Anomalous behavior of impurity centers in $Pb_{1-x}Sn_xTe(Ga)$ alloys subjected to pressure

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It was discovered that a localization of electrons at impurity centers occurs in single-crystal, Ga-doped $Pb_{1-x}Sn_xTe$ alloys subjected to hydrostatic compression at $T = 4.2$ K. In n-type alloys the Fermi level suddenly moves into the valence band with an increase in pressure.

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1. In many cases the use of external pressure as an independent physical parameter makes it possible to obtain new information about the nature of the impurity states in semiconductors. Usually, the charge state of the introduced impurities and the density of free carriers in the semiconductor do not change due to the influence of pressure. Cases in which the band structure near the Fermi level is determined by quasi-local (resonance) impurity levels are an exception. Such a situation is realized, for example, in $Pb_{1-x}Sn_xTe(In)$ alloys, where an external pressure at $T = 4.2$ K induces semiconductor-metal-semiconductor transitions.[1] These studies made it possible to establish unequivocally the presence of a large-capacity impurity level within the limits of the forbidden band of the $Pb_{1-x}Sn_xTe(In)$ alloys. In our work described in this paper, we have found in $Pb_{1-x}Sn_xTe(Ga)$ alloys a new, unusual behavior of the impurity centers due to the action of pressure.

2. In our work we investigated the galvanomagnetic and oscillation effects in $Pb_{1-x}Sn_xTe(Ga)$ alloys from the interval $(0.19 \lesssim x \lesssim 0.30)$ in magnetic fields up to 60

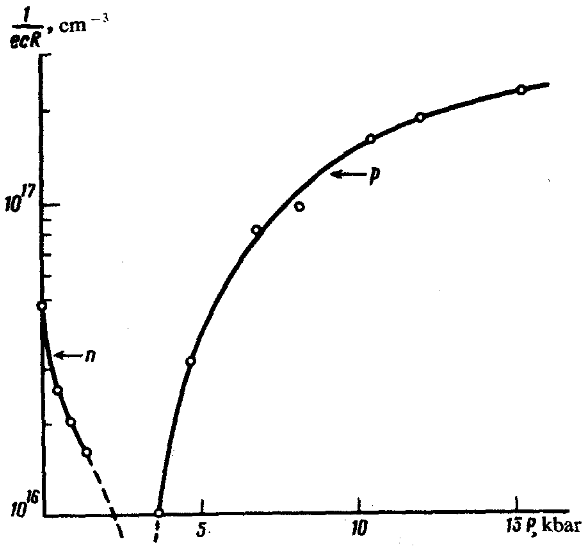

FIG. 1. Pressure dependence of the charge carrier density, $n, p = 1/ec|R|$ in the $Pb_{0.81}Sn_{0.19}Te(Ga)$ alloy. $T = 4.2$ K.

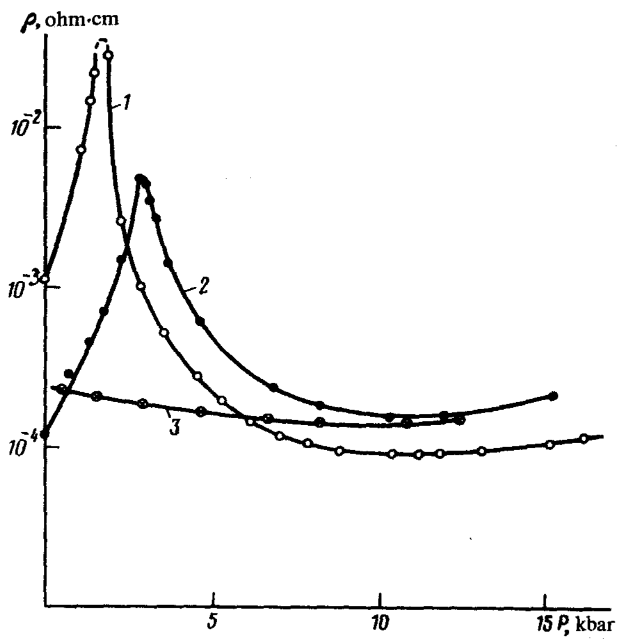

FIG. 2. Pressure dependence of resistivity in $Pb_{1-x}Sn_xTe(Ga)$ alloys at $T = 4.2$ K: $1 - x = 0.19$; $2 - x = 0.20$; $3 - x = 0.25$.

kOe, which were subjected to pressures up to 16 kbar in the temperature range of 2 to 300 K.

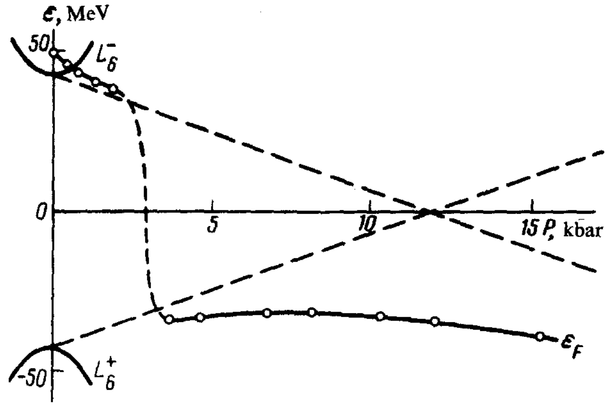

FIG. 3. Location of the Fermi level ϵ_F relative to the L band in the $Pb_{0.81}Sn_{0.19}Te(Ga)$ alloy as a function of the pressure.

The initial $Pb_{1-x}Sn_xTe$ alloys were grown by the Czochralski method. Ga was introduced into the ~1-mm-thick, single-crystal wafers by means of an isothermal annealing in GaTe vapors. The annealing temperature (~650°) and duration (~10 days) were the same for all alloy compositions. Some alloys were grown from the gaseous phase. In this case the Ga was introduced directly into the growth charge. The Ga in the alloys, according to analysis estimates and results, amounts to a few tenths of a percent.

3. In the absence of an impurity the $Pb_{1-x}Sn_xTe$ alloys, regardless of their composition, exhibited p-type conductivity with a hole density of $p \sim 10^{18}$–10^{19} cm^{-3}. The Ga impurity in these compounds carries a certain donor character; however, the resulting carrier density at $T = 4.2$ K depends on the alloy composition. Alloys with $x = 0.19$ and $x = 0.20$ exhibit n-type conductivity with an electron density of $n \sim 5 \times 10^{16}$ cm^{-3} and $\sim 10^{16}$ cm^{-3}, respectively. The $Pb_{1-x}Sn_xTe(Ga)$ alloys from the interval $0.22 \lesssim x \lesssim 0.30$ had p-type conductivity, with the hole density increasing drastically with an increase in the amount of SnTe from $p \approx 10^{16}$ cm^{-3} ($x = 0.22$) to $p \approx 10^{19}$ cm^{-3} ($x = 0.30$). We note that in the $Pb_{1-x}Sn_xTe(Ga)$ alloys in the vicinity of the transition from n- to p-type conductivity the insulator state, which was observed in the $Pb_{1-x}Sn_xTe(In)$ alloys, is not realized at low temperatures.[2] The temperature dependence of the resistivity ρ in the investigated alloys is metallic in nature throughout the entire temperature interval.

4. The oscillation and galvanomagnetic effects were investigated at pressures up to 16 kbar in alloys with $x = 0.19$, $x = 0.20$, and $x = 0.25$. It was expected that the pressure dependence of the carrier density would remain constant if the Ga impurity is a usual, shallow impurity, or it would be described by a parabolic function, as in the $Pb_{1-x}Sn_xTe(In)$ alloys, if the Ga impurity stabilizes the Fermi level. The experimental pressure dependence of the carrier density of the alloy with $x = 0.19$, for example, is shown in Fig. 1. The electron density decreases sharply, with increasing pressures and then at $P = P_i \approx 2.8$ kbar the electron conductivity is replaced by hole conductiv-

ity; a further increase in pressure leads to an increase in the hole density up to a value of $p \sim 2 \times 10^{17}$ cm^{-3}. As far as we know, such large density variation due to pressure has no analogies in other materials, in whose spectrum the resonance levels are missing. The curve in Fig. 1 is typical for all alloys having n-type conductivity. In the alloy with $x = 0.25$ (p-type) a monotonic increase is observed in the hole density from $p \approx 9 \times 10^{17}$ to $p \approx 3 \times 10^{18}$ cm^{-3} as the pressure is changed from 1 kbar to 16 kbar.

The region of inversion of the sign of the Hall coefficient R is characterized by an abrupt (~ 50 fold) increase in resistivity (Fig. 2). For the alloy with $x = 0.25$ (initial p-type conductivity) the $\rho(P)$ dependence at $T = 4.2$ K is a monotonic function (curve 3 in Fig. 2).

We note that all the studies alloys are sufficiently homogeneous: their electron spectrum is described by degenerate statistics at $T = 4.2$ K and throughout the entire range of pressures except for the narrow inversion region (Fig. 1); Shubnikov-de Haas oscillations are clearly observed. Using the experimentally obtained cross sections for the Fermi surface and the cyclotron carrier masses, we calculated, within the framework of the two-band approximation, the location of the Fermi level ϵ_F relative to the L band in the spectrum of the alloys. Figure 3 is an example of this calculation for the alloy with $x = 0.19$. A characteristic feature of this relationship is almost discontinuous jump of the Fermi level from the conduction band to the valence band within some narrow pressure interval near $P = P_i$.

It is important to note that beyond the ultraquantum limit of magnetic fields in the regions $P < P_i$ and $P > P_i$, there is no increase of the carrier density with increasing magnetic field, as for the $Pb_{1-x}Sn_xTe(In)$ alloys with a stabilized Fermi level.[3]

5. The obtained data show that the Ga in the $Pb_{1-x}Sn_xTe$ alloys, unlike In, apparently does not form a quasi-local impurity level and, at the same time, it is not the usual shallow impurity, but possesses fundamentally new properties. It can be assumed that a transition of the Ga atoms from an electrically active state to a neutral state occurs due to the action of the external pressure and, possibly, as a result of increasing SnTe concentration, as a result of which the number of carriers introduced by Ga decreases monotonically to zero.

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