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Investigation of the effective mass of electrons in solid solutions $Hg_{1-x-y-z}A_xB_yC_zTe$

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Abstract. This paper presents theoretical investigation on the influence of manganese and zinc in solid solutions of $Hg_{1-x-y-z}A_xB_yC_zTe$ on changes in the electron effective mass.

Keywords: solid solution, electron effective mass.

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Semiconductor solid solutions of $Hg_{1-x-y-z}A_xB_yC_zTe$ type have been actively studied in the course of recent 20 years. Such a stable interest is largely attributable to the unique properties of these materials, allowing their successful use for manufacturing IR detectors, filters and other instruments operating in the ranges of 3-5 and 8-14 μm.

Alongside with traditional materials of this type, including, in our opinion, HgCdTe and HgMnTe, growing popularity is gained by 4-component solid solutions HgCdMnTe and HgCdZnTe, possessing, as shown in [1-2], a better temporal and thermal stability and greater crystal perfection. The reason for this is a smaller ion radius Mn^{2+} and Zn^{2+} as compared to cadmium.

It is clear that the effect of manganese and zinc additions is not restricted to the above phenomena. This effect should also extend to band parameters of materials and electrophysical phenomena occurring therein.

The purpose of this paper is to study the effect of manganese and zinc in solid solution $Hg_{1-x-y-z}A_xB_yC_zTe$ on electron effective mass.

As shown in [3-5], effective electron mass near the bottom of conduction band in the nondegenerate case in materials of $Hg_{1-x-y-z}A_xB_yC_zTe$ type is described by expression:

$$m^*_e = m_0\left[1+E_P\frac{E_g+2\Delta/3}{E_g(E_g+\Delta)}\right]^{-1}. \qquad (1)$$

Here $E_P = 2m_0P^2/\hbar^2$, Δ is the spin-orbit band splitting, P is matrix element of pulse momentum operator, E_g is the bandgap, m_0 is the free electron mass.

The effective electron mass in a fully degenerate case was calculated as follows [3]:

$$\left(\frac{m^*_e}{1-m^*_e}\right)^2 = 32.5\cdot10^{-32}E_g^2/P^4 + 8.27\cdot10^{-30}n^{2/3}/P^2, \qquad (2)$$

where n is the electron concentration.

The bandgap, the matrix element of pulse momentum operator, the distance to split out band were calculated by the method described in [4].

Figs 1 and 2 show the composition dependences of a parabolic equivalent of the electron effective mass for HgCdMnTe (Fig. 1) and HgCdZnTe (Fig. 2) at $T = 300$ K. As can be seen from these figures, the effective electron mass in the nondegenerate case varies much more with a change in the amount of manganese and zinc, than with a change in the cadmium amount.

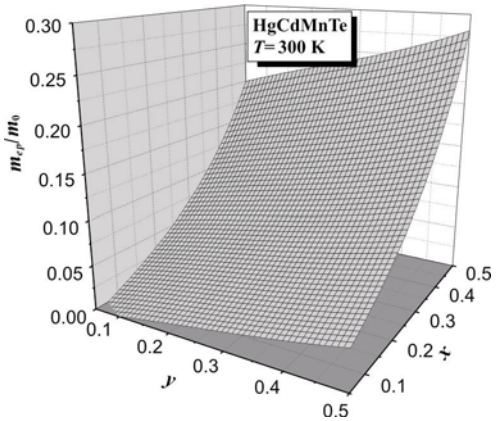

Fig. 1. Composition dependence of the parabolic equivalent of the effective electron mass in $Hg_{1-x-y}Cd_xMn_yTe$ at $T = 300$ K.

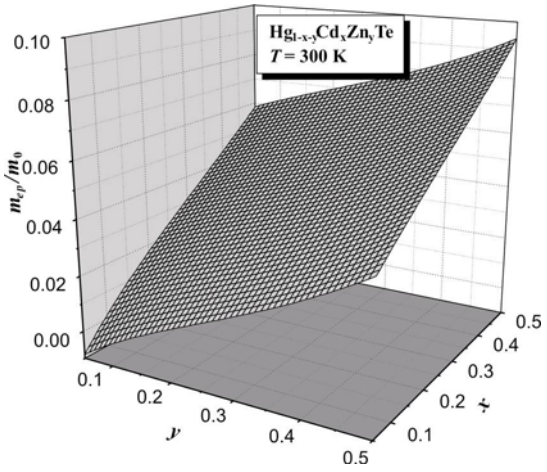

Fig. 2. Composition dependence of the parabolic equivalent of the effective electron mass in $Hg_{1-x-y}Cd_xZn_yTe$ at $T = 300$ K.

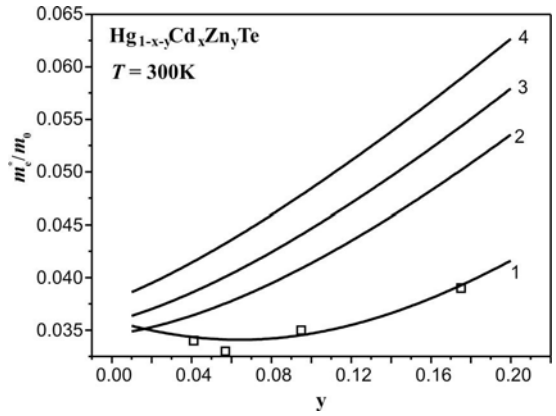

Fig. 3. Effective electron mass in $Hg_{1-x-y}Cd_xZn_yTe$ of various compositions. Curve 1 – $x = 0$; 2 – $x = 0.15$; 3– $x = 0.2$; 4 – $x = 0.25$. Experimental data (points) – from [6]. The carrier concentration was chosen as $n = 10^{18}$ cm^{-3}.

In a completely degenerate case, the effective electron mass should be calculated using the formula (2).

Figs 3 and 4 show the results of comparison between the effective electron mass values calculated by this formula in the fully degenerate case and the experimental data. As is obvious from the figures, the theory is in a satisfactory agreement with the experiment, despite the fact that it was performed for extreme cases of HgZnTe and HgMnTe. Thus, in our view, the formula (2) is also suitable for description of the effective mass of solid solutions under study.

In this connection, it is also interesting to compare effective electron masses in HgCdMnZnTe and HgCdTe for crystals with an identical bandgap. Table 1 presents calculation results as compared to the data [7] at room temperature.

From the table, it can be concluded that the effective electron mass in HgCdMnZnTe somewhat exceeds that in HgCdTe, this difference becoming greater as the content of manganese and zinc increases. It agrees well with the conclusion made in [8] when comparing the effective electron masses in HgMnTe and HgCdTe. Comparison of our calculations with the results of [8] at $T = 300$ K is shown in Table 2. It can be seen that the effective electron mass in HgCdMnZnTe is somewhat smaller (by about 15%) than in HgMnTe.

As regards the considerable divergence for samples with $E_g = 0.054$ eV, a similar disagreement between the theory and experiment can be also observed in [8], and also towards a greater side. The reason apparently lies in the fact that this theory would not work well with E_g approaching zero.

Thus, as can be concluded from our research, the introduction of manganese and zinc into solid solution HgCdTe increases not only the bandgap, but also the effective electron mass.

Table 1. Results of calculations of effective electron masses in comparison with [7].

$Hg_{1-x-y-z}Cd_xMn_yZn_zTe$ composition	E_g, eV	Carrier concentration, N, cm^{-3}	m_e/m_0, Eq. (2)	m_e/m_0, theor. [7]	m_e/m_0, exper. [7]	$Hg_{1-x}Cd_xTe$ composition [7]
x=0.14; y=0.014; z=0.01	0.131	$2.4\cdot10^{18}$	0.049	0.045	0.049	0.18
x=0.166; y=0.02; z=0.01	0.182	$6.7\cdot10^{17}$	0.034	0.035	0.033	0.22
x=0.16; y=0.03; z=0.02	0.223	$2.8\cdot10^{18}$	0.052	0.049	0.048	0.25

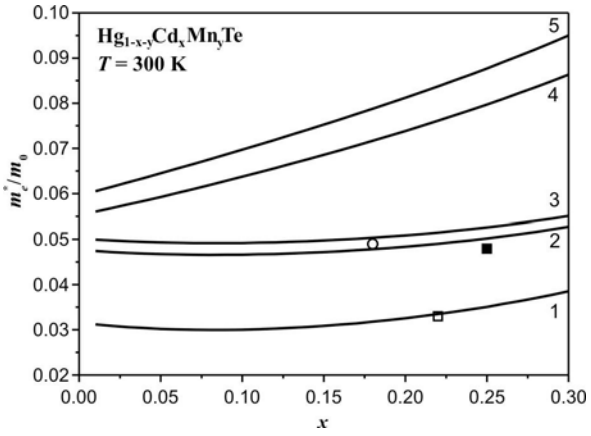

Fig. 4. Effective electron mass in $Hg_{1-x-y}Cd_xMn_yTe$ of various compositions. Curve 1 – $y = 0$, $n = 6.7\cdot10^{17}$ cm^{-3}; 2 – $y = 0$, $n = 2.4\cdot10^{18}$ cm^{-3}; 3 – $y = 0$, $n = 2.8\cdot10^{18}$ cm^{-3}; 4 – $y = 0.13$, $n = 2\cdot10^{18}$ cm^{-3}; 5 – $y = 0.15$, $n = 2\cdot10^{18}$ cm^{-3}. Experimental data for HgMnTe (points) – from [7].

Table 2. Results of calculations of effective electron masses in comparison with [8].

$Hg_{1-x-y-z}Cd_xMn_yZn_zTe$ composition	E_g, eV	Carrier concentration, N, cm^{-3}	m_e/m_0, Eq. (6)	m_e/m_0, theor. [8]	m_e/m_0, exper. [8]	$Hg_{1-x}Mn_xTe$ composition [8]
x=0.092; y=0.01; z=0.01	0.054	$1.5\cdot10^{17}$	0.019	0.019	0.0162	0.06
x=0.14; y=0.014; z=0.01	0.131	$6.0\cdot10^{16}$	0.017	0.0194	–	0.09
x=0.16; y=0.015; z=0.01	0.158	$5.5\cdot10^{17}$	0.031	0.0345	0.036	0.1

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