-parabolic and non-standard energy bands. The band non-parabolicity can alone explain the energy dependence of the effective mass but cannot account for the dependence of the effective mass on the size quantum number at any given value of the electron energy. However, it may be noted that it is this energy dependent effective mass which plays the most dominant role in explaining the experimental results of all types of scattering mechanisms, Faraday rotation and various low field *AC* and *DC* transport coefficients, respectively, in ultrathin films of Bi. The dependence of the effective mass on the size quantum number is due to the combined effect of the p_2^4 term and the energy dependent p_2^2 term of the modified electron energy spectrum.

The determination of the effective electron mass at the Fermi level corresponding to a given subband would require the electron statistics which in turn can be expressed, in the range of very low temperatures and neglecting the small tilt angles, as

$$n_0 = \frac{2 \times 3}{(2\pi)^2} \sum_{n=1}^{n_{max}} [\Phi (E_F)]. \tag{6}$$

3. *Results and discussion*

Using the appropriate equations together with the parameters[8] $m_1 = 0.00194\, m_0$, $m_2 = 0.235\, m_0$, $m_3 = 0.0024\, m_0$, $m_2' = 0.236\, m_0$ and $E_g = 0.015$ eV we have computed the normalized Fermi level masses for the electrons of the first three sub-bands at low temperatures as functions of the film thickness in ultrathin films of bismuth corresponding to an electron concentration of 10^{17} m^{-2} as shown in Fig. 1. In Fig. 2, with the same parameters, we have computed the normalized Fermi level masses for the electrons of the first three sub-bands at low temperatures as functions of the electron concentration per unit area corresponding to a film thickness of 30 nm. The effect of size quantization is immediately apparent from Fig. 1 since the effective Fermi level mass has become strongly dependent on the thickness of the film which is in direct contrast to that observed in bulk specimens of Bi. It has further been observed that the different effective masses corresponding to different electric sub-bands closely approach each other, for a given film thickness and, for a given electron concentration with increasing film thickness. These are in conformity with expectations since both with increasing electron concentration at a given film thickness and with increasing film thickness for a given electron concentration, the effects of size quantization gradually become less and less significant[9]. It may further be noted that if the direction normal to the film is taken as one of the transverse directions and not as a longitudinal direction as assumed in the present work, the effective mass at the Fermi level corresponding to any given sub-band would be different analytically. Nevertheless, the arbitrary choice of the direction normal to the film would not result in a change of the basic qualitative features of the index-dependent effective electron mass of Bi at the Fermi level corresponding to a particular sub-band. It may finally be remarked that, the general features of the effects of size quantization on the effective

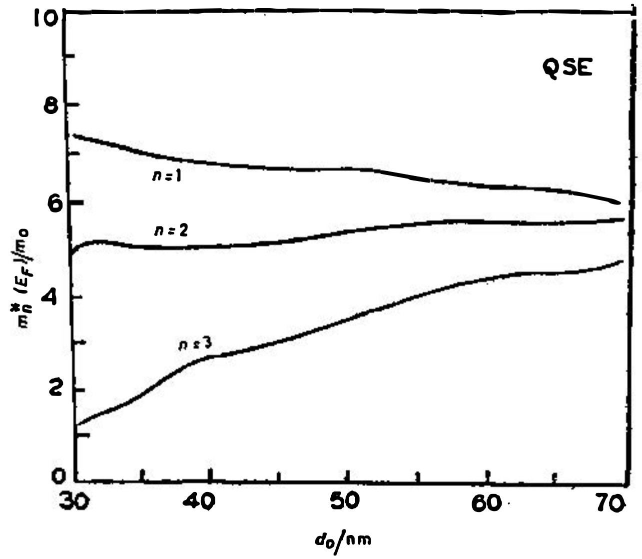

Fig. 1. Plot showing the dependence of the normalized effective mass at the Fermi level of the electrons of the first three sub-bands on film thickness in ultrathin film of Bi at low temperatures corresponding to an electron concentration of 10^{17} m^{-2}.

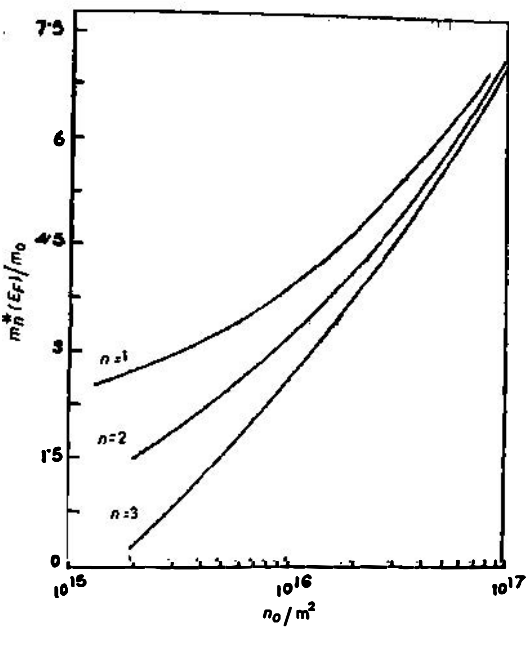

Fig. 2. Plot showing the dependence of the normalized effective mass at the Fermi level of the first three sub-bands on electron concentiation per unit area in ultrathin films of Bi at low temperatures corresponding to a film thickness of 30 nm.

electron mass as discussed here would also be valid with only exception that the same mass will be independent of size quantum number for most of the Kane--type semiconductors[10] having spherical constant-energy surfaces.

References

1) A. N. Chakravarti, K. P. Ghatak, K. K. Ghosh and H. M. Mukherjee, Phys. Stat. Sol. (b) **116** (1963) 17 and the references cited therein;
2) A. C. Sharma, M. M. Ravindra, S. Auluck and V. K. Srivastava, Phys. Stat. Sol. (b) **120** (1983) 715 and the references cited therein;
3) M. Singh, P. R. Wallace, S. D. Jog and E. Arushanov, J. Phys. Chem. Solids **45** (1984) 409;
4) U. Rossler, Solid State Commun. **49** (1984) 409;
5) M. H. Cohen, Phys. Rev. **121** (1961) 387;
6) D. R. Lovett, *Semimetals and Narrow Band Gap Semiconductors*, Pion Limited,London (1977);
7) R. J. Dinger and A. W. Lawson, Phys. Rev. **B1** (1970) 2418;
8) J. Rose and R. Schudhardt, Phys. Stat. Sol. (b) **117** (1983) 213;
9) R. Dingle, *Festkörperprobleme*, Pergamon-Vieweg, **15** (1975) 21;
10) E. O. Kane, J. Phys. Chem. Solids. **1** (1957) 249.

UTJECAJ KVANTNIH EFEKATA VELIČINE NA EFEKTIVNU MASU ELEKTRONA U VRLO TANKIM FILMOVIMA BIZMUTA

MANABENDRA MONDAL i KAMAKHYA P. GHATAK

Department of Pure Physics, University College of Science and Technology, 92, Acharya P. C. Road, Calcuta — 700 009, India

UDK 538.915

Originalni znanstveni rad

Istražen je utjecaj kvantnih efekata veličine na efektivnu masu elektrona u vrlo tankim filmovima bizmuta. Na bazi Cohen-ovog modela, nađeno je da efektivna masa elektrona na Fermijevom nivou ovisi o veličinskom kvantnom broju i pod jakim je utjecajem debljine filma.