IMPROVEMENT OF ELECTRICAL PROPERTIES OF $Hg_{1-x}Zn_xSe$ UPON DOPING WITH Fe

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Results of measurements of electron concentration and mobility in mixed crystals of $Hg_{1-x}Zn_xSe$ ($0 \leq x \leq 0.07$) doped with resonant Fe donors ($0 \leq n_{Fe} \leq 5 \times 10^{19}$ cm^{-3}) at liquid helium temperatures are presented. The data show that there is a considerable improvement of the electrical properties of the material when Fe impurities are present. The analysis of the mobility in terms of the scattering from ionized centers (accounting for possible spatial correlation of impurity charges) and the alloy scattering is in agreement with the measured data.

PACS numbers: 72.80.Ey, 72.20.Fr, 71.55.Fr

Mixed crystals of II–VI semiconductors containing Zn have attracted recently a great deal of interest. This is related to the fact that the presence of Zn in, say, HgTe improves considerably mechanical [1] and electrical [2] properties compared to the case of, e.g., Cd containing compounds. Therefore, we have studied mixed crystals of $Hg_{1-x}Zn_xSe$ doped with resonant Fe hoping that the improvement related to the stabilizing effect of Zn observed by Cobb et al. [2] will combine with a similar effect related to the presence of Fe [3] and result in a particularly attractive semiconducting material from the point of view of possible applications. Furthermore, doping with iron is known to lead to an increased mobility, as evidenced by the study of the case of HgSe:Fe in the mixed valence regime [4]. The existence of similar enhancement in $Hg_{1-x}Zn_xSe$:Fe was confirmed in the course of our study.

The highest molar fraction x attained in the crystals grown by the modified Bridgman method was 0.072. The Zn fraction in the studied samples was determined by energy dispersive X-ray analysis. The concentration of intentional Fe donors ranged from $n_{Fe} = 0$ (undoped samples), through intermediate Fe concentrations (corresponding to completely ionized system of donors at low temperatures), up to $n_{Fe} = 5 \times 10^{19}$ cm^{-3}, when only a fraction of Fe donors were ionized (mixed valence regime).

Electron conductivity and the Hall effect at liquid helium temperatures were measured and from those values the concentration of conduction electrons as well as their mobility were determined. As in HgSe:Fe, there is an increase in the electron concentration together with the amount of Fe impurities present in the

crystals, followed by a saturation (at high Fe doping levels) whose value depends on Zn molar fraction. The latter dependence shows that there is a relative shift of the resonant Fe level and the bottom of the conduction band induced by alloying with Zn. The observed mobility values, particularly in the samples with high concentrations of Fe, are quite high — indicating good quality of the crystals studied here. There are clear indications that the mechanism of the mobility enhancement, seen previously in HgSe:Fe [4], is also active in the present case of $Hg_{1-x}Zn_xSe:Fe$.

To analyze the data quantitatively we have to incorporate in the appropriate model of the band structure the variation of the $\Gamma_8 - \Gamma_6$ energy gap, E_0, as well as the variation of the relative position (with respect to the conduction band edge) of the resonant Fe level, E_{Fe}, with the composition of the crystals. We made use of the determination of the triple degeneracy point (i.e., the composition corresponding to $E_0 = 0$) of Potapov et al. [5] who give its value as $x_0 \cong 0.06$ at 4.2 K. Let us note that this value shows that the variation of the energy gap in $Hg_{1-x}Zn_xSe$ is markedly nonlinear (a linear interpolation between the energy gap in HgSe and ZnSe would correspond to $x_0 \cong 0.10$). With the above variation of the energy gap we can calculate the Fermi level position* corresponding to the measured electron concentrations. Figure 1 shows results of such calculation for the samples in the saturation region. Assuming that the Fermi level in these samples is pinned to the Fe resonant level one can compare these results with an estimate of the position of the iron level obtained, in the spirit of the Langer–Heinrich rule [6], from the known values of this energy in the end point materials ($E_{Fe} \cong 0.2$ eV above the Γ_8 conduction band edge in HgSe [7] and $E_{Fe} = 0.6 \div 0.8$ eV above the Γ_8 valence band edge in ZnSe [8]) and deduce the shift (in the absolute energy scale) of the Γ_8 edge upon addition of Zn to HgSe. The comparison shows again that the shift depends on x in a nonlinear way. The difference between the values of E_{Fe} in HgSe and ZnSe with respect to the Γ_8 band edges determines the value of the parameter W which we shall need further when calculating the contribution to the scattering rate due to disorder scattering [9].

Our analysis of mobility assumed that only two scattering mechanisms of the conduction electrons are effective at low temperatures: the scattering from ionized impurities (whose number was assumed to be equal to the number of ionized Fe donors and whose screening was taken to be given by the Thomas–Fermi screening radius) and the alloy scattering. One obtains, then, the values of the mobility shown by squares in Fig. 2. It is clear that in the case of strong doping, corresponding to the mixed valence regime, there is an efficient reduction of the scattering rate. When the mechanism of the scattering reduction related to the spatial correlation of the impurity charges is taken into consideration within the short-range correlation approach [4], one obtains values of mobility shown in Fig. 2 by empty circles. The agreement is fair, indicating that there are no other scattering mechanisms, apart from those already included in the analysis, contributing significantly to the total scattering rate. In contrast to the latter samples, the mobility measured in $Hg_{1-x}Zn_xSe$ doped only very lightly (or undoped) with Fe is considerably

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*We used the three band Kane model of the band structure with the effect of the higher bands included — the values of the parameters were taken as in HgSe, except of E_0 and the momentum matrix element P which was also allowed to depend on the Zn content [5], see inset to Fig. 1.
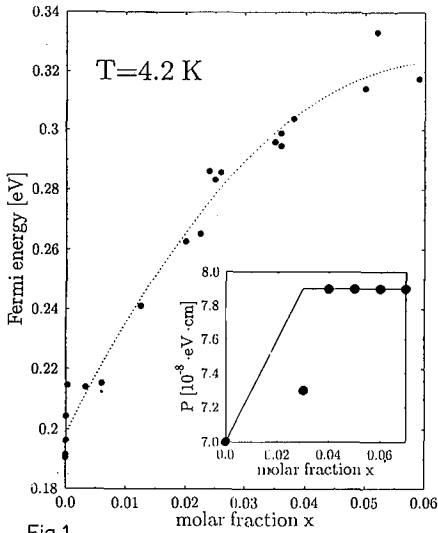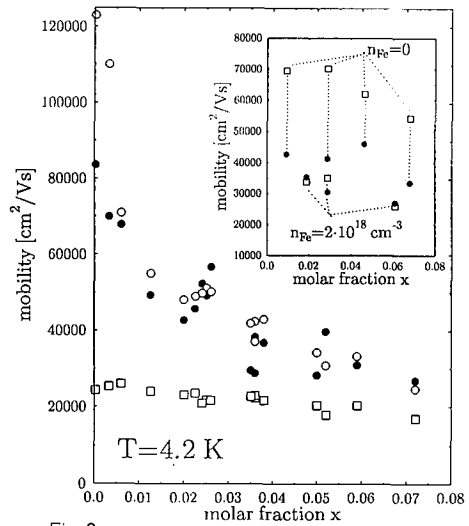
Fig.1

Fig.2

Fig. 1.   Fermi level in $Hg_{1-x}Zn_xSe$ as a function of molar fraction x corresponding to electron concentration at 4.2 K in samples strongly doped with Fe ($n_{Fe} \geq 8 \times 10^{18}$ cm^{-3}). The calculation was performed for highly degenerate electron gas within the 3-band model of the band structure with higher bands included perturbatively (higher bands parameters and the spin orbit splitting parameter $\Delta = 0.39$ eV were taken as for HgSe from Ref. [10], $E_0(x) = -0.270 + 4.59x - 1.52x^2$ [eV], and the momentum matrix element P as shown in the inset).

Fig. 2.   The electron mobility in $Hg_{1-x}Zn_xSe$ at liquid helium temperature as a function of molar fraction x for samples strongly doped with Fe ($n_{Fe} \geq 8 \times 10^{18}$ cm^{-3}) and (in the inset) slightly doped with Fe (n_{Fe} given in the figure). Experimental values are shown by full circles, calculated values taking into account screened ionized impurity scattering ($N_{scatt} = n_e$) and disorder scattering ($W = -0.5$ eV, $V = 2.6$ eV) are shown by squares when no spatial correlation of impurities charges were included or by empty circles when the spatial correlation was accounted for within the short-range correlation model.

smaller than the calculated value. Obviously, other scattering mechanisms impede the conductivity in this case. This fact shows again that the presence of iron donors has a "healing" effect on the electrical properties probably by making formation of structural defects less probable [1]. The healing effect is particularly evident when one compares the mobility in the samples without Fe that have smaller conduction electron concentration (and, nevertheless smaller mobility values) with the samples having even small amount of Fe, whose mobility is substantially greater despite their greater conduction electron concentrations.

Acknowledgments

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