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INFLUENCE OF BAND TAILS ON THE ELECTRONIC CONTRIBUTION TO ELASTIC CONSTANTS OF DEGENERATE TERNARY SEMICONDUCTORS

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An attempt is made to study the electronic contribution to elastic constants of degenerate ternary semiconductors on the basis of a newly derived dispersion law taking into account the influence of band tails. It is found, taking n-$Hg_{1-x}Cd_xTe$ as an example that mentioned contribution increases with increasing carrier degeneracy in different manner and that the formation of band tails decreases the contribution in both the cases. The corresponding results for well-known non-degenerate parabolic energy bands in the absence of any such tails have been obtained from our results under certain limiting conditions.

1. Introduction

In recent years, there has been considerable interest in studying the various electronic features of degenerate materials having highly degenerate electron concentration because of their importance in device technology[1,2]. Under the conditions of high carrier degeneracy, the band tails are formed and as a consequence all the physical properties of degenerate semiconductors become modified. It appears from the literature that the electronic contributions to elastic constants have relatively been less investigated for small-gap materials[3]. Therefore it would be of much interest to study the same contributions for ternary semiconductors having Kane type bands since the above class of materials are being increasingly studied for their peculiar physical characteristics. We wish to note that Keyes[4] developed a theory for determining the electronic contribution to elastic constants of degenerate materials (neglecting the formation of band tails) on the basis of deformation potential model. It was shown that the electronic contribution to elastic constants depends on the density-of-states function. Thus in degenerate semiconductors having non-parabolic energy bands with the formation of band tails as a consequence of heavy doping, the electronic contribution to elastic constants will be significant since the density-of-states function in non-parabolic materials having band-tails increases much more rapidly with carrier energy than when the bands are parabolic in the absence of tail formation. In this communication, we shall study the electronic contribution to second and third order elastic constants of ternary semiconductors as a function of carrier degeneracy by formulating the new dispersion law, taking n-$Hg_{1-x}Cd_xTe$ as a example. The compound $Hg_{1-x}Cd_xTe$ is the classic very narrow-gap semiconductor and is a very important optoelectronic material because its band-gap can be varied to over the entire spectral range from 0.8 to 30 μm by adjusting the alloy composition[5]. $Hg_{1-x}Cd_xTe$ finds extensive applications in infrared detector materials and photovoltaic detector arrays in 8—12 μm wave bands[6]. This spurred a $Hg_{1-x}Cd_xTe$ technology for the production of high-mobility crystals and the same material is ideally suited for studying the physics of narrow gap materials since the relevant physical parameters are within easy experimental reach[6].

2. *Theoretical background*

In a strained semiconductor, only the second and third order elastic constants (hereafter referred to as C_{44} and C_{456}) are affected[3]. The electronic contribution to C_{44} and C_{456} is[3]

$$\Delta C_{44} = ((\overline{a})^2/9) \int_0^\infty N(E) \left[\frac{\partial f_0(E)}{\partial E} \right] \mathrm{d}E \tag{1}$$

and

$$\Delta C_{456} = ((\overline{a})^3/27) \int_0^\infty N(E) \left[\frac{\partial^2 f_0(E)}{\partial E^2} \right] \mathrm{d}E \tag{2}$$

where a is the deformation potential constant, $N(E)$ is the density-of-states function and $f_0(E)$ is the Fermi-Dirac occupation probability factor. The dispersion relation of the unperturbed conduction electrons in small-gap materials having Kane type energy bands can be written[7] as

$$E = a_0 k^2 - b_0 k^4 \tag{3}$$

where E is the energy as measured from the edge of the unperturbed conduction band in the vertical upward direction, $a_0 \equiv \hbar^2/2m^*$, $\hbar$ is Planck's constant, m^* is the effective electron mass at the edge of the unperturbed conduction band,

$$b_0 \equiv \left(1 - \frac{m^*}{m_0}\right)^2 a^2 [3E_g^2 + 4\bar{\Delta}E_g + 2\bar{\Delta}^2] [E_g (E_g + \bar{\Delta})(2\bar{\Delta} + 3E_g)]^{-1},$$

m_0 is free electron mass, E_g is unperturbed band gap and $\bar{\Delta}$ is the spin-orbit splitting. The modified electron energy spectrum due to heavy doping can be expressed, following the method of D. K. Roy[8] as a result of first and second order perturbation as

$$E = a_0 k^2 - b_0 k^4 - \Phi(k), \tag{4}$$

where

$$\Phi(k) \equiv (4\pi N_t A_s/N\Omega a^2) + \frac{4\pi A_s^2 N_t m^*}{N\Omega a \hbar^2} \cdot \frac{(1 + 2b_0 k^2 a_0^{-1})}{(a^2 + 4k^2)} +$$

$$+ (N_t/N\Omega 4\pi^2)(4\pi A_s/a_0)^2 (b_0 \pi/a a_0),$$

N_t are the numbers of impurity atoms per N atoms of the crystal, Ω is the volume of unit cell, $A_s = e^2/4\pi\varepsilon_s$, e is electron charge, ε_s is the semiconductor permitivity and

$$a \equiv (\pi\varepsilon_s)^{1/2} (\pi/3)^{1/6} \cdot \left(N^{-1/3} \frac{\hbar^2}{m_0 e^2}\right)^{1/2}.$$

For $E_g \to \infty$ as for parabolic energy bands and $b_0 \to 0$, Eqs. (3) and (4) get simplified as

$$E = \hbar^2 k^2/2m^* \tag{5}$$

and

$$E = \frac{\hbar^2 k^2}{2m^*} - \frac{4\pi N_t A_s}{N\Omega a^2} - \frac{4\pi A_s^2 N_t m^*}{N\Omega a \hbar^2 (a^2 + 4k^2)}. \tag{6}$$

Eq. (6) was derived for the first time by D. K. Roy[8].

Furthermore for $N_t \to 0$, Eqs. (6) and (5) become identical. The use of Eq. (4) leads to the expression of density-of-state function as

$$N(E) = 4\pi (2m^*/h^2)^{3/2} (\sqrt{\gamma(E)})\, \gamma'(E), \tag{7}$$

where

$$\gamma(E) \equiv G - \sqrt{H - IE}, \qquad G \equiv Aa_0/2B, \qquad A \equiv [a_0 - b_0 \alpha + \beta D_0],$$

$$D_0 \equiv \frac{4\pi A_s^2 N_t m^*}{N\Omega a^3 \hbar^2}, \qquad \alpha \equiv 2b_0/a_0, \qquad \beta \equiv 4/a^2, \qquad B \equiv b_0 - Da\beta,$$

$$D \equiv C_0 + D_0, \qquad C_0 \equiv \frac{4\pi N_i A_s}{N\Omega a^2} - \frac{N_i a_0^{-3}}{N\Omega 4\pi^2}\left(\frac{b_0 \pi}{a}\right)(4\pi A_s)^2, \qquad H \equiv H_0 a_0,$$

$$H_0 \equiv [(A^2/4B^2) - DB^{-1}], \qquad I \equiv I_0 a_0^2, \qquad I_0 \equiv B^{-1}$$

and

$$\gamma'(E) \equiv I/\sqrt{H - IE}.$$

Under the conditions $E_g \to \infty$ and $N_i \to 0$ equation (7) assumes the well-known form[9] as

$$N(E) = 4\pi (2m^*/h^2)^{3/2} \sqrt{E}. \tag{8}$$

Using the equations (1), (2) and (7) we can write

$$\Delta C_{44} = -C_1 [U(E_F) + V(E_F)] \tag{9}$$

and

$$\Delta C_{456} = C_2 [X(E_F) + Y(E_F)] \tag{10}$$

where

$$C_1 \equiv (4\pi(\bar{a})^2/a)\left(\frac{2m^*}{h^2}\right)^{3/2}, \qquad U(E_F) \equiv [\gamma'(E_F)\sqrt{\gamma(E_F)}],$$

E_F is the corresponding Fermi energy,

$$V(E_F) = \sum_{r=1}^{s} V_r [U(E_F)], \qquad V_r \equiv 2\left[(k_B T)^{2r}(1 - 2^{1-2r})\zeta(2r)\frac{d^{2r}}{dE_F^{2r}}\right],$$

r is the set of integers, $\zeta(2r)$ is the zeta function of order $2r$[10],

$$C_2 \equiv \frac{4\pi(\bar{a})^3}{27}(2m^*/h^2)^{3/2}, \quad X(E_F) \equiv \left\{\{\gamma'(E_F)\}^2/2\sqrt{\gamma(E_F)} - \right.$$

$$\left. - \frac{I\gamma'(E_F)}{2(H - I E_F)^{3/2}}\right\}$$

and

$$Y(E_F) \equiv \sum_{r=1}^{s} V_r [X(E_F)].$$

It appears then that the evaluation of ΔC_{44} and ΔC_{456} from equations (9) and (10) requires an expressions of electron concentration which can, in turn, be written as

$$n_0 = e_1 [p_1(E_F) + q_1(E_F)] \tag{11}$$

where

$$e_1 \equiv (3\pi^2)^{-1}(2m^*/\hbar^2)^{3/2}, \qquad p_1(E_F) \equiv [\gamma(E_F)]^{3/2}$$

and

$$q_1(E_F) \equiv \sum_{r=1}^{s} V_r [p_1(E_F)].$$

Under the conditions $E_g \to \infty$ and $N_t \to 0$, Eqs. (9), (10) and (11) assume the forms

$$\Delta C_{44} = -((\overline{a})^2 N_C/qk_BT) F_{-1/2}(\eta) \quad (12)$$

$$\Delta C_{456} = [(\overline{a})^3 N_C/27(k_BT)^2] F_{-3/2}(\eta), \quad (13)$$

and

$$n_0 = N_C F_{1/2}(\eta), \quad (14)$$

where

$$N_C \equiv 2(2\pi m^* k_B T/h^2)^{3/2}, \qquad \eta \equiv E_F/k_BT$$

and $F_j(\eta)$ is the one parameter Fermi-Dirac integral of order j as defined by Blakemore[9]. Under the condition of non-degeneracy $\eta \ll -1$ and $F_j(\eta) = \exp(\eta)$ for all j[9]. Thus using Eqs. (12), (13) and (14) we finally get[3]

$$\Delta C_{44} = -n_0(\overline{a})^2/9k_BT \quad (15)$$

$$\Delta C_{456} = n_0(\overline{a})^3/9k_B^2T^2 \quad (16)$$

and

$$n_0 = N_C \exp(\eta). \quad (17)$$

3. *Results and discussion*

Using the appropriate equations together with the parameters[11–14]

$$E_g(x) = [-0.3045 \times 10^{-4}\, T + (1.914 - 10^{-3}\, T)\, x] \text{ eV},$$

$$m^*(x) = 3\hbar^2 E_g(x)/4P^2(x), \quad P(x) = [(\hbar^2/2m_0)(18 + 3x)]^{1/2}$$

$$\Delta = 0.9 \text{ eV}, \quad T = 4.2 \text{ K}, \quad \varepsilon_{sc}(x) = (20.262 - 14.812x + 5.2795x^2)\,\varepsilon_0,$$

$$\Omega = \frac{L^3}{4}, \quad L \text{ (lattice constant)} = (6.4614 + 0.0084x + 0.0168x^2 -$$

$$- 0.0057x^3) \cdot (10^{-1}) \text{ nm}, \quad x = 0.5, \quad N = 8/L^3 \quad \text{and} \quad n_0 = N_t,$$

we have plotted ΔC_{44} versus n_0 in the presence and absence of band tails in n-$Hg_{1-x}Cd_xTe$ as shown by plots a and b of Fig. 1 in which the plots d and c exhibit the same dependence in accordance with parabolic energy band both in the presence and absence of band tails for the purpose of comparison. Using the same parameters as used in obtaining Fig. 1, we have plotted in Fig. 2 the normalized ΔC_{456} versus n_0 in accordance with the aforementioned cases.

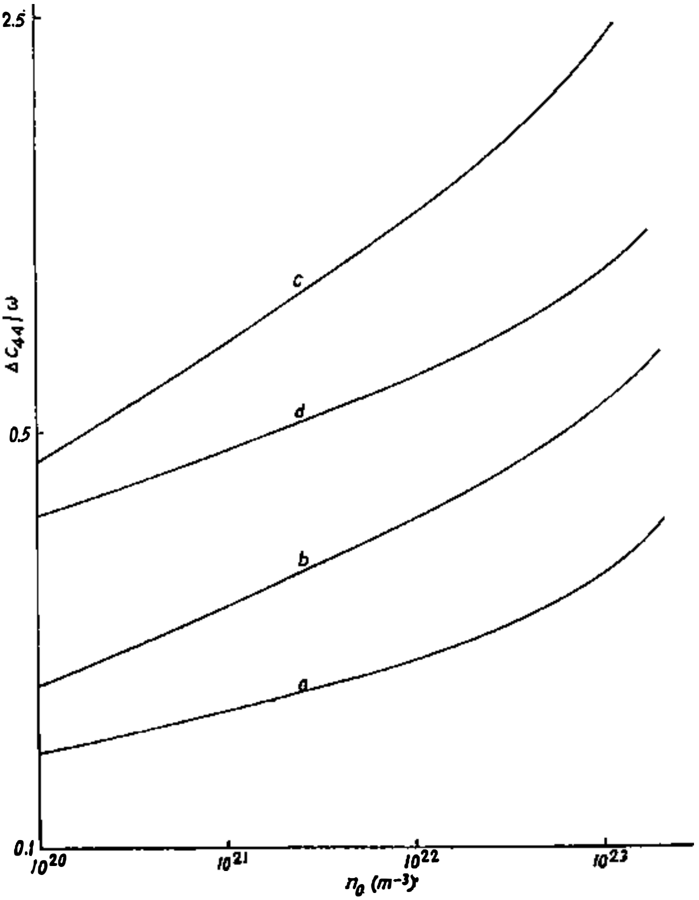

Fig. 1. Plot of $\Delta C_{44}/\omega$ ($\omega = -n_0 (\bar{a})^2/9\, k_B T$) versus n_0 in n-$Hg_{1-x}Cd_xTe$ in accordance with: curve a, presence of band tails and band non-parabolicity; curve b, absence of band tail and presence of band non-parabolicity; curve c, absence of band tail and with band parabolicity and curve d, presence of band tails and with band parabolicity.

The basic dispersion relation of degenerate Kane-type materials having band tails as given by equation (4) is most complicated and the density-of-states function in accordance with the equation (7) changes with carrier energy significantly. Again the expressions for ΔC_{44} and ΔC_{456} are monotonous increasing functions of Fermi energy. The influence of band tails decreases the numerical values of ΔC_{44} and ΔC_{456} in accordance with both parabolic and non-parabolic bands. The influence of band non-parabolicity on the variations of ΔC_{44} and ΔC_{456} is also apparent from the figures. We wish to note that in view of the large changes of the elastic constants with n_0, detailed experimental work on second and third order elastic constants as functions of carrier degeneracy would be interesting for small-gap materials for assessing the band structure of doped materials. It may also be suggested that the experiments on the velocity of sound involving the shear mode as a function of carrier concentration may exhibit the carrier contribution to elastic constants of ternary semiconductors. Our numerical computations are valid for $x > 0.16$ since for $x < 0.16$, the band gap in $Hg_{1-x}Cd_xTe$ becomes negative leading to semimetallic state. Though we have taken ternary materials as an example our results can be used for III—V semiconductors in general with the different values of the experimentally available band parameters. Finally it may be noted that the basic aim of the present paper is not solely to formulate the ΔC_{44} and ΔC_{456} but also to develop the dispersion relation of doped non-parabolic semiconductors since it is the dispersion relation which controls the carrier transport and the formulation of the different physical features under different physical conditions are directly based on the carrier energy spectrum in such materials.

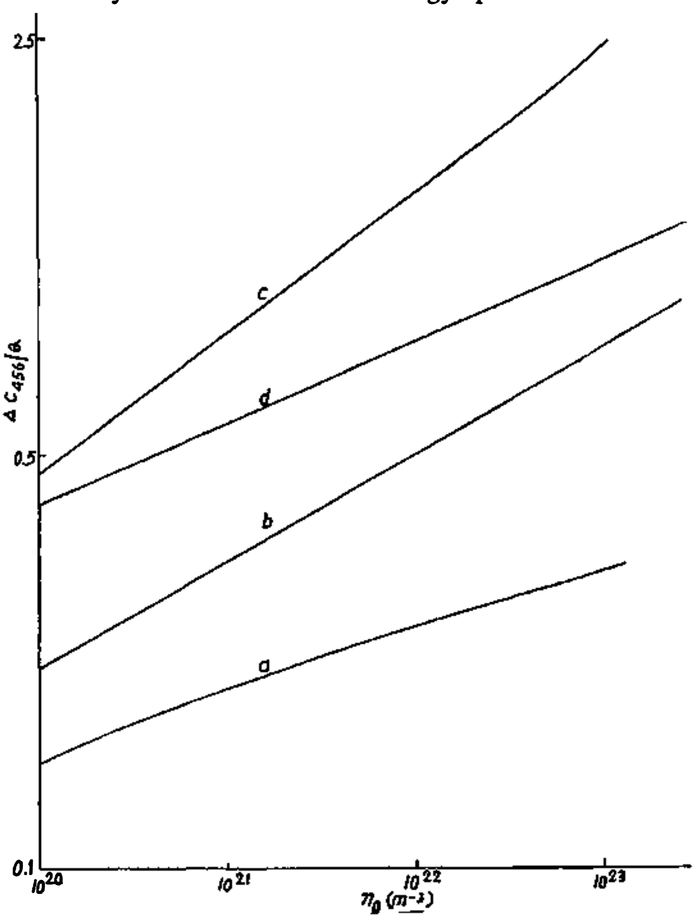

Fig. 2. Plot of $\Delta C_{456}/\Theta$ ($\Theta = n_0 (\bar{a})^3/27 (k_B T)^2$ versus n_0 in n-$Hg_{1-x}Cd_xTe$ in accordance with: curve a, presence of band tails and band non-parabolicity; curve b, absence of band tails and presence of band non-parabolicity; curve c, absence of band tails and with band parabolicity; curve d, presence of band tails and absence of band non-parabolicity.

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UTJECAJ REPOVA VRPCI NA ELEKTRONSKI DOPRINOS KONSTANTAMA ELASTIČNOSTI U DEGENERIRANIM TERNARNIM POLUVODIČIMA

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Razmatran je elektronski doprinos elastičnim konstantama u degeneriranim ternarnim poluvodičima na osnovu nove disperzione relacije koja uzima u obzir utjecaj repova vrpci. Uzevši n-$Hg_{1-x}Cd_xTe$ kao primjer nađeno je da elektronski doprinos raste s porastom degeneracije nosilaca naboja a da formiranje repova u vrpci smanjuje taj doprinos.