THE FERMI LEVEL IN $Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$ AND $PbS_{1-x}Se_x$

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Results are presented of calculations of the dependence of the Fermi level on the concentration of carriers for $Pb_{1-x}Sn_xTe$ ($0 \leqslant x \leqslant 0.30$), $Pb_{1-x}Sn_xSe$ ($0 \leqslant x \leqslant 0.12$) and $PbS_{1-x}Se_x$ ($0 \leqslant x \leqslant 1$) in the temperature range 50 to 300 K. The calculations have been performed in terms of the Kane model, using the generalized Fermi-Dirac integral.

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1. Introduction

The development of the technology of $Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$ and $PbS_{1-x}Se_x$ solid solutions is related to the wide use of those materials in infrared techniques. In view of some specific properties characteristic of semiconductors with a small and controlled energy gap (very small effective masses, high carrier mobilities, anomalous values of the dielectric constant, etc.) these compounds have been widely investigated. However, to interpret some of their optical and electric properties it is necessary to know the relationship between the Fermi level and the concentration of carriers for various molar compositions x in a wide range of temperatures.

In the present work the calculations of the Fermi level have been performed for $Pb_{1-x}Sn_xTe$ ($0 \leqslant x \leqslant 0.30$), $Pb_{1-x}Sn_xSe$ ($0 \leqslant x \leqslant 0.12$) and $PbS_{1-x}Se_x$ ($0 \leqslant x \leqslant 1$) for several carrier concentrations, and temperatures, 50–300 K. Also calculations of the temperature dependence of the carrier concentrations where the Fermi level touches the band edges are performed.

2. Calculations and results

In vicinity of the energy gap in lead chalcogenides we observe a system of three conduction bands and three valence bands which should be accounted for in accurate calculations of the bands structure. The Dimmock model provides for them by precisely

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taking into account the interactions between the nearest extremes of the valence band L_6^+ and conduction band L_6^-, and accounting for the interaction with more remote bands in the second approximation in terms of the perturbation theory [1]. It occurs, however, that the generalized Kane model is much simpler for interpreting experimental results. This model is in good agreement with experiment and is a common working model [2, 3].

For the generalized Kane model, the relationship between the Fermi level and carrier concentration can be expressed as [4]

$$n = \frac{(2m_{do}^* kT)^{3/2}}{3\pi^2 h^2} \int_0^\infty \left(-\frac{\partial f}{\partial z} \right) (z+\beta z^2)^{3/2} dz = \frac{(2m_{do}^* kT)^{3/2}}{3\pi^2 h^2} {}^0L_0^{3/2}, \tag{1}$$

where m_{do}^* is the density-of-states effective mass at the band edge, k is Boltzmann's constant, h is Planck's constant, $f = [\exp(z-\eta)+1]^{-1}$ is the Fermi-Dirac distribution function, $z = E/kT$ is the reduced energy, $\eta = E_F/kT$ is the Fermi level reduced energy, $\beta = kT/E_g$, E_g is the energy gap. The integral in expression (1) denoted as ${}^0L_0^{3/2}$ is a specific form of the general Fermi-Dirac integrals ${}^mL_K^n(\eta, \beta)$ tabularized in [5] and describing the thermodynamic, magnetic and transport properties of carriers in non-parabolic bands. The density-of-states effective mass can be obtained from the longitudinal and transverse mass components according to $m_d^* = N_v^{2/3}(m_l^* m_t^{*2})^{1/3}$ where $N_v = 4$ is the number of equivalent band extrema.

The effective masses are determined by a contribution due to the conduction valence band interaction, m_{cv}^*, and a far band contribution m_F^*. The longitudinal and transverse m_{cv}^* and m_F^* data are known from Shubnikov-de Haas measurements in $Pb_{1-x}Sn_xTe$ [6, 7] and $Pb_{1-x}Sn_xSe$ [8, 9] at liquid helium temperature. In the first approximation the temperature and x-dependence of the effective masses are due to the variation of the band gap, which influences m_{cv}^*. The x and T dependencies of the four effective masses: m_{ct}^* (conduction band, transverse), m_{vt}^* (valence band, transverse), m_{cl}^* (conduction band, longitudinal), m_{vl}^* (valence band, longitudinal) may then be obtained from the general expression [9]

$$\frac{1}{m^*(x, T)} = \frac{1}{m_{cv}^*} \frac{E_g(0, 0)}{E_g(x, T)} + \frac{1}{m_F^*}. \tag{2}$$

These functions are summarized in Table I for $Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$ and $PbS_{1-x}Se_x$ according to paper [9]. It is important to keep in mind that these expressions hold only for the band edges.

Exact knowledge of $E_g(x, T)$ dependences for the ternary compounds is required for reliable calculations over a wide range. However, quite different relationships for the energy gap especially for $Pb_{1-x}Sn_xSe$, can be found in the literature [9]. The $E_g(x, T)$ expressions given in Table I [9] showed very good agreement with experimental data for $Pb_{1-x}Sn_xTe$ [10–14] $Pb_{1-x}Sn_xSe$ [15–18] and $PbS_{1-x}Se_x$ [19].

The calculations of the dependence of the Fermi level on carrier concentration were performed on a computer using relation (1) and taking into account the $m^*(x, T)$ and $E_g(x, T)$ expressions given in Table I. In the calculations of m_{do}^* (see Eq. (1)) the values of

TABLE I

Band parameters of $Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$ and $PbS_{1-x}Se_x$

	$E_g\ (x,\ T)$ [meV]	$\frac{m^*_{c1}(x,\ T)}{m_0}$	$\frac{m^*_{v1}(x,\ T)}{m_0}$	$\frac{m^*_{c1}(x,\ T)}{m_0}$	$\frac{m^*_{v1}(x,\ T)}{m_0}$
$Pb_{1-x}Sn_xTe$	$171.5-535x$ $+\sqrt{(12.8)^2+0.19(T+20)^2}$	$\left(30.58\frac{E_g(0,0)}{E_g(x,\ T)}+14.29\right)^{-1}$	$\left(30.58\frac{E_g(0,0)}{E_g(x,\ T)}+10.0\right)^{-1}$	$\left(\frac{30.58}{10.25+6.56x}\frac{E_g(0,0)}{E_g(x,\ T)}+2.42\right)^{-1}$	$\left(\frac{30.58}{10.25+6.56x}\frac{E_g(0,0)}{E_g(x,\ T)}+1.25\right)^{-1}$
$Pb_{1-x}Sn_xSe$	$125-1021x$ $+\sqrt{400+0.256T^2}$	$\left(20.7\frac{E_g(0,0)}{E_g(x,\ T)}+4.3\right)^{-1}$	$\left(20.7\frac{E_g(0,0)}{E_g(x,\ T)}+8.7\right)^{-1}$	$\left(11.4\frac{E_g(0,0)}{E_g(x,\ T)}+2.9\right)^{-1}$	$\left(11.4\frac{E_g(0,0)}{E_g(x,\ T)}+3.3\right)^{-1}$
$PbS_{1-x}Se_x$	$263-138x$ $+\sqrt{400+0.256T^2}$	$\left(10.6\frac{E_g(0,0)}{E_g(x,\ T)}+1.9+2.4x\right)^{-1}$	$\left(10.6\frac{E_g(0,0)}{E_g(x,\ T)}+2.7+6.0x\right)^{-1}$	$\left(5.8\frac{E_g(0,0)}{E_g(x,\ T)}+3.7-0.8x\right)^{-1}$	$\left(5.8\frac{E_g(0,0)}{E_g(x,\ T)}+3.7-0.4x\right)^{-1}$

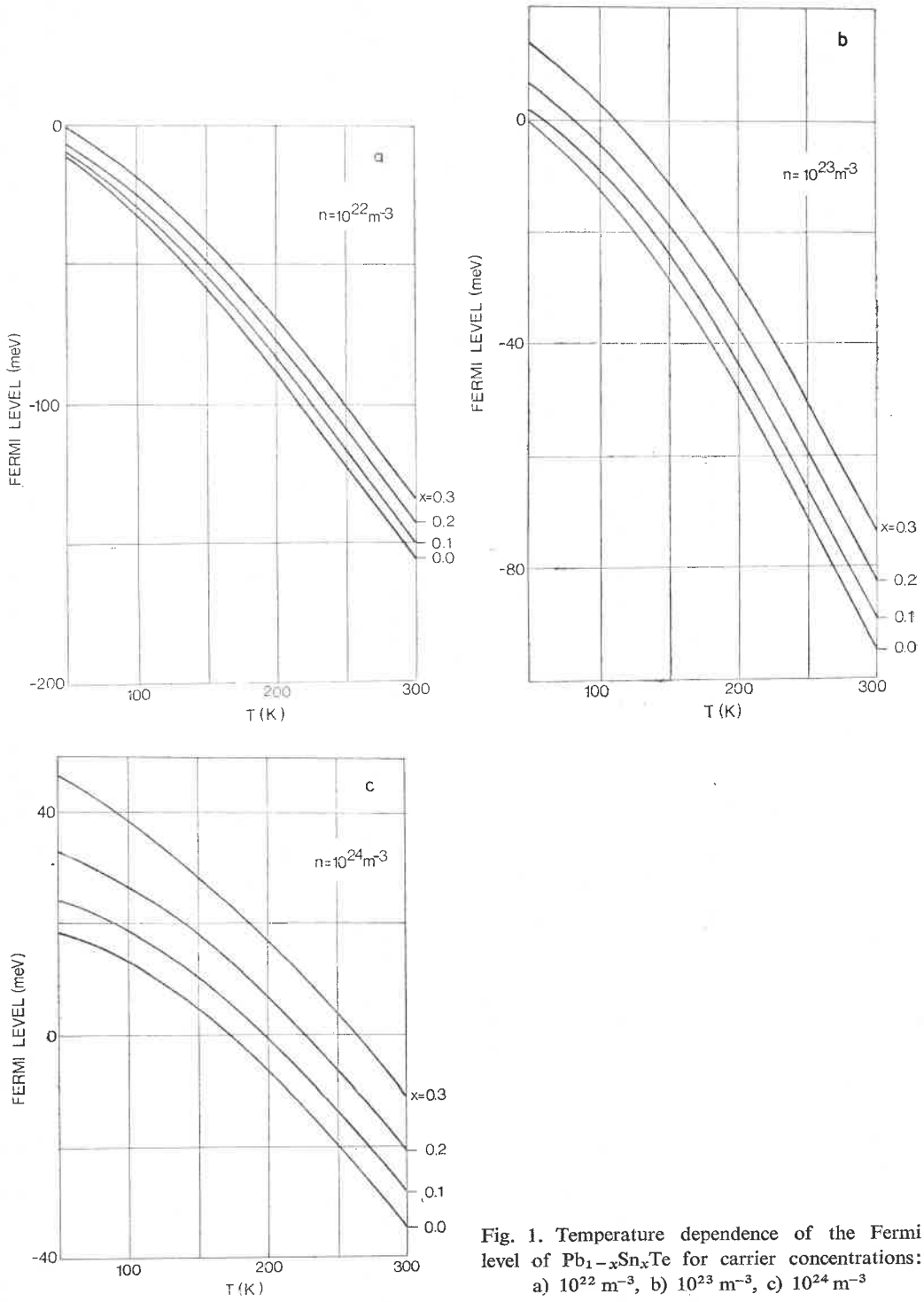
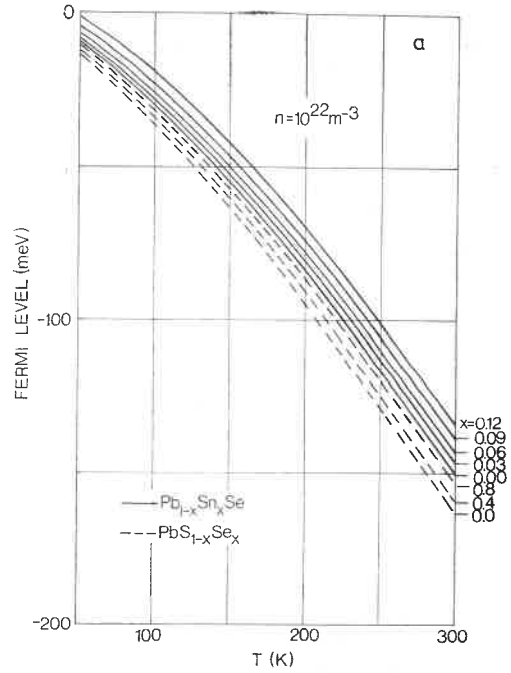
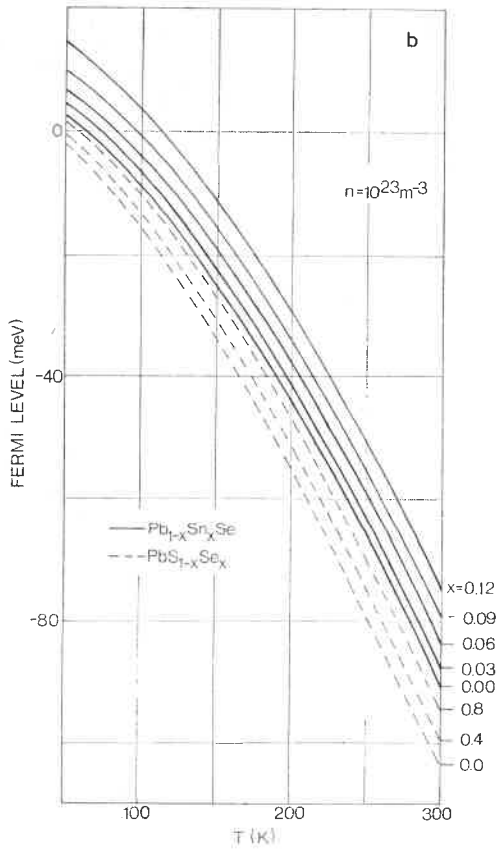


Fig. 1. Temperature dependence of the Fermi level of $Pb_{1-x}Sn_xTe$ for carrier concentrations: a) 10^{22} m^{-3}, b) 10^{23} m^{-3}, c) 10^{24} m^{-3}





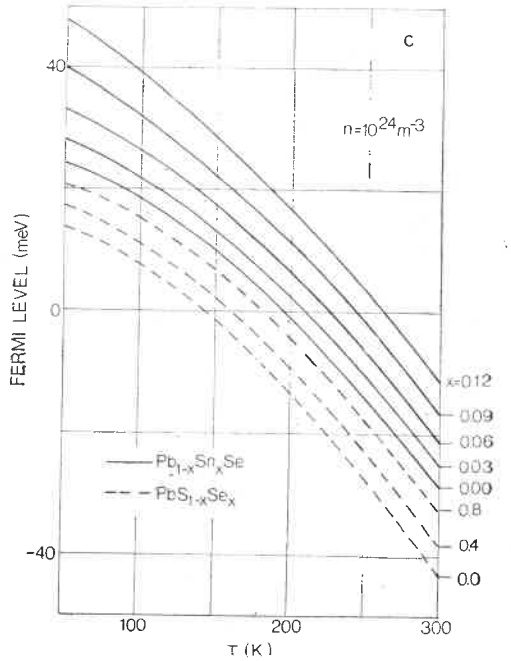


Fig. 2. Temperature dependence of the Fermi level of $Pb_{1-x}Sn_xSe$ and $PbS_{1-x}Se_x$ for carrier concentrations: a) 10^{22} m^{-3}, b) 10^{23} m^{-3}, c) 10^{24} m^{-3}

the effective masses of electrons were taken. For the case of the mirror-symmetric band structure of lead chalcogenides, the values of the effective masses of electrons and holes are almost identical (see Table I).

The temperature dependences of the Fermi level for $Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$ and $PbS_{1-x}Se_x$ for carrier concentrations 10^{22} m^{-3}, 10^{23}–m^{-3} and 10^{24}–m^{-3} are plotted in

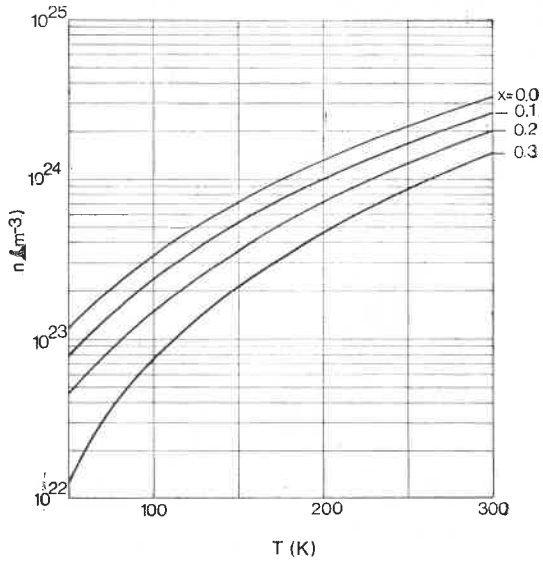


Fig. 3. Temperature dependence of the carrier concentrations for which the Fermi level of $Pb_{1-x}Sn_xTe$ touches the bottom of the conduction band

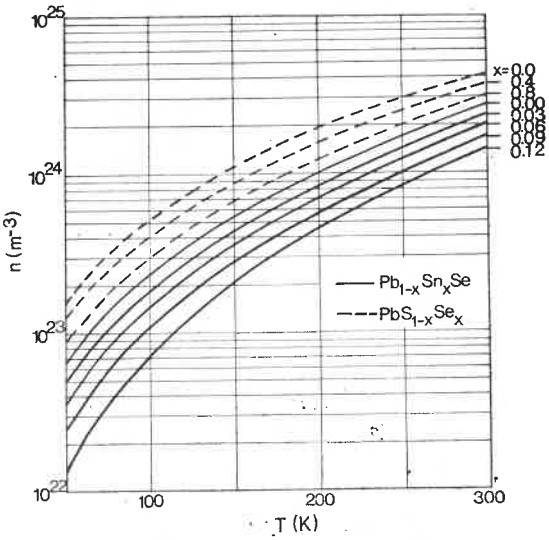


Fig. 4. Temperature dependence of the carrier concentrations for which the Fermi level of $Pb_{1-x}Sn_xSe$ and $PbS_{1-x}Se_x$ touches the bottom of the conduction band

Figs 1, 2. In Figs 3, 4 the temperature dependences of the carrier concentrations for which the Fermi level touches the bottom of the conduction band for the above ternary compounds are presented.

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