

**INFLUENCE OF THE BAND-BAND INTERACTION ON THE  
DISPERSION AND DENSITY OF STATES OF SURFACE CARRIERS  
IN  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  AT FINITE TEMPERATURE**

**Ivo Nachev**

*Institute of Microelectronics,  
Department of Process and Device Modelling,  
Sofia-1784, Bulgaria*

الخلاصة :

لقد تمّت دراسة تأثير المفاعلة بين شريط المواسلة  $\Gamma_6^c$  وشريط التكافؤ  $\Gamma_8^v$  على التشتت  $E_r^{\pm}(k)$  وأيضاً على كثافة المستويات  $D_r(E)$  لغاز اليكتروني شبيه البعدين في طبقة معكوسة على  $p\text{-Hg}_{1-x}\text{Cd}_x\text{Te}$  وذلك باستخدام طريقة درجة الحرارة المحددة والتوافق الذاتي . وكتيجة لهذه المفاعلة وُجد أنّ التشتت وكثافة المستويات لجزء شريطي من المستويات أصبح غير مكافئ . ووُصفت الخاصية غير المكافئة ولُوَحظ أنها تزداد مع زيادة دليل الجزء الشريطي ( $r = 0, 1, 2, \dots$ ) وتتناقص مع ارتفاع درجة الحرارة  $T$  ومركبات السبيكة  $x$  .

**ABSTRACT**

The influence of the interaction between the conduction band  $\Gamma_6^c$  and the valence band  $\Gamma_8^v$  (band-band interaction) on the dispersion  $E_r^{\pm}(k)$  and the density of states  $D_r(E)$  of the quasi-two-dimensional electron gas in inversion layers on  $p\text{-Hg}_{1-x}\text{Cd}_x\text{Te}$  is investigated, using a finite-temperature self-consistent procedure. As a result of the band-band interaction the dispersion and the density of states of the sub-band states become non-parabolic. The non-parabolicity is described quantitatively and it is shown that it increases with the sub-band index  $r = 0, 1, 2, \dots$ , and decreases with the temperature  $T$  and the alloy composition  $x$ .

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### 1. INTRODUCTION

In a previous paper [1] the dispersion relation of the ground sub-band, the density of states, and the surface potential in an  $n$ -inversion layer on the ternary compound  $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$  were studied at zero temperature.

The purpose of this work is the investigation of the dispersion  $E_r^\pm(\mathbf{k})$  and the density of states  $D_r(E)$  of the first sub-bands  $r = 0, 1, 2$  in an  $n$ -inversion layer on  $p$ - $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  at finite temperature in order to obtain more complete and realistic description of the carriers confined in narrow surface channels on the small-gap semiconductor  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ . For this reason we have generalized our model [1] to account for the finite temperature  $T$  and for several occupied sub-bands.

Since inversion layers on  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  are used in infra-red devices, understanding of their properties is presently of importance [2]. Compared to the silicon inversion layers, which have been studied intensively for many years [3] and are referred to as a standard system, due to their wide applications in the micro-electronic industry, the properties of surface carriers on  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  are more complex, difficult to describe, and less understood. One reason for this is that it is difficult to prepare a good interface between the semiconductor  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  and the insulator in the MIS (Metal – Insulator – Semiconductor) structure. The other reason is more fundamental. It stems from the proximity of the conduction and the valence bands of  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  near the  $\Gamma$ -point, *i.e.* on the small energy gap  $E_G$  of this material for values of the stoichiometric composition  $x \approx 0.2$ . As a consequence the bands interact and this interaction influences strongly the properties of the surface carriers, as pointed out by many authors, see for instance the review of Koch [4]. One manifestation of this influence is the deviation of the dispersion from the simple parabolic law. A way to treat the non-parabolicity of  $E_r^\pm(\mathbf{k})$  and  $D_r(E)$  quantitatively is undertaken here.

Another motivation to study  $E_r^\pm(\mathbf{k})$  and  $D_r(E)$  in detail is that they are essential ingredients of the self-consistent procedure used to calculate quantized surface states on  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  and this formalism is best suited to describe the recently developed quantum alloy  $\text{HgCdTe}$  [5], produced by advanced experimental techniques.

### 2. THE PHYSICAL MODEL AND DISCUSSION OF THE RESULTS

The dispersion of the surface carriers on  $\text{HgCdTe}$  is obtained by diagonalizing the multi-band Schrödinger equation

$$[H_{n \times n}(\mathbf{k}) - \mathbf{1}_{n \times n}V(z) - E]\Psi(\mathbf{k}, z) = 0, \quad (1)$$

where  $H_{n \times n}$  is the Kane  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian, which describes the band-band interaction near the  $\Gamma$ -point  $V(z)$  is the surface potential,  $\Psi$  is an  $n$ -component spinor of the envelope wave functions of the conduction and valence bands, and  $\mathbf{1}_{n \times n}$  is a unit matrix. We consider here the six-band model ( $n=6$ ) of the band structure of  $\text{HgCdTe}$  near the  $\Gamma$ -point, which takes into account the coupling between the two-fold, spin-degenerate conduction band  $\Gamma_6^c$  and the four-fold degenerate valence band  $\Gamma_8^v$ . The surface potential  $V(z)$  is a solution to Poisson equation, and the calculations are Hartree-type self-consistent, as described in [1], but generalized to the case of finite temperature.

The non-parabolic dispersion  $E_r^\pm(\mathbf{k})$ , where  $r$  denotes the sub-band states and the signs  $\pm$  correspond to the two spin directions, can be written as a power series of the wave vector  $\mathbf{k}$

$$E_r^\pm(\mathbf{k}) = \sum_{m=0}^P A_{r,m}^\pm k^m. \quad (2)$$

The density of states  $D_r(E)$  reads

$$D_r(E) = \sum_{\pm} D_r^\pm(E) = \sum_{\pm} \left( \frac{k}{2\pi} \right) \left[ \frac{dE_r^\pm(\mathbf{k})}{dk} \right]^{-1}. \quad (3)$$

Since the wave vector  $\mathbf{k}$  enters explicitly in (3) we have to use the inverse function of (2) in order to obtain only the quasi-particle energy  $E$  on the r.h.s. of the definition (3). We see therefore that the expression (3) is awkward and unpleasant for practical calculations of the density of states  $D_r(E)$  for sub-bands with non-parabolic dispersion. As a reasonable approximation for  $D_r(E)$  in this case we use the following expression

$$D_r(E) = (a_r E + b_r) \Theta(E - E_r(k=0)), \quad (4)$$

where  $\Theta(E)$  is the Heaviside step-function,  $E_r(k=0)$  is the bottom of the  $r$ th sub-band and the coefficients

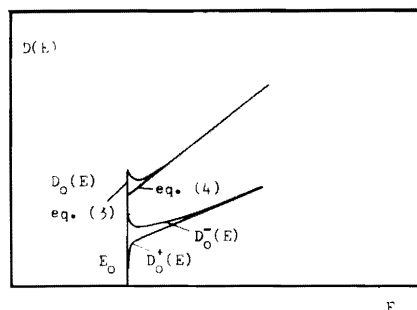


Figure 1. The Density of States of the Ground Sub-Band  $D_0(E)$  Calculated with the Definition (3) and With the Approximation (4).

$a_r$  and  $b_r$  account for the non-parabolicity. For the parabolic case we have  $a_r = 0$  and  $b_r = 1$ , where  $D_r(E)$  is measured in units  $\frac{m^*}{\pi\hbar^2}$  and  $m^*$  is the effective mass. As one can see from Equations (2) and (4), the non-parabolicity of the dispersion and the density of states, resulting from the band-band interaction, is described through the coefficients  $A_{r,m}^\pm$  for the dispersion (2) and by  $a_r$  and  $b_r$  for the density of states (4). Sub-bands with stronger non-parabolicity are characterized with higher values of  $a_r$  and lower  $b_r$ . In Figure 1, comparison between the approximation (4) and the exact expression (3) for the density of states of the ground sub-band ( $r=0$ ) is given. One can see that they deviate only in a small energy region at the bottom of the sub-band. From this comparison we conclude that (4) is a reasonable approximation. The approximation (4) was tacitly used by Ohkawa and Uemura [6].

The dependence of  $a_r$  and  $b_r$  on the physical parameters of the system is presented next.

The physical parameters of our system are the doping  $N_A$ , the carrier concentration in the inversion layer  $N_s$ , the temperature  $T$  and the alloy composition  $x$ . The acceptor energy is  $E_A = 20$  (meV), and the Fermi level  $E_F$  is pinned above the valence band in the bulk,  $E_F = E_v(d) + E_A$ , because of the acceptor levels presented there. The depth of the depletion layer is denoted by  $d$ .

The dispersion  $E_r^\pm(\mathbf{k})$  of the first three sub-bands  $r = 0, 1, 2$  of  $n$ -inversion layer on  $p$ - $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ , and the total density of states  $D(E) = \sum_r D_r(E)$  are shown on Figure 2 for  $N_A = 3 \times 10^{22}$  ( $\text{m}^{-3}$ ),  $N_s = 8 \times 10^{15}$  ( $\text{m}^{-2}$ ),  $x = 0.2$  and  $T = 300$  (K). The energy reference point is in the middle of the gap and we consider 7 terms in the decomposition (2), *i.e.*,  $p = 6$ . This is

enough for the convergence of the series (2), as our experience with practical calculations has convinced us, for the usual range of the values of the physical parameters of the system. The coefficients  $A_{r,m}^\pm$  in (2) are determined by obtaining  $E_r^\pm(\mathbf{k})$  first numerically, solving Equations (1), then performing interpolations using Chebyshev polynomial and finally rearranging the terms in ascending powers of the wave vector  $k = |\mathbf{k}|$ .

Figure 3 shows the temperature dependence of  $a_r$  and  $b_r$  for  $N_A = 3 \times 10^{22}$  ( $\text{m}^{-3}$ ),  $N_s = 8 \times 10^{15}$  ( $\text{m}^{-2}$ ), and  $x = 0.2$ . We see that the following conditions are fulfilled

$$\begin{aligned} a_2 &> a_1 > a_0, \\ b_2 &< b_1 < b_0, \end{aligned} \quad (5)$$

which means that the non-parabolicity of the higher sub-bands is more strongly expressed. The non-parabolicity decreases with  $T$  because the gap increases and the band-band interaction becomes weaker. As noted above,  $D_r(E)$  is measured in units  $\frac{m^*}{\pi\hbar^2}$  [3], and since the effective mass  $m^* = \frac{\hbar^2 E_G}{4P_0^2}$  increases with  $T$ , through the gap  $E_G$ , which in turn increases with the temperature [7], the vertical unit in Figure 3 changes with  $T$  (the matrix element  $P_0$  is a constant) and therefore Figure 3 shows the combined effect of the influence of the temperature on the considered entities. The temperature dependence of  $a_r$  and  $b_r$  will be smaller should we measure  $D_r(E)$  in absolute units ( $\text{J}^{-1}\text{m}^{-2}$ ), but this is not customary [3].

It is known that the gap of  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  increases with  $x$  [7] and therefore we expect that the non-parabolicity will decrease with  $x$ . Figure 4 shows the dependence of  $a_r$  and  $b_r$  on the alloy concentration  $x$  for  $N_A = 5 \times 10^{22}$  ( $\text{m}^{-3}$ ),  $N_s = 10^{16}$  ( $\text{m}^{-2}$ ) and  $T = 77$  (K). We note that the conditions (5) are fulfilled again and the non-parabolicity really decreases with  $x$ .

The temperature dependence of the spin-splitting  $\Delta_r(\mathbf{k}) = E_r^+(\mathbf{k}) - E_r^-(\mathbf{k})$  ( $r = 0, 1, 2$ ) is shown on Figure 5 for  $N_A = 3 \times 10^{22}$  ( $\text{m}^{-3}$ ),  $N_s = 8 \times 10^{15}$  ( $\text{m}^{-2}$ ),  $x = 0.2$  and for two values of the wave vector  $\mathbf{k}$ . The spin-splitting decreases with  $T$  and this is again a consequence of the weaker band-band interaction at higher temperatures.

In summary, we have investigated numerically the non-parabolicity of the dispersion and the density of

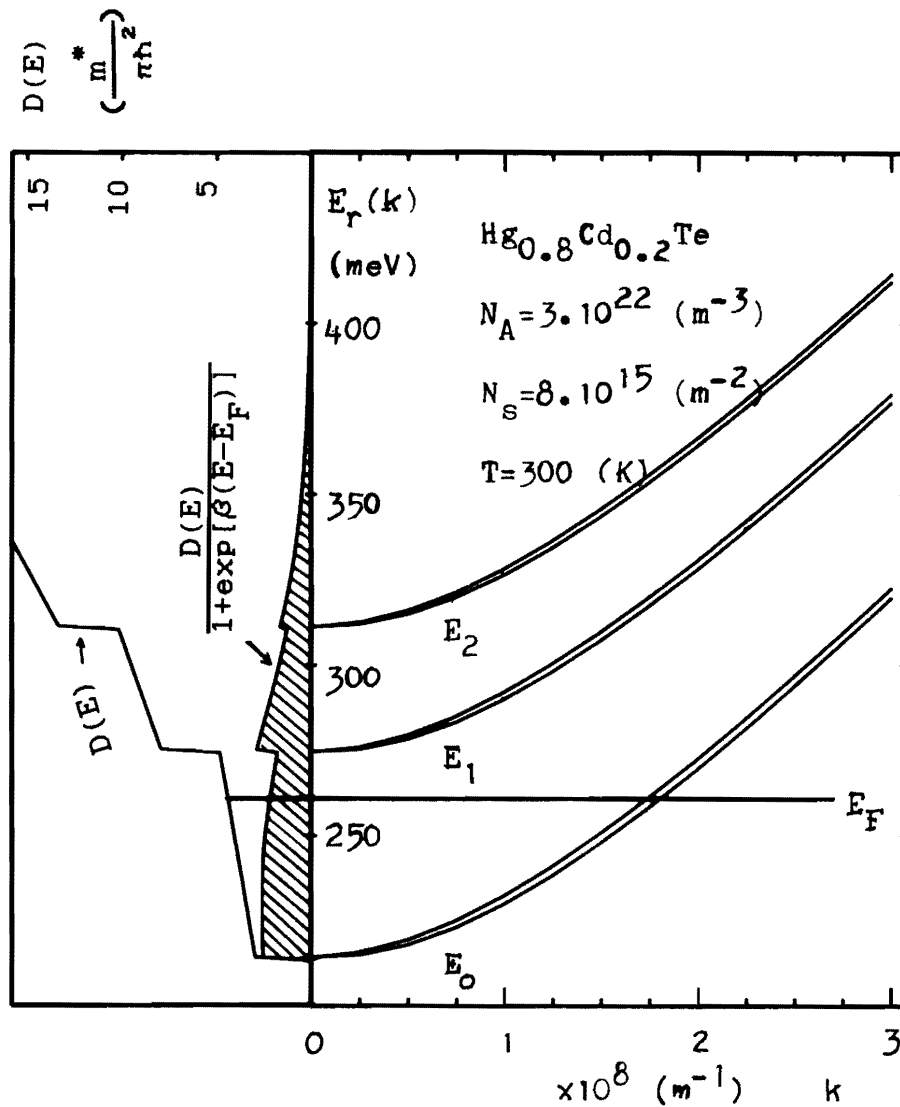


Figure 2. The dispersion of the First Three Sub-Bands  $E_r^\pm(k)$ , ( $r = 0, 1, 2$ ) is Shown on the Right Side. The spin-splitting of each sub-band is a consequence of the influence of the surface potential  $V(z)$ , which breaks the crystal symmetry near the surface. The total density of states  $D(E) = \sum D_r(E)$  is plotted on the left side. Because of the non-parabolicity of the dispersion, the density of states of each sub-band  $D_r(E)$  is not constant. The integral over the shaded area gives the electron concentration  $N_s$ . Due to the tail of the Fermi-distribution, these carriers spread over several sub-bands at finite temperature.  $\beta$  denotes the inverse temperature ( $\beta = k_B T/q$ )<sup>-1</sup>.

states of the sub-band states in  $n$ -inversion layers on  $p$ - $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  at finite temperature. This is a generalization of the previous zero-temperature treatments of this problem [1, 8–10]. We show that the non-parabolicity increases with the sub-band index and decreases with  $T$  and  $x$  due to the weaker band–band interaction at higher temperatures and alloy concentrations.

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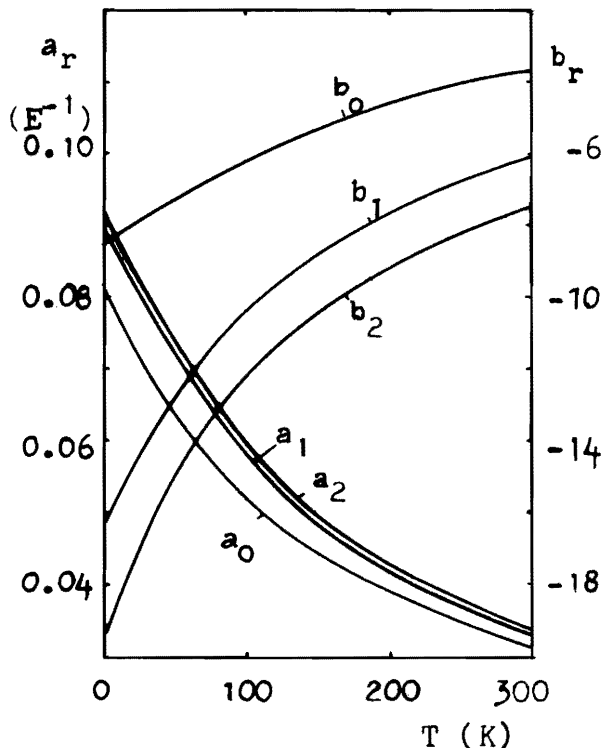


Figure 3. The Temperature Dependence of the coefficients  $a$ , and  $b$ , Describing the Non-parabolicity of  $D(E)$  According to the Linearized Approximation (4). The numbers on the  $a$ -axis are given assuming that the quasi-particle energy  $E$  in Equation (4) is measured in (meV).

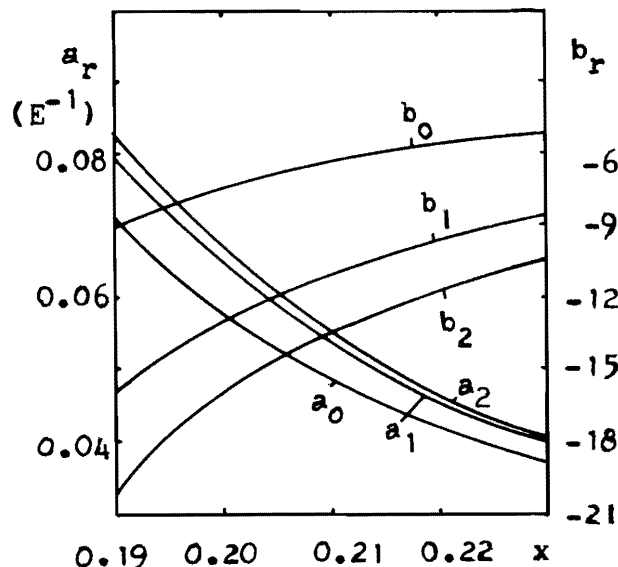


Figure 4. Dependence of  $a$ , and  $b$ , on the Alloy Composition  $x$ .

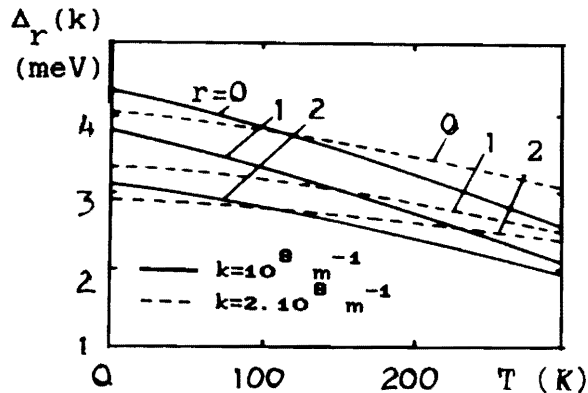


Figure 5. Temperature Dependence of the Spin Splitting  $\Delta$ , of the Dispersion of HgCdTe.

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