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THEORETICAL STUDY OF THE EFFECTIVE ELECTRON MASS IN QUASI-ONE-DIMENSIONAL SYSTEMS OF BISMUTH

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An attempt is made to investigate theoretically the effective electron mass in quasi-one-dimensional systems of bismuth by using the dispersion relation of Takaoka et al. which includes various types of anisotropies in the energy spectrum and has been stated in the literature to be the most valid model of Bi. It is found that the effective electron mass at the Fermi level depends both on the quantum number and the Fermi energy due solely to the influence of band non-parabolicity. Besides, the corresponding results of anisotropic parabolic energy bands are also obtained from the expressions derived.

1. Introduction

In recent years considerable work has already been done in the literature on the various physical properties of bismuth having non-parabolic and non-standard energy bands[1-4]. Nevertheless, there still remain many 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 effective electron mass since it is this mass which plays the most dominant role in all types of electron transport and has also been investigated in the literature under various physical conditions[5-14)]. Nevertheless, the effective electron mass in quasi-one-dimensional systems of bismuth has yet to be theoretically worked out for the more difficult case which occurs from the use of the dispersion relation as proposed by Takaoka et al.[15)] and has also been stated in the literature to be the most valid model of Bi. This is very important since the above model not only includes various types of anisotropies in the energy spectrum of bismuth but also it explains a large number of experimental data. Furthermore, the importance of quasi-one-dimensional conduction and the role of bismuth in such conductor as a promising candidate are already well known[16)].

In what follows, we shall first derive an expression of the effective electron mass in quasi-one-dimensional systems of bismuth by using the dispersion relation as proposed by Takaoka et al.[15)]. Besides, for the purpose of investigating the doping dependence on such mass we shall derive the corresponding electron statistics. It may be stated in this context that the various transport phenomena and the derivation of the expressions of the different physical parameters are based on the corresponding electron statistics in such materials. Incidentally, it may be stated that we shall consider the effective electron mass at the Fermi level since in bismuth particularly at low temperatures where the quantum effects become prominent the electrons at the Fermi surface are the major participants in electron transport.

1. Theoretical background

The energy spectrum of the conduction electrons in bismuth in the absence of any quantization can be expressed according to Takaoka et al.[15)] as

$$E(1+\lambda)=\frac{\beta(E)\,p_2^2}{2M_2}+\frac{\gamma\,p_2^4}{4M_2^2E_g}+\frac{p_1^2}{2m_1}+\frac{p_3^2}{2m_3} \tag{1}$$

where E is the electron energy as measured from the edge of the conduction band in the absence of any quantization, $\lambda\equiv aE$, $a\equiv 1/E_g$, E_g is the band gap, $\beta(E)\equiv$ $\equiv 1+\lambda-\lambda\gamma+\delta$, $\gamma\equiv M_2/M_2'$, $\delta\equiv M_2/m_2$ and the other symbols are defined in the above reference. Incidentally, the modified electron energy spectrum of quasi-one-dimensional systems of bismuth can be written, following Brum[17)] and using Eq. (1), as

$$E(1+\lambda)=\frac{\beta(E)\,\hbar^2}{2M_2}\left(\frac{n_2\pi}{d_2}\right)^2+\frac{\gamma\,\hbar^4}{4M_2^2E_g}\left(\frac{n_2\pi}{d_2}\right)^4+\frac{1}{2m_1}\left(\frac{\hbar\,n\,\pi}{d_1}\right)^2+\frac{p_3^2}{2m_3} \tag{2}$$

where $n_1, n_2\equiv 1, 2, 3, \ldots$, $\hbar\equiv h/2\pi$, h is the Planck's constant, d_1 and d_2 are the dimensions of the rectangular quantum well wire of bismuth.

The use of Eq. (2) leads to the expression of the effective electron mass at the Fermi level E_F as

$$m^*(E_F)=m_3\left[1+2aE_F-(1-\gamma)\,a\,\frac{\hbar^2}{2M_2}\left(\frac{n_2\pi}{d_2}\right)^2\right]. \tag{3}$$

It appears then that the evaluation of the effective mass at the Fermi level as a function of electron concentration requires an expression of the electron statistics which, in turn, is determined by the density-of-states function. Incidentally, using equation (2) the density-of-states function can be expressed as

$$N_{1D} = \frac{g_v \cdot \sqrt{2m_3}}{h} \sum_{n_1=0}^{n_{1max}} \sum_{n_2=0}^{n_{2max}} [\psi(E)]^{-1} \Bigg[1 + 2aE - \\ - (1-\gamma)\frac{a\hbar^2}{2M_2}\left(\frac{n_2\pi}{d_2}\right)^2 \Bigg] H(E-E') \tag{4}$$

where g_v is the valley degeneracy,

$$\psi(E) \equiv \Bigg[E(1+\lambda) - \frac{\beta(E)}{2M_2}\left(\frac{n_2\pi\hbar}{d_2}\right)^2 - \frac{\gamma\hbar^4}{4E_g M_2^2}\left(\frac{n_2\pi}{d_2}\right)^4 - \\ - \frac{1}{2m_1}\left(\frac{\hbar n_1 \pi}{d_1}\right)^2 \Bigg]^{1/2},$$

H the Heaviside step function and E is obtained by putting $p_3 = 0$ and $E = E'$ in Eq. (2). Thus combining Eq. (4) with the Fermi-Dirac occupation probability factor, the electron concentration per unit length is given by

$$n_0 = \frac{g_v \sqrt{2m_3}}{\pi\hbar} \sum_{n_1=0}^{n_{1max}} \sum_{n_2=0}^{n_{2max}} [\psi(E_F) + \Delta(E_F)] \tag{5}$$

where

$$\Delta(E_F) \equiv \sum_{r=1}^{s} 2(k_B T)^{2r}[1 - 2^{1-2r}]\,\zeta(2r)\frac{d^{2r}}{dE_F^{2r}}[\psi(E_F)],$$

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

Incidentally under the substitution $a \to 0$ and $\delta \gg 1$ Eq. (1) takes the well-known form

$$E = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3}. \tag{6}$$

Thus under the above substitutions, Eqs. (3), (4) and (5) assume the following forms:

$$m^*(E_F) = m_3 \tag{7}$$

$$N_{1D}(E) = \frac{g_v \sqrt{2m_3}}{h} \sum_{n_1=0}^{n_{1max}} \sum_{n_2=0}^{n_{2max}} \frac{H(E-a)}{\sqrt{(E-a)}} \tag{8}$$

and

$$n_0 = \frac{g_v}{h} \sqrt{2m_3 \pi k_B T} \sum_{n_1=0}^{n_{1max}} \sum_{n_2=0}^{n_{2max}} F_{-\frac{1}{2}}(\eta) \tag{9}$$

where

$$a \equiv \frac{\hbar^2}{2m_1} \left(\frac{n_1 \pi}{d_1}\right)^2 + \frac{\hbar^2}{2m_2} \left(\frac{n_2 \pi}{d_2}\right)^2, \quad \eta \equiv \left[\frac{E_F - a}{k_B T}\right].$$

$F_j(\eta)$ is the Fermi-Dirac integral of order j as defined by Blakemore[18].

3. *Results and discussion*

Using Eq. (5) together with the parameters[15]

$$m_1 = 0.00109\, m_0,\ m_2 = 0.401\, m_0,\ m_3 = 0.00204\, m_0,\ M_2 = 1.28\, m_0,$$

$$M_2 = 0.80\, m_0,\ E_g = 0.0135 \text{ eV and } T = 4.2 \text{ K},$$

we have plotted the Fermi energy as a function of electron concentration per unit length in 1-D systems of bismuth as shown in Fig. 1 in which the same dependence has also been plotted for parabolic energy bands for the purpose of comparison. Using the same parameters as used in obtaining Fig. 1 we have also plotted in Fig. 2 the normalized effective electron masses corresponding to first three sub-bands as functions of electron concentration in which the concentration axis corresponds to the same dependence for parabolic energy bands. It appears from Fig. 1 that the Fermi energy increases monotonically with electron concentration, as expected in degenerate semiconductors, though the rate of variations are solely band-structure dependent. However, the numerical values of the Fermi energy in 1-D systems of parabolic energy bands increases drastically. Besides it appears from Fig. 2 that the effective electron mass in 1-D bismuth at Fermi level depends both on the quantum number and electron concentration due solely to the effect of band non-parabolicity which can be demonstrated by comparing Eqs. (3) and (7). Furthermore, the effective Fermi level mass increases with increasing quantum number. Besides, they increase with increasing electron concentration as expected for degenerate non-parabolic bands and different effective masses at the Fermi level converge to a single value for relatively higher values of the carrier degeneracy in the whole range of concentrations considered. Incidentally it may be mentioned that if the direction of one-dimensional motion be taken as either k_x or k_y and not as k_z 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 of free one-dimensional motion would not result in a change of the basic qualitative features of the index dependent effective electron mass in bismuth at the Fermi level corresponding to a particular sub-band. It may also be stated that the SdH oscillations which occur in degenerate semiconductors would further be influenced by the index dependent effective electron mass in bismuth and its contribution to the oscillatory mobility would be impor-

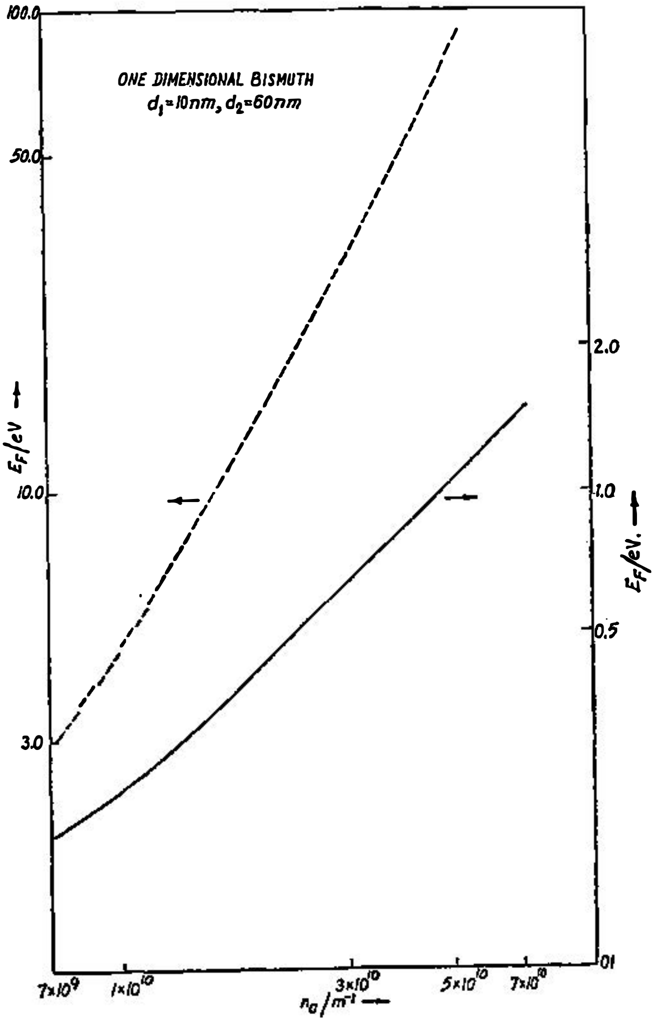

Fig. 1. Plot of the Fermi energy as a function of electron concentration per unit length in one-dimensional systems of bismuth. The dotted plot corresponds to the same dependence for the corresponding anisotropic parabolic energy bands.

tant. Though the experimental verification of the basis content of our paper is not available to the best of our knowledge the importance of the effective electron mass in the whole field of semiconductor physics is already well-known. Finally it may be mentioned that though in a more rigorous treatment the many-body effects should be considered along with a self-consistent procedure, this simplified analysis exhibits the basic qualitative features of the index dependent effective electron mass in 1-D bismuth with reasonable accuracy.

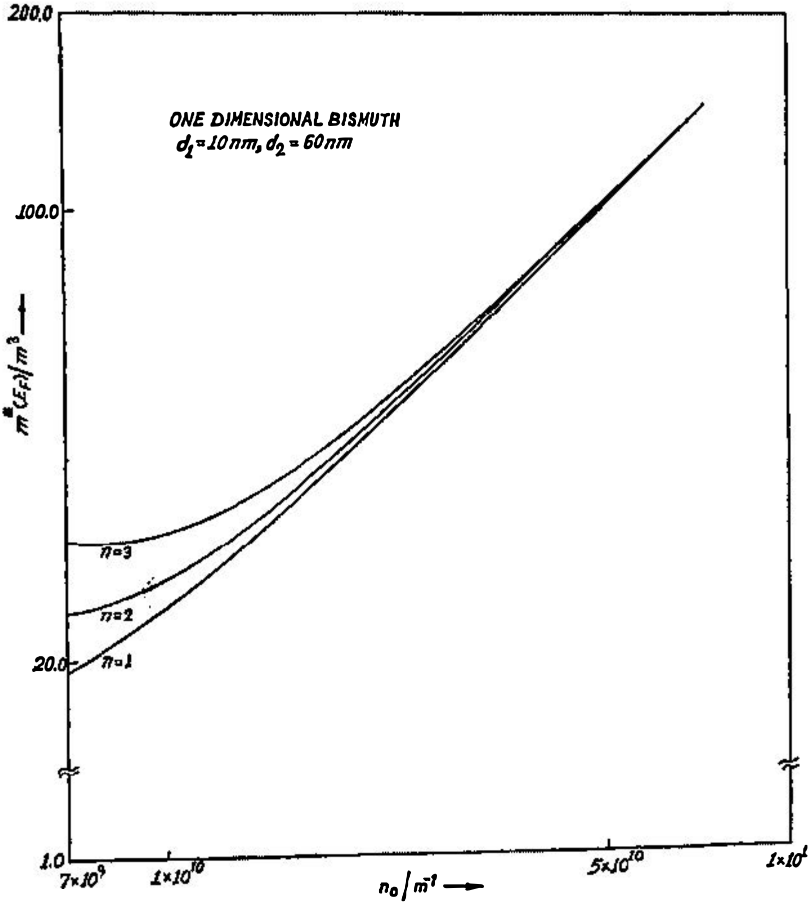

Fig. 2. Plot of the normalized effective masses at the Fermi level for first three sub-bands as functions of electron concentration per unit length in one-dimensional systems of bismuth. The dotted plot corresponds to the same dependence for the corresponding anisotropic parabolic energy bands.

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TEORIJSKA STUDIJA EFEKTIVNE ELEKTRONSKE MASE U KVAZI-JEDNO-DIMENZIONALNIM SUSTAVIMA BIZMUTA

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Koristeći disperzivnu relaciju Takaoke i dr. koja uključuje različite tipove anizotropija u energetskom spektru, i koja je u literaturi bila naznačena kao najvaljaniji model za Bi, napravljen je pokušaj da se teorijski istraži efektivna elektronska masa u kvazi-jedno-dimenzionalnim sustavima bizmuta. Pronađeno je da efektivna elektronska masa na Fermijevom nivou ovisi i o kvantnom broju i o Fermijevoj energiji samo uslijed utjecaja neparaboličnosti vrpce. Osim toga, iz izvedenih izraza su također dobiveni odgovarajući rezultati za anizotropne parabolične energetske vrpce.