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INFLUENCE OF CARRIER DEGENERACY ON THE ELASTIC CONSTANTS OF GAP LESS SEMICONDUCTORS

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We study the carrier contribution to the elastic constants in gapless semiconductors, taking n-HgTe as an example. It is found that both the elastic constants increase with increasing electron concentration and the electron-electron interaction enhances their numerical values. In addition, the theoretical results are in agreement with the suggested experimental method of determining both the elastic constants in degenerate materials having arbitarary carrier dispersion laws.

1. Introduction

In recent years, there has been considerable interest in studying the various physical properties of non-parabolic semiconductors having different band structures because of their importance in device technology [1]. Nevertheless, it appears from the literature that the carrier contribution to elastic constants in semiconductors having still smaller bandgap like zero gap semiconductors has yet to be properly worked out. This is important since the various physical properties of zero-gap semiconductors have recently been studied [2,3]. It is wellknown that the carrier contribution to the elastic constants depends on the density-of-states function [4]. Therefore, in gap-less materials the carrier contribution to the elastic constants will be rather significant due to the complicated variation of the density-of-states function as compared to parabolic energy bands. In the following, we study the carrier contribution to the second - and third-order elastic constants of gapless semiconductors. We suggest an experimental method of determining such contributions in degenerate materials having arbitrary dispersion laws. We investigate the doping dependence of the above contributions taking n-HgTe as an example, for the purpose of numerical computation which has many applications in optoelectronics [5].

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2. Theoretical background

In a strained semiconductors only the second- and third-order elastic constants (hereafter referred to as C_{44} and C_{456}) are affected. The carrier contribution to C_{44} and C_{456} can, respectively, be written [4] as

$$\Delta C_{44} = (a_0^2/9)\int_0^\infty N(E)\left[\frac{\mathrm{d}f_0(E)}{\mathrm{d}E}\right]\mathrm{d}E \tag{1}$$

and

$$\Delta C_{456} = (a_0^3/27)\int_0^\infty N(E)\left[\frac{\mathrm{d}^2 f_0(E)}{\mathrm{d}E^2}\right]\mathrm{d}E \tag{2}$$

Where a_0 is the deformation potential constant, E is total energy of the carriers as measured from the band edge, $N(E)$ is the density-of-states function, $f_0(E) = [1 + exp((E-E_F)/k_BT)]^{-1}$, E_F is the corresponding Fermi energy, k_B is Boltzmann constant and T is temperature. It appears then that the evaluation of ΔC_{44} and ΔC_{456} requires an expression of $N(E)$ which, in turn, is determined by the carrier energy spectrum. In gapless materials, the carrier dispersion law can be expressed [2] as

$$E = Ak^2 + Bk \tag{3a}$$

where $A = \hbar^2/2m^*$, $\hbar = h/2\pi$, h is Planck constant, m^* is the effective carrier mass at the bandedge, $|k|$ is the carrier wave vector, $B = 3e^2/128\epsilon_s$, e is the magnitude of the carrier charge and ϵ_s is the semiconductor permittivity. The use of eq.(3a) leads to the expression of the density-of-states function as

$$N(E) = 4\pi(2m^*/h^2)^{3/2}(C(E))^{\frac{1}{2}}P(E) \tag{3b}$$

where $C(E) = [-B + (B^2 + 4AE)^{\frac{1}{2}}]^2/4A$ and $P(E) = [1 - B.(B^2 + 4AE)^{-\frac{1}{2}}]$ Thus using Eqs. (1), (2) and (3), the expressions of ΔC_{44} and ΔC_{456} for gapless materials are, respectively, given by

$$\Delta C_{44} = [-((k_BT)^{3/2}(a_0^2/9))/(2\pi^2.A^{3/2})][C_1(t) - (a)^{\frac{1}{2}} + ac_2(t)] \tag{4}$$

and

$$\Delta C_{456} = (a_0^3/27)(k_BT)^{\frac{1}{2}}(2\pi^2.A^{3/2})^{-1}[C_3(t) - 2F_{-1}(t).(a)^{\frac{1}{2}} + ac_4(t)] \tag{5}$$

where

$$C_1(t) = [(a+t)^{\frac{1}{2}} + \sum_{r=1}^{S} L_r(Y)], \quad a = B^2/4Ak_BT,$$

$$t = (E_F/k_BT), \quad L_r = \left[2(k_BT)^{2r}.(1-2^{1-2r})Z(2r)\frac{\mathrm{d}^{2r}}{\mathrm{d}E_F^{2r}}\right],$$

r is the set of real positive integers, $Z(2r)$ is the zeta function of order $2r$ [6],

$$\begin{aligned}
Y &= (3/2-2r)(a+t)^{-1}Y_1(t)\\
Y_1(t) &= (-1)^{2r-2}[1.3 \ldots\ldots (|4r-5|)]\,[2^{r-1}.(a+t)^{2r-3/2}]^{-1},\\
C_2(t) &= (a+t)^{-\frac{1}{2}} + \sum_{r=1}^{S} L_r(u)\\
u &= [V(t)(\frac{1}{2}-2r)/(a+t)],\\
V(t) &= (-1)^{2r-1}.[1.5.9. \ldots\ldots (4r-3)]\,[2^{2r-1}.(a+t)^{2r-\frac{1}{2}}]^{-1},\\
C_3(t) &= [(2.(a+t)^{\frac{1}{2}})]^{-1} + \sum_{r=1}^{S} L_r(G)\\
G &= [-Y.(a+t)^{-1}]\\
C_4(t) &= (-1/2.(a+t)^{3/2}) + \sum_{r=1}^{S} L_r(H)\\
H &= [-u/(a+t)]
\end{aligned}$$

and $F_j(t)$ is the one-parameter Fermi-Dirac integral of order j [7] which can be written as

$$F_j(t) = \frac{1}{\Gamma_{j+1}}\int_0^\infty [1+\exp(x-t)]^{-1}.x^j\mathrm{d}x \ for\ j > -1;$$

or for all j, analytically continued as a complex contour integral around the negative axis

$$F_j(t) = (\Gamma_{-j}/2\pi.(-1)^{\frac{1}{2}})\int_{(-\infty)}^{(0+)} x^j[1+\exp(-x-t)]^{-1}\mathrm{d}x$$

It appears then that, the evaluation of ΔC_{44} and ΔC_{456} as a function of carrier degeneracy require as expression of the carrier statistics which can, in turn, be expressed following eq. (3b) as

$$n_0 = (2\pi^2)^{-1}(k_BT/A)^{3/2}[L_1(t) + L_2(t)] \tag{6}$$

where

$$\begin{aligned}
L_1(t) &= (2/3)[(a+t)^{3/2} - a^{3/2}] + \sum_{r=1}^{S} L_rY_1(t)\\
L_2(t) &= (a/B)[BL_3(t) - 4F_0(t).(Ak_BT)^{\frac{1}{2}}]
\end{aligned}$$

and

$$L_3(t) = 2[(a+t)^{\frac{1}{2}} - (a)^{\frac{1}{2}}] + \sum_{r=1}^{S} L_r(V(t))$$

Under the special case $B \to 0$, as for parabolic energy bands, the expressions for ΔC_{44}, ΔC_{456} and the carrier concentration get simplified as [4]

$$\Delta C_{44} = -(a_0^2/9k_BT)N_cF_{-\frac{1}{2}}(t) \tag{7}$$

$$\Delta C_{456} = (a_0^3.N_c/27k_B^2T^2)F_{-3/2}(t) \tag{8}$$

and

$$n_0 = N_cF_{\frac{1}{2}}(t);\ N_c = 2(2\pi m^* k_BT/h^2)^{3/2} \tag{9}$$

In this context, we shall suggest a method for the experimental determination of the carrier contribution to the elastic constants in degenerate materials having arbitrary dispersion laws. The thermoelectric power of the carrierss in degenerate materials in the presence of a classically large magnetic field can be written as [8]

$$G = (\pi^2k_B^2T/3en_0)\left(\frac{dn_0}{dE_F}\right) \tag{10}$$

Using eqs. (1), (2) and (10) we get

$$\Delta C_{44} = -en_0a_0^2G/3\pi^2k_B^2T \tag{11}$$

and

$$\Delta C_{456} = (a_0^3n_0eG^2/3\pi^4k_B^3T)[1 + (n_0/G)\left(\frac{dG}{dn_0}\right)] \tag{12}$$

Thus we can determine ΔC_{44} and ΔC_{456} from the experimental values of G which is an easily measurble experimental quantity [9].

3. Results and discussion

Using eqns. (4), (5) and (6) and taking n-HgTe together with the material constants [2] $m^* = 0.025m_0$, $a_0 = 4eV$, $\epsilon_S = 20\epsilon_0$ and $T = 4.2K$ we have plotted Fig. 1, $\Delta C_{44}/T_1$ ($T_1 = (-n_0a_0^2/k_BT)$ and $\Delta C_{456}/T_2$ ($T_2 = (n_0a_0^3)/[27.(k_BT)^2]$) as functions of n_0 in which the same dependences have also been computed for parabolic energy bands for the purpose of assessing the influence of many-body effects on ΔC_{44} and ΔC_{456} respectively. The circular plots correspond to the same dependences obtained by using eqs.(11) and (12) and taking the experimental values of the thermoelectric power of the electrons in n-HgTe in the presence of classically large magnetic field [9].

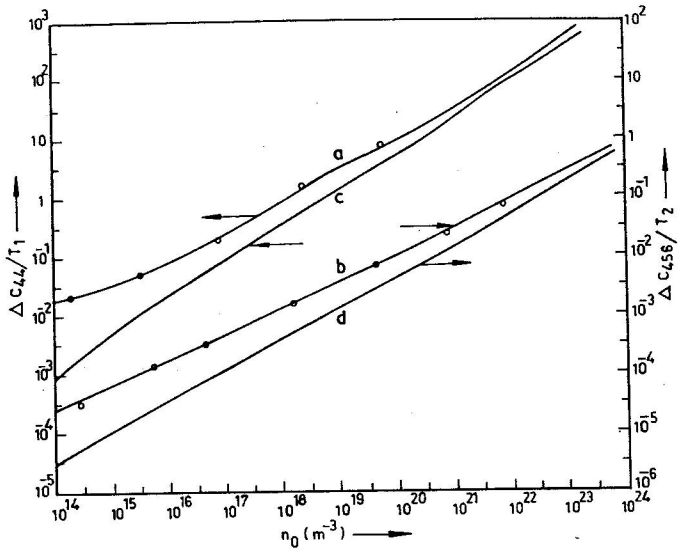

Fig. 1. Plots a and c show the variations of $\Delta C_{44}/T_1$ as a functions of n_0 in n-HgTe for both $B \neq 0$ and $B = 0$. Plots b and d exhibit the variations of $\Delta C_{456}/T_2$ for both $B \neq 0$ and $B = 0$. The circular plots exhibit the same dependence as obtained using (11) and (12) and taking the experimental value of the thermoelectric power of the electrons in the presence of a classically large magnetic field.

ΔC_{44} and $\Delta C456$ are functions of the Fermi energy, which increases with increasing carrier concentration. Therefore ΔC_{44} and ΔC_{456} will increase with increasing n_0. Since the differentiation of a monotonous increasing function decreases the curvature, ΔC_{456} changes almost linearly with n_0. It appears that the electron electron interaction term Bk enhances the values of ΔC_{44} and ΔC_{456} in n-HgTe as compared to $B = 0$ for relatively low values of concentrations that are considered. We note that the influence of many-body effects on ΔC_{44} and ΔC_{456} has been neglected, in general, in the analyses of the physical properties of small-gap semiconductors. In this paper we have formulated ΔC_{44} and ΔC_{456} without any approximations among the band parameters of gapless materials in which the many-body effects play the dominant role. The dispersion relation of the zero gap semiconductors cannot be derived as a special case of any dispersion relation of the carriers of any semiconductors under zero-gap condition, $E_g = 0$. From Fig.1 it appears that the theoretical results and our experimental suggestion for determining the ΔC_{44} and ΔC_{456} are in close agreement.

Our experimental suggestion for the determination of ΔC_{44} and ΔC_{456} for any semiconductor with arbitrary dispersion laws given by eqs. (11) and (12) do not contain any band parameter excluding G. Only the experimental values of G for any model as a function of n_0 at a constant temperature will given the experimental values of ΔC_{44} and ΔC_{456} for that range of carrier concentration for that model. We wish to note that

in view of the large changes of the elastic constants with n_0, detailed experimental work on the second and third order elastic constants as a function of carrier degeneracy would be interesting in gapless semiconductors. It may finally be noted that the experiments on the velocity of sound involving the shear mode as a function of carrier concentration may exhibit the carrier contribution to the elastic constant of zero gap materials which is another suggestion of the experimental determinations of ΔC_{44} and ΔC_{456}, besides the already suggested method.

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