The method for calculation of carrier concentration in narrow-gap n-type doped $Cd_xHg_{1-x}Te$ structures

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Abstract **A simple method for the computation of carrier concentration in n-type doped $Cd_xHg_{1-x}Te$ structures is proposed. The method is based on the postulate on the existence of donor bands. In our model the donor bands are postulated to have a Gaussian distribution of density of states characterized by two parameters only (energy being the centre of gravity for this distribution and standard deviation). These parameters are taken as well as good consistency could be obtained with experimental data, which were comprised of a wide range of doping levels for various kinds of dopants**.

I Introduction

When the density of impurity atoms is large enough, the interaction between dopants is the reason for the creation of dopant bands. This essentially changes the electrical properties and particularly influences the concentration of charge carriers. The strict quantum theory of dopant bands is a very complex problem and requires the consideration of multi-electron models. In the case of narrow-bandgap semiconductors, additional difficulties occur related to both experimental verification and the development of a theoretical model. Important and plentiful information about this issue one can found in the monograph of Shklovskii and Efros [1]. In strong doped semiconductors, a large impurity band must have a considerable effect on the density of electron states in the original conduction band. This effect should be most pronounced at the lower energy states for the conduction band, making that band non-parabolic [2]. It is commonly known that for strongly n-type doped $Cd_xHg_{1-x}Te$ structures there are large differences between the experimental data of electron concentration and the numerical results obtained by using the Kane's model of band structure [3]. Usually the numerical results are almost over one order lower than those obtained experimentally. Usually the numerical results are almost over one order lower than those obtained experimentally. Thus it is the reason for the discrepancies between the values of the detector's performances measured experimentally and those calculated numerically. To omit this issue some simple procedures are used to increase the values of the electron concentration. Sometimes the values of the electron effective mass are assumed to be much higher than the real values to increase the density of states in the conduction band [4], or instead of Kane's model, a hyperbolic model is applied [5]. In this model the wave vector dependence of the conduction band energy differs significantly from Kane's results [3].
Those "tricks" have no physical interpretation, and the reason for the discrepancies could be found in another way. This work has been done in order to find a correct and possible simple way for the numerical calculation of the charge carrier concentration in doped structures (primarily those doped with donors). If we apply classical methods (see for example [6]) based on the assumption that isolated donor levels exist, this leads to results which are very much underrated in relation to the experimental results and it is impossible to explain why. On the other hand,the assumption in this case that the total ionization of donors takes place giving the incorrect values of the Fermi energy. In p-type materials, these difficulties can occur in practice only at the very high concentrations of acceptors.

In this paper the simple method for the computation of carrier concentration in n-type doped $Cd_xHg_{1-x}Te$ structures is proposed. It is based on the assumption that donor bands are created overlapping the conduction band and have the effective density of states at least twice as high as the donor concentration. An approximate estimation based on the hydrogen-like model of donor states shows that the overlapping of electron wave function of the donor ground states takes places even for donor concentrations below 10^{15} cm^{-3}.

II Numerical results

Due to the fact that the ground donor level is degenerated β_1-fold, the donor band being created should contain $\beta_1 N_D$ energy levels. If the ground donor level is an s-like donor state with $\beta_1 = 2$. There should also exist the bands corresponding to the excited states of the donor level. The energy distance between the individual states of the donor level can be easily estimated on the basis of a hydrogen-like model. We have assumed that the density of ground states exhibits the Gaussian distribution with standard deviation W determined by relation (2), however n_{D_1}, the electron concentration in this band, is determined by the relation (1):

$$n_{D_1} = \int_{E_c - E_D - 3W}^{E_c - E_D + 3W} \frac{\beta_1 N_D}{\sqrt{2\pi}W} e^{\frac{-(E - E_c - E_D)^2}{2W^2}} \frac{1}{1 + \exp\left(\frac{E - F}{k_B T}\right)} dE$$

The centre of gravity for this distribution may occur at an energy equal to E_C-E_D (E_C is the energy of bottom of conduction band and E_D is mean ionization energy of donors).

F denotes the Fermi energy. According to the well-known model [7] the standard deviation W caused by interaction of the electron with all the other electric carriers inside the cubic meter of semiconductor volume is approximated by the relation:

$$W = \frac{e}{2\pi\hbar}\frac{e^2}{(\varepsilon\varepsilon_0)^2}(k_B T)^{\frac{1}{4}}(N_D + N_A)^{\frac{1}{4}} \qquad (2),$$

where e is the elementary charge, ε is the permittivity and ε_0 is the permittivity of free space. N_D and N_A is the donor and acceptor concentration respectively.

In the hydrogen-like model the radius of the first excited state is four time higher than that for the unexcited state, thus the overlapping of the electron wave function may occur even for the low concentration of donor atoms. This is why we have assumed that it creates the additional donor band. We have also assumed that the density of states in this band also exhibits the Gaussian distribution with the standard deviation determined by relation (9), however n_{D_2}, the electron concentration in this band is determined by the relation:

$$n_{D_2} = \int_{E_C-3W}^{E_C+3W} \frac{\beta_2 N_D}{\sqrt{2\pi}W} e^{\frac{-(E-E_C)^2}{2W^2}} \frac{1}{1+\exp\left(\frac{E-F}{k_B T}\right)} dE \qquad (3)$$

The overlap between impurity wave-functions is strong enough so that the impurity band must cover an appreciable range of energy. The centre of gravity for this distribution may occur at an energy above or equal to E_C.(We have assumed equal to E_C) The presence of this large impurity bands must have a considerable effect on the density of the electron states $g(E)$ for the original conduction band. The idea of this is shown in Figs. 1. β_2 is the degeneracy of the first excess hydrogen-like donor state. Because it is orbital p , then β_2 should be equal to 6.

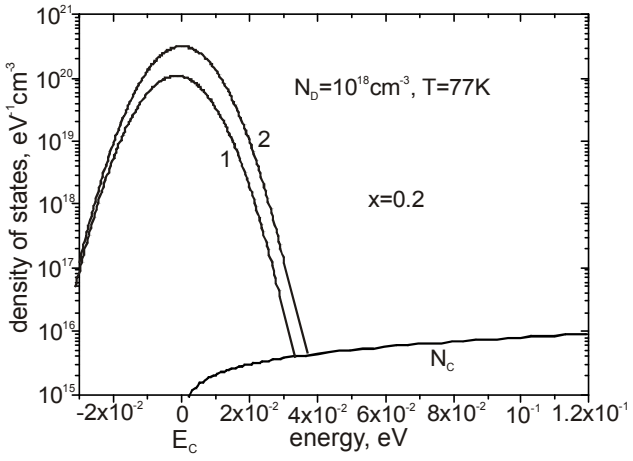
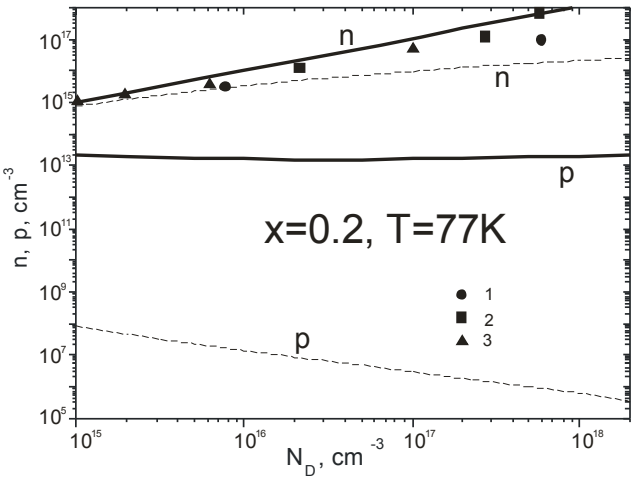


Fig.1. The density of states (in $eV^{-1}cm^{-3}$) as a function of energy in material of mole fraction x=0,2 and donor concentration $N_D = 10^{18}cm^{-3}$ at 77K. The curve marked by N_C presents the density of states in conduction band . Te value of energy denoted as E_c is the edge of the conduction band. Curve indicated by the number 1 shows the density of states in the donor band connected with ground donor states, and this indicated by number 2 shows the density of states in the donor band connected with the excess states.

Fig.2. Lines denoted as n show electron concentration and these denoted as p the hole concentration respectively as a function of donor concentration for $Cd_xHg_{1-x}Te$ with CdTe mole fraction x=0.2 at 77K. Experimental data are shown for epitaxial $Cd_xHg_{1-x}Te$ structures with near 0.2 mole fraction grown by MOCVD technology doped in iodine; 1-[8], 2-[9] structures deposited on CdZnTe (100)4° substrate, 3-[10] structures deposited on CdZnTe (211)B substrate. Dashed lines show calculated results obtained without assumption of the existence of donor bands. Solid lines are obtained under the assumption that two donor bands exist, one connected with donor



ground states and the second connected with donor excess states.

III SUMMARY

A simple method for computing the concentration of charge carriers in $Cd_xHg_{1-x}Te$ structures doped with donors has been proposed. It is based on the assumption that donor bands are created overlapping the conduction band and have the effective density of states at least twice as high as the donor concentration. An approximate estimation based on the hydrogen-like model of donor states shows that the overlapping of electron wave function of the donor ground states takes places even for donor concentrations below 10^{15} cm^{-3}. Our calculations have shown that in n-type doped $Cd_xHg_{1-x}Te$ narrow-gap structures, the electrons populated states located both in donor bands and in the conduction band. The electron concentration is practically equal to the concentration of donor atoms. These results are consistent with the experimental data.

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