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Parameters of Yb-Induced Deep Level in $Pb_{1-x}Ge_xTe$ Doped with Yb

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The effect of pressure ($P \leq 12 \times 10^8$ Pa) on the galvanomagnetic properties (4.2 K $\leq T \leq$ 300 K, $B \leq 7$ T) of $Pb_{1-x}Ge_xTe$ ($x = 0.038$) alloy doped with Yb has been investigated. Under pressure the insulator–metal transition and the sharp increase in the free hole concentration in the alloy were revealed. On the basis of obtained experimental results the model of reconstruction of the energy spectrum of the alloy under pressure has been proposed. In the frame of this model by comparing the theoretical and experimental pressure dependences of Fermi energy and free hole concentration the main parameters of the Yb-induced deep level were determined.

1. Introduction

It was found recently that doping of $Pb_{1-x}Ge_xTe$ ($x \leq 0.06$) alloys with Yb leads to the formation of a deep Yb-induced level, the energy position of which strongly depends on the alloy composition [1 to 3]. In PbTe this level situates in the valence band near its top. Upon the increase in Ge content the level moves to the top of the valence band with the rate $d(\Delta E_{Yb})/dx \approx 7$ meV/at% [4], intersects it at $x \approx 0.01$ and enters into the forbidden gap.

Application of hydrostatic compression induces a decrease of $Pb_{1-x}Ge_xTe$ forbidden gap. So one can expect that in alloys with $x > 0.01$ it will lead to the approach of the Yb impurity level to the valence band edge and entrance of this level into the valence band. In this case the redistribution of electrons between the valence band and free states in the deep level may give the possibility to observe an insulator–metal transition induced by pressure and to reconstruct the energy spectrum of $Pb_{1-x}Ge_xTe\ \langle Yb\rangle$ under pressure.

In order to prove these assumptions and to determine the main parameters of the Yb impurity states in $Pb_{1-x}Ge_xTe$ alloys in the present work the effect of high hydrostatic pressure on galvanomagnetic properties of $Pb_{1-x}Ge_xTe$ ($x = 0.038$) doped with Yb was investigated.

2. Experiment

$Pb_{1-x}Ge_xTe\langle Yb\rangle$ single crystals, grown by the modified Bridgman technique described in [1] were studied. The parameters of the investigated samples at the atmospheric pressure are given in Table 1. For each sample the temperature dependences of resistivity ϱ and the Hall constant R_H (4.2 K $\leq$ 300 K, $B \leq 0.1$ T) were measured in a chamber shielded from the external background illumination.

Table 1.
Parameters of the investigated $Pb_{1-x}Ge_xTe$ ($x = 0.038$) samples at $T = 4.2$ K

sample	C_{Yb} (at.%)	type	R_H (cm^3/C)	ϱ (Ω cm)	p, (cm^{-3})	μ_H, (cm^2/V s)
Yb60-1	0.86	p	$>5 \times 10^7$	$>6 \times 10^4$	$<10^{11}$	$>8 \times 10^2$
Yb60-2	0.86	p	$>2 \times 10^6$	$>8 \times 10^2$	$<10^{12}$	$>3 \times 10^3$

The sample Yb60-1 was then investigated under high hydrostatic pressure. Pressures up to 12×10^8 Pa were obtained in the heat-treated beryllium bronze chamber with kerosene–oil–pentane pressure transmitting medium. At pressures $P > 4 \times 10^8$ Pa the Shubnikov-de Haas effect ($T = 4.2$ K, $B \leq 7$ T) were also studied.

3. Results and Discussion

The temperature dependences of resistivity ϱ and Hall constant R_H measured under the atmospheric pressure exhibit activation character in the whole investigated temperature range (Fig. 1). With increase of pressure the slope of the activation region decreases and becomes zero at some critical pressure P^*. From the slope of the activation regions on $R_H(1/T)$ dependences the activation energy of the Yb-induced level $\Delta E_{Yb} = E_{Yb} - E_v$ was determined (Fig. 2). It was found that under pressure ΔE_{Yb} decreases almost line-

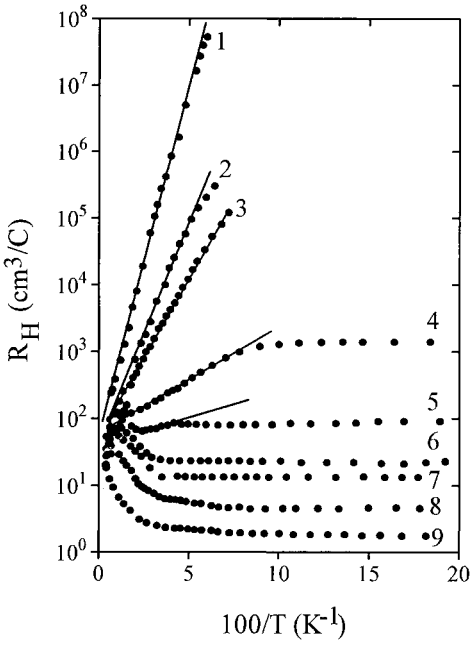

Fig. 1

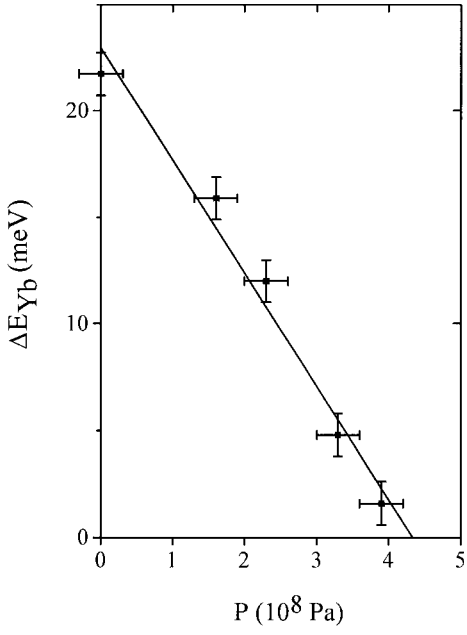

Fig. 2

Fig. 1. Temperature dependence of Hall constant in $Pb_{1-x}Ge_xTe\langle Yb\rangle$ ($x = 0.038$) under various pressures. P (10^8 Pa): (1) 0, (2) 1.6, (3) 2.3, (4) 3.3, (5) 3.9, (6) 4.4, (7) 6.8, (8) 8.7, (9) 12.0
Fig. 2. Dependence of the activation energy of Yb-induced deep level in $Pb_{1-x}Ge_xTe\langle Yb\rangle$ ($x = 0.038$) on pressure

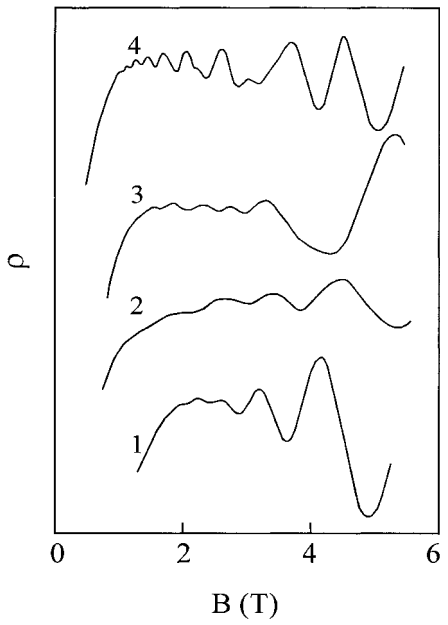

Fig. 3

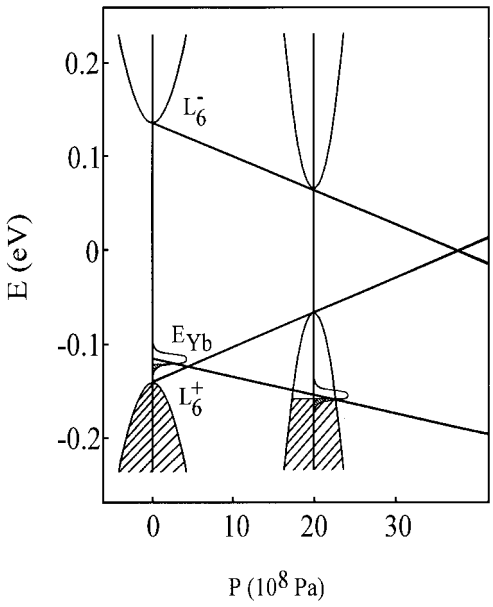

Fig. 4

Fig. 3. Transverse magnetoresistance oscillations in $Pb_{1-x}Ge_xTe\langle Yb\rangle$ ($x = 0.038$) under various pressures. P (10^8 Pa): (1) 4.7, (2) 6.8, (3) 8.7, (4) 12

Fig. 4. Reconstruction of the energy spectrum of $Pb_{1-x}Ge_xTe\langle Yb\rangle$ ($x = 0.038$) under pressure at $T = 4.2$ K

arly with the rate $d(\Delta E_{Yb})/dP \approx 5 \times 10^{-8}$ meV/Pa and becomes zero at pressure $P = P^* = 4.5 \times 10^8$ Pa.

At pressure P^* on the $R_H(1/T)$ dependences the saturation region at low temperature emerges, indicating the appearance of free holes in the valence band at $T = 4.2$ K. At the same pressure in the magnetic field dependence of resistivity Shubnikov-de Haas oscillations were revealed (Fig. 3). Upon further increase of pressure the values of R_H and the period of Shubnikov-de Haas oscillations at $T = 4.2$ K decrease, pointing toward the increase of the free hole concentration in the alloy under pressure.

The obtained experimental results allow one to conclude that under pressure the deep Yb-induced level moves to the top of the valence band, intersects it and enters into the valence band, inducing an insulator–metal transition due to the flow of electrons from the valence band to the free states in the impurity level (Fig. 4). For the further consideration it is very important that the emergence of the appreciable free hole concentration takes place at $P < P^*$, under which the activation energy of the Yb-induced level becomes zero. This fact allows us to suggest that the Yb-induced level (impurity band) should have a considerable width and should be filled with electrons less than half under atmospheric pressure. In any other case the free holes must emerge in the valence band exactly at pressure P^*, when the activation energy ΔE_{Yb} becomes zero.

In order to determine the main parameters of the Yb-induced band the comparison between theoretical and experimental pressure dependences of the free hole concentra-

tion was carried out (Fig. 5). The experimental values of the free hole concentration (points in Fig. 5) were calculated from the values of the Hall constant at $T = 4.2$ K. In the calculation of the theoretical dependences we consider that under pressure the sum of free hole concentration in the valence band $p(P)$ and the density of empty states in the impurity band $p_{\mathrm{Yb}}(P)$ is constant and equal to the initial concentration of empty states in the impurity band under atmospheric pressure $p_{\mathrm{Yb}}(0)$,

$$p_{\mathrm{Yb}}(0) = p(P) + p_{\mathrm{Yb}}(P)\,. \tag{1}$$

The concentration of the free holes was obtained in terms of the Kane energy–momentum relation with the values of parameters typical of $Pb_{1-x}Sn_xTe$ ($x \approx 0.2$) presented in [5]. The concentration of empty states in the Yb-induced band was calculated under the assumption that the density of impurity states function $g_{\mathrm{Yb}}(E)$ can be approximated by the Gaussian-type curve and under atmospheric pressure the impurity band is partially filled with electrons,

$$p_{\mathrm{Yb}}(P) = \int_{E_{\mathrm{F}}}^{\infty} g_{\mathrm{Yb}}(E)\,\mathrm{d}E\,, \tag{2}$$

$$g_{\mathrm{Yb}}(E) = \left(\frac{N_{\mathrm{Yb}}}{\sigma\sqrt{2\pi}}\right) \exp\left[-\frac{(E - E_{\mathrm{Yb}})^2}{2\sigma^2}\right], \tag{3}$$

$$p_{\mathrm{Yb}}(0) = N_{\mathrm{Yb}}(1 - k)\,, \tag{4}$$

where σ is the width of the Yb-induced band, N_{Yb} the total capacity of the band and k is the occupancy of the band with electrons under atmospheric pressure.

To estimate the value of N_{Yb} we suppose that every impurity atom takes part in the formation of impurity states and gives one electronic state to the impurity band. In our

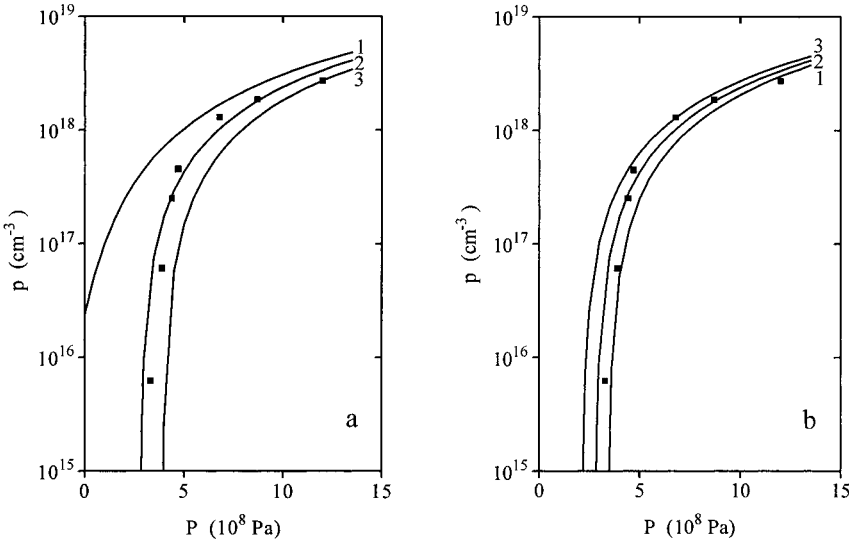

Fig. 5. Dependence of the free hole concentration in $Pb_{1-x}Ge_xTe\langle Yb\rangle$ ($x = 0.038$) on pressure. Theoretical dependences (curves 1 to 3) were obtained in the frame of the model given by Eq. (1) to (4). a) $\sigma = 7$ meV, k: (1) 0, (2) 1/8, (3) 3/8; b) $k = 1/8$, σ (meV): (1) 4, (2) 7, (3) 10

calculations the total capacity $N_{Yb} \approx 10^{20}\,cm^{-3}$ obtained in such a way was fixed and only two parameters (σ and k) were varied.

It was found that the variation of the initial occupancy of the impurity band with electrons k leads to more appreciable changes in the $p(P)$ dependence, than the variation of σ (Fig. 5). With increase of k the insulator–metal transition point shifts toward higher values of pressure and a sharper increase of the free hole concentration in the metallic phase takes place. The best agreement between theoretical and experimental dependences was reached with the values of parameters $k \approx 1/8$ and $\sigma \approx 7\,meV$ (curves 2 in Fig. 5).

4. Conclusion

The obtained experimental results allow us to conclude that in investigated $Pb_{1-x}Ge_xTe$ ($x \approx 0.038$) alloy the Yb-induced deep level is partially filled with electrons ($k \approx 1/8$) and under atmospheric pressure situated above the valence band top ($E_{Yb} \approx E_v + 22\,meV$). Under pressure the impurity level moves toward the valence band top with the rate $d(\Delta E_{Yb})/dP \approx 5 \times 10^{-8}$ meV/Pa, intersects it and the insulator–metal transition occurs due to the flow of electrons from the valence band to the impurity states. The Yb-induced level (impurity band) has a considerable width $\sigma \approx 7\,meV$ and a total capacity $N_{Yb} \approx 10^{20}\,cm^{-3}$. The density of states function in the impurity band can be satisfactorily described by a Gaussian-type curve.

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