EFFECT OF CARRIER DEGENERACY ON THE SCREENING LENGTH IN DEGENERATE TERNARY CHALCOPYRITE SEMICONDUCTORS

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An attempt is made to study the effect of carrier degeneracy on the screening length under the Thomas-Fermi approximation of the carriers in ternary chalcopyrite semiconductors, taking degenerate n-$CdGeAs_2$ as an example. It is found on the basis of the Kildal model that the screening length under the Thomas-Fermi approximation decreases with increasing carrier concentration as expected for degenerate semiconductors and the crystal field parameter effectively reduces the same length. The corresponding results for parabolic semiconductors are also obtained from the expressions derived.

ВЛИЯНИЕ НОСИТЕЛЕЙ ВЫРОЖДЕНИЯ НА ДЛИНУ ЭКРАНИРОВАНИЯ В ВЫРОЖДЕННЫХ ТРОЙНЫХ ХАЛЬКОПИРИТОВЫХ ПОЛУПРОВОДНИКАХ

В работе сделана попытка изучить влияние носителей вырождения на длину экранирования в случае аппроксимации Томаса-Ферми для носителей в тройных халькопиритовых полупроводниках, когда в качестве образца взят вырожденный кристалл n-$CdGeAs_2$. На основе модели Кильдаля обнаружено, что длина экранирования в аппроксимации Томаса-Ферми падает с увеличением концентрации носителей, как этого и следовало ожидать для вырожденных полупроводников, и параметр кристаллического поля эффективно снижает ту же самую длину. На основе данных выражений получены также соответствующие результаты для параболических полупроводников.

INTRODUCTION

It is well known that the Debye screening length of the carriers in semiconductors is a very important basic parameter, characterizing the screening of the Coulomb field of the ionized impurity centres by the free carriers. Moreover, it affects many of the special characteristics of semiconductor devices, the carrier mobilities under different mechanisms of scattering and the carrier plasmas in semiconductors. Besides, the screening length is a very good approximation to the accurate self-consistent screening in the presence of band tails [1]. It may be mentioned in this context that the screening length is also connected with the diffusivity-mobility ratio [2, 3] and the use of a screened Coulomb potential to represent the effect of an impurity ion in a lattice has extensively been adopted to illustrate the interaction between two colliding carriers in Auger effects in semi-conductors [4]. Furthermore, the screening length has also been shown [5] to be significantly modified by the conditions of carrier degeneracy and has been investigated [6—12] for degenerate semi-conductors under various physical conditions. Nevertheless, the effect of carrier degeneracy on the screening length in ternary chalcopyrite semiconductors having non-parabolic and non-standard energy bands has yet to be theoretically investigated. This will make our analysis a generalized one since from the results we can obtain the corresponding expressions for the isotropic parabolic energy bands. This is done in what follows by taking n-$CdGeAs_2$ as an example since this has widely been investigated in the recent years for its different physical aspect [13—24]. Moreover, these semiconductors are being increasingly used as non-linear optical materials [13—15] and light emitting diodes [16]. Idencidentally, Rowe and Shay [17] have demonstrated that the quasi-cubic model [18] can be used to explain the observed splitting and symmetry properties of the conduction and valence bands at the zone centre of the ternary chalcopyrite semiconductors. The s-like conduction band is singly degenerate and the p-like valance band is triply degenerate. The latter splits into three sub-bands because of spin-orbit and crystal-field interactions. The largest contribution to the crystal-field splitting of the valence band occurs from the non-cubic potential [19]. In $CdGeAs_2$ incorporating the anisotropic crystal potential to the Hamiltonian and the special features of the ternary chalcopyrite semiconductors, Kildal [20—21] proposed an E-$\boldsymbol{k}$ relation for the conduction electrons in the same semiconductor, based on the generalized Kane theory, with the assumption of an isotropic momentum matrix element and spin-orbit splitting. Furthermore, the experimental data of the absorption constant [20], the effective masses and the optical third order susceptibility [24] in $CdGeAs_2$ have provided strong evidence for the validity of the Kildal [19] model according to which the conduction band corresponds to a single ellipsoid at the zone centre in the k-space with the anisotropy dependent on energy. It would therefore be of much interest to investigate the effect of carrier degeneracy on the screening length of the electrons under the Thomas-Fermi approximation for the above class of materials. Incidentally, it may be noted that in ternary chalcopyrite semiconductors the screening length is anisotropic since the dielectric permittivity (ϵ_s) is anisotropic in such materials [25]. However, the two principal elements coincide in such semiconductors, i.e. $\epsilon_{11} = \epsilon_{22} \neq \epsilon_{33}$. Nevertheless, for the purpose of numerical computations we shall plot one such principal element of the anisotropic screening length as

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a function of carrier degeneracy for n-$CdGeAs_2$ by using some average value of the permittivity as has often been done in literature [29].

II. THEORETICAL BACKGROUND

The Debye screening length of the electrons in ternary chalcopyrite semiconductors can be expressed [25] as

$$\hat{L}_D = \begin{bmatrix} L_{D1} & 0 & 0 \\ 0 & L_{D1} & 0 \\ 0 & 0 & L_{D2} \end{bmatrix} \tag{1}$$

where $L_{D1} \equiv (e^2/\epsilon_{11})^{-1/2} (\partial n_0/\partial E_F)^{-1/2}$, e is the electron charge, n_0 is the electron concentration, E_F is the Fermi energy as measured from the edge of the conduction band and $L_{D2} \equiv (e^2/\epsilon_{33})^{-1/2} (\partial n_0/\partial E_F)^{-1/2}$.

It appears then that, for evaluating the screening length using eq. (1), one has to obtain an expression for the electron concentration in terms of the Fermi energy. Incidentally, in ternary chalcopyrite semiconductors the E-$\boldsymbol{k}$ dispersion relation can be expressed [20], neglecting the free electron term, as

$$\gamma(E) = f_1(E) k_T^2 + f_2(E) k_Z^2 \tag{2}$$

where

$$\gamma(E) \equiv E(E - E_g') \left[E(E + \Delta) + \delta \left(E + \frac{2}{3} \Delta \right) \right],$$

$$f_1(E) \equiv P^2 \left[E\left(E + \frac{2}{3} \Delta \right) + \delta \left(E + \frac{1}{3} \Delta \right) \right], \quad k_T^2 \equiv k_x^2 + k_y^2,$$

$$f_2(E) \equiv P^2 \left[E \left(E + \frac{2}{3} \Delta \right) \right], \quad E_g' \equiv E_g + E_1, \quad E_1 \equiv \frac{1}{2} \left[\sqrt{(\delta + \Delta)^2 - \frac{8}{3} \Delta\delta} - (\Delta + \delta) \right]$$

E is the electron energy as counted from the edge of the conduction band, E_g is the bandgap, δ is the crystal field splitting parameter, Δ is the spin-orbit splitting and P is the momentum-matrix element. Thus, the electron concentration can be written as

$$n_0 = \int_0^\infty Z(E) \left[-\frac{\partial f(E)}{\partial E} \right] dE \tag{3}$$

where $Z(E) \equiv \dfrac{2}{(2\pi)^2} \displaystyle\int_0^{k_{Z\,max}} k_T^2 \, dk_L$

and $f(E)$ is the Fermi-Dirac occupation probability factor. Therefore combining eqs. (2) and (3) and using the generalized Sommerfield lemma [26], the electron concentration in degenerate ternary chalcopyrite semiconductors can be expressed as

$$n_0 = \omega_0 [\Phi(\eta) + L(\eta)] \tag{4}$$

where $\omega_0 \equiv (k_B T)^3/(3\pi^2 P^3)$, k_B is the Boltzmann constant, T is the temperature, $\Phi(\eta) \equiv \left[\eta(\eta - \bar{E}_g) \left\{ \eta\left(\eta + \frac{3}{2} M' \right) + \delta'(\eta + M') \right\} \right]^{3/2} \left[\left\{ \eta(\eta + M') + \delta'\left(\eta + \frac{M'}{2} \right) \right\} \sqrt{\eta(\eta + M')} \right]^{-1}$, $\eta \equiv E_F/k_B T$, $\bar{E}_g \equiv E_g/k_B T$, $M' \equiv 2\Delta'/3$, $\Delta' \equiv \Delta/k_B T$, $\delta' \equiv \delta/k_B T$ and $L(\eta) \equiv \left[\dfrac{\pi^2}{6} \dfrac{d^2}{d\eta^2} \{\Phi(\eta)\} + \dfrac{7\pi^4}{360} \dfrac{d^4}{d\eta^4} \{\Phi(\eta)\} + \dfrac{31\pi^6}{5120} \dfrac{d^6}{d\eta^6} \{\Phi(\eta)\} \right]$.

Combining eqs. (1) and (4), we therefore get the screening length of the electrons under the Thomas-Fermi approximation in degenerate ternary chalcopyrite semiconductors as

$$\hat{L}_D = \begin{bmatrix} \delta_1(\eta) & 0 & 0 \\ 0 & \delta_1(\eta) & 0 \\ 0 & 0 & \delta_2(\eta) \end{bmatrix} \tag{5}$$

where $\delta_1(\eta) \equiv [e^2 \omega_0 \varrho(\eta)/\epsilon_{11} k_B T]^{-1/2}$, $\varrho(\eta) \equiv \left[\dfrac{d}{d\eta} \{L(\eta)\} + \dfrac{d}{d\eta} \{\Phi(\eta)\} \right]$ and $\delta_2(\eta) \equiv [e^2 \omega_0 \varrho(\eta)/\epsilon_{33} k_B T]^{-1/2}$. Incidentally, under the substitutions $\delta = 0$, $\Delta = 0$, $P^2 = \dfrac{\hbar^2}{2m_n} |E_g|$ ($-E_g$ being replaced by $|E_g|$ and taking m_n to be the bandedge effective mass), eq. (2) takes the form

$$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2m_n}, \qquad \alpha \equiv [|E_g|]^{-1} \tag{6}$$

which is the standard dispersion relation for the two-band Kane model [28]. Therefore, using the above substitutions, eq. (4) assumes the form

$$n_0 = C_0 [\Psi(\eta) + D(\eta)] \tag{7}$$

where $C_0 \equiv \dfrac{(k_B T)^3}{3\pi^2} [\hbar^2 |E_g|/2m_n]^{-3/2}$, $\Psi(\eta) \equiv [\eta(\eta + E_G)]^{3/2}$, $E_G \equiv |E_g|/k_B T$ and $D(\eta) \equiv \left[\dfrac{\pi^2}{6} \dfrac{d^2}{d\eta^2} \{\Psi(\eta)\} + \dfrac{7\pi^4}{360} \dfrac{d^4}{d\eta^4} \{\Psi(\eta)\} + \dfrac{31\pi^6}{5120} \dfrac{d^6}{d\eta^6} \{\Psi(\eta)\} \right]$. Equation (7) represents the electron statistics for the isotropic two-band Kane model at a finite temperature and should be used as such for calculations of different physical parameters in non-parabolic semiconductors where the electron energy is comparable to the band gap (e.g. in n-$Hg_{1-x}Cd_xTe$). Moreover, under the above

mentioned substitutions and for isotropic semiconductor permittivity eq. (5) takes the form

$$\frac{1}{L_D^2}=\frac{c_0e^2}{\epsilon_s k_B T}\left[\frac{\mathrm{d}}{\mathrm{d}\eta}\{\Psi(\eta)\}+\frac{\mathrm{d}}{\mathrm{d}\eta}\{D(\eta)\}\right]. \tag{8}$$

Incidentally, under the approximation $(\alpha E_F)\ll 1$, eqs. (7) and (8) can be simplified using binomial expansions and neglecting a higher order term as

$$n_0\approx N_c\left[F_{1/2}(\eta)+\frac{15\alpha k_B T}{4}F_{3/2}(\eta)\right] \tag{9}$$

and

$$\frac{1}{L_D^2}=\frac{e^2N_c}{\epsilon_s k_B T}\left[F_{-1/2}(\eta)+\frac{15\alpha k_B T}{4}F_{1/2}(\eta)\right] \tag{10}$$

where $N_c\equiv 2(2\pi m_n k_B T/h^2)^{3/2}$ and $F_j(\eta)$ stands for the Fermi-Dirac integrals of order j as defined by Blakemore [30]. Equations (9) and (10) have already been reported in literature [7] for the Kane-type non-parabolic energy bands. Furthermore, for $\alpha\to 0$, the eqs (9) and (10) assume the following well-known forms:

$$n_0=N_cF_{1/2}(\eta) \tag{11a}$$

and

$$L_D=[e^2N_cF_{-1/2}(\eta)/\epsilon_s k_B T]^{-1/2}. \tag{11b}$$

III. RESULTS AND DISCUSSION

For n-$CdGeAs_2$ using eq. (4) and the parameters [21] $\Delta=0.34$ eV, $\delta=-0.21$ eV, $E_g=0.57$ eV, $P=8\times10^{-10}$ eV — m and $T=4.2$ K, we have computed the Fermi energy as a function of the electron concentration as shown in Fig. 1, in which the same dependence is also plotted by taking the crystal-field parameter as zero for the purpose of comparison. In the same figure, the plots corresponding to the degenerate Kane-type band and the plot for a degenerate parabolic and with an effective electron mass ($m_n=0.02\ m_0$), which is of the order of mass [21] at the bandedge of n-$CdGeAs_2$, are also shown. Using the appropriate equations together with the above parameters used for obtaining Fig. 1 and taking $\epsilon_{11}=14\,\epsilon_0$ [29] we have further plotted the first principal element of the anisotropic Debye screening length as a function of the electron concentration in Fig. 2, in which the same dependence is also shown for $\delta=0$ such that the effect of the crystal field splitting on the same length could be immediately apparent. The simplified cases of a degenerate non-parabolic band and that of a degenerate parabolic band have further been considered in fig. 2.

It appears from Fig. 1 that the Fermi energy increases with increasing carrier concentration at a rate lower than that corresponding to the zero value of the crystal-field splitting parameter. Moreover for relatively low values of the electron concentration, the effect crystal-field splitting decreases whereas the same parameter affects significantly the Fermi energy for relatively high values of the carrier degeneracy. Besides, the crystal-field splitting parameter lowers the value of the

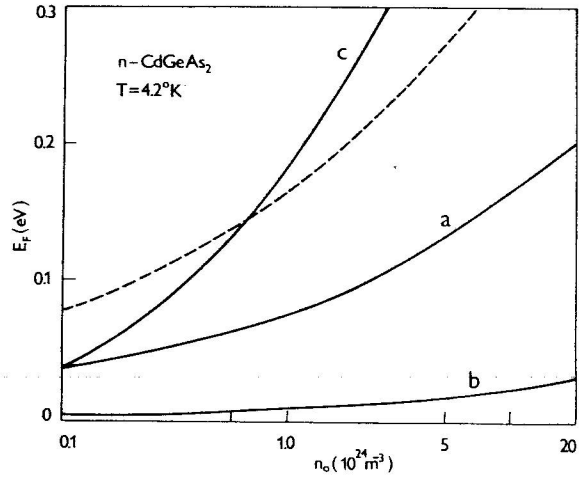

Fig. 1.

Fermi energy in degenerate ternary chalcopyrite semiconductors as compared with that corresponding to $\delta=0$ at a given value of the electron concentration in the whole range of the concentrations considered. Furthermore for concentrations below 1×10^{23} m^{-3}, it is apparent from the same figure that the Fermi energies are in close agreement with each other and the effect of energy dependent mass anisotropy decreases. It is again noted that though the Fermi energy also increases nonlinearly with concentration in the cases of the degenerate non-parabolic and the parabolic band, the rates of increase are quite different from that in the Kildal band. That the dotted curve in Fig. 1 is somewhat different from the plot for the degenerate parabolic band is due exclusively to the effect of mass anisotropy. It is seen in Fig. 2 that the screening length decreases with increasing electron concentration as expected for degenerate semiconductors. It is also seen that the crystal-field parameter effects the screening length of the electrons under the Thomas-Fermi approximation quite significantly in degenerate ternary chalcopyrite semiconductors and for a fixed value of the electron concentration the screening length of the electrons is smaller as compared to that in the absence of

crystalline field effects in the whole range of concentrations considered. It is observed that the dependence of the screening length on concentration is also determined by the bandshape because of its direct relevance to the Fermi energy. Besides, from Fig. 2 we can also compare the screening length according to both the Kildal and the Kane-type band models since many authors have continued to interpret the experimental data in terms of the Kane model. It is noted that the

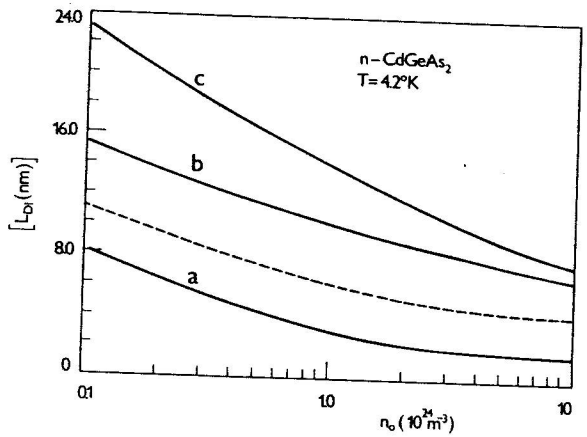

Fig. 2.

Kane model gives larger values of the screening length as compared to these obtained from the Kildal model from the whole range of concentrations considered. Besides, the difference between the screening lengths as determined from these two models can be seen to decrease with increasing electron concentration. This suggests that the Kildal model has to be strictly considered for relatively low values of the electron concentration so far as the screening effects are concerned. It is again noted that the effect of electron-electron interactions which become increasingly important with increasing electron concentration have not been considered in the present analysis. These considerations would certainly improve the accuracy of the results. However, even in the absence of such interactions, the crystal-field splitting significantly affects the screening length of the electrons in degenerate ternary chalcopyrite semiconductors in the whole range of concentrations considered. Moreover, without consideration of such interactions, the two models give widely different screening length which become closer with increasing electron concentration. It is, therefore, felt that the two models would still give widely different screening lengths in the presence of electron electron interactions. Furthermore, it is apparent from Fig. 2 that the two model will give screening lengths in close agreement with each other only at very large values of the electron

concentration due to reasons which are incidental and not due to electron-electron interaction effects. It is then likely that the results of the two models would not be in close agreement even at large electron concentrations if the electron-electron interaction effects are taken into consideration. Incidentally, it may be stated that the screening length under the Thomas-Fermi approximation represents a rough picture for the complicated problem of many particle screenings. The requirement for the Thomas-Fermi model is that the potential should vary slowly enough in an electron wave length so that many electrons can be localized within a volume over which the potential changes by a small fraction of itself [31]. However, this basic condition of the Thomas-Fermi screening length is not satisfied in semiconductors as pointed out in literature [31]. Nevertheless, a satisfactory genèralized theory is still not available. It may finally be noted that the basic purpose of the present work is not solely to illustrate graphically the simplified result of the screening length of the electrons in degenerate ternary chalcopyrite semiconductors according to the Kildal model but also to formulate the electron statistics at a finite temperature since the various electron transports and the derivation of the expressions for many important physical parameters are based on the electron statistics in such materials.

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