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THE LOCAL HEAVY-HOLE INTERACTION WITH CRYSTAL LATTICE DEFECTS IN INDIUM ANTIMONIDE

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The processes of heavy-hole scattering on the short-range potential caused by interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, static strain and ionized impurities in zinc blende p-InSb samples with carrier concentration $\sim 5\times10^{13}\div2\times10^{19}\,\mathrm{cm}^{-3}$ are considered. The temperature dependences of heavy-hole mobility and Hall factor in the range $11-520\,K$ are calculated.

Key words: transport phenomena, charge carrier scattering, indium antimonide.

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Introduction

Usually the heavy-hole scattering in indium antimonide was considered in relaxation time approximation or using the variational method. The common feature of these methods is the using of the long-range charge carrier scattering models for the description of the transport phenomena in this semiconductor. In these models it is supposed that either the charge carrier interacts with all the crystal (electron -phonon interaction) or it interacts with the defect potential of the impurity the action radius of which is equal to $\sim 10\div1000a_0$ (a_0 – lattice constant). However, such an assumption has next contradictions: a) it contradicts the special relativity according to which the charge carrier would interact only with the neighbouring crystal region; b) it contradicts the atomistic hypothesis according to which the charge carrier interacts (and transfers the energy respectively) only with one atom but not simultaneously with many atoms which are situated in different points of space. To eliminate these contradictions it is necessary to consider the following question – what object in the crystal absorbs the energy during the charge carrier scattering process? It can be either ionized (neutral) impurity atom or an atom which oscillates in the lattice site. During the scattering process all of these objects do not leave the boundaries of the elementary cell. Therefore the short-range charge carrier scattering models in zinc-blende II-VI [1,2] and in wurtzite III-V [3,4] semiconductors were proposed where it has been supposed that the carrier interacts with the defect potential only within the limits of one elementary cell. Here the following physical reasons were used: during the scattering the electron interacts only with neighboring crystal region (the short-range principle), after the scattering on this region the electron interacts with the next neighboring crystal region, etc. The aim of the present paper is the use of short-range models to describe the heavy-hole scattering on the various crystal lattice defects in indium antimonide.

I. Theory

According to the short-range scattering models in zinc-blende structure semiconductor the carrier transition probability from state $\mathbf{k}$ to state $\mathbf{k}'$ caused by the interaction with polar optical (PO), nonpolar optical (NPO), piezooptic (POP) and piezoacoustic (PAC), acoustic (AC) phonons, static strain (SS) potential, ionized impurity (II) looks like [1,2]:

$$W_{PO}(\mathbf{k},\mathbf{k}')=\frac{64\pi^7\gamma_{PO}^{10}e^4}{225\varepsilon_0^2G}\frac{M_{In}+M_{Sb}}{M_{In}M_{Sb}}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{LO})+\right.\right.$$
$$\left.\left.+\ (N_{LO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{LO})\right]+\frac{2}{\omega_{TO}}\left[N_{TO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{TO})+(N_{TO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{TO})\right]\right\};\quad(1)$$

$$W_{NPO}(\mathbf{k},\mathbf{k}')=\frac{\pi^3E^2}{288G}\frac{M_{In}+M_{Sb}}{M_{In}M_{Sb}}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{LO})+\right.\right.$$
$$\left.\left.+\ (N_{LO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{LO})\right]+\frac{2}{\omega_{TO}}\left[N_{TO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{TO})+(N_{TO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{TO})\right]\right\};\quad(2)$$

$$W_{POP}(\mathbf{k},\mathbf{k}') = \left(\frac{32}{75}\right)^2 \frac{\pi^9 e^2 e_{14}^2 \gamma_{PZ}^{10}}{\varepsilon_0^2 G} \frac{M_{In}+M_{Sb}}{M_{In}M_{Sb}} \left\{ \frac{1}{\omega_{LO}} [N_{LO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{LO}) + \right.$$
$$\left. + (N_{LO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{LO})] + \frac{2}{\omega_{TO}} [N_{TO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{TO}) + (N_{TO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{TO})] \right\}; \quad (3)$$

$$W_{PAC}(\mathbf{k},\mathbf{k}') = \frac{a_0^{10}}{\left(\frac{a_0+c_0}{2}\right)^8} \frac{128\pi^7 e^2 e_{14}^2 \gamma_{PZ}^{10} k_B T}{225\varepsilon_0^2 \hbar G[M_{In}+M_{Sb}]} \left(\frac{1}{c_\parallel}+\frac{2}{c_\perp}\right)^2 \delta(\varepsilon'-\varepsilon); \quad (4)$$

$$W_{AC}(\mathbf{k},\mathbf{k}') = \frac{\pi^3 k_B T E^2}{144\hbar G[M_{In}+M_{Sb}]} \left(\frac{1}{c_\parallel}+\frac{2}{c_\perp}\right)^2 \delta(\varepsilon'-\varepsilon); \quad (5)$$

$$W_{SS}(\mathbf{k},\mathbf{k}') = \frac{2^5 3^4 \pi^3 C^2 e^2 e_{14}^2 N_{SS}}{V\varepsilon_0^2 \hbar} \frac{1}{q^2} \delta(\varepsilon'-\varepsilon); \quad (6)$$

$$W_{II}(\mathbf{k},\mathbf{k}') = \frac{\pi e^4 Z_i^2 N_{II} \gamma_{II}^4}{2\varepsilon_0^2 \hbar V} \delta(\varepsilon'-\varepsilon); \quad (7)$$

where M_{In}, M_{Sb} – the atom masses; G – the number of unit cells in a crystal volume; ϵ_0 – the vacuum permittivity; e – the elementary charge; k_B – the Boltzmann constant; $\hbar$ – the Planck constant; N_{LO}, N_{TO} – the number of longitudinal (LO) and transverse (TO) phonons with a frequency ω_{LO} and ω_{TO} respectively; e_{14} – the component of the piezoelectric tensor; c_{LO}, c_{TO} – the respective sound velocities; V – the crystal volume; N_{II}, N_{SS} – the ionized impurities and strain centers concentration respectively; Z_i – the impurity charge in electron-charge units; E_{AC}, E_{NPO} – the acoustic and optical deformation potentials respectively (valence band); γ_{PO}, γ_{PZ}, γ_{II} – the fitting parameters determining the action radius of short-range potential ($R = \gamma a_0$, $0 \le \gamma_{PO}$, $\gamma_{PZ} \le 0.86$, $0 \le \gamma_{II} \le 1$); $q = |\mathbf{k}'-\mathbf{k}|$; $C \approx 0.1$.

It must be noticed that the strong power dependence of parameters γ_{PO}, γ_{PZ}, γ_{II} sharply limits the choice opportunities of their numerical values.

The heavy-hole scattering on NPO and AC phonons was described on the basis of the effective deformation potentials defined in [15-16]:

$$E_{NPO} = \frac{M_{In}+M_{Sb}}{2(M_{In}M_{Sb})^{1/2}} \left[\frac{C_t \left(\frac{C_l}{C_t}+2\right)}{2\rho\omega_{LO}^2 \left(\frac{a_0+c_0}{2}\right)^2} \right]^{1/2} d_0; \quad (8)$$

$$E_{AC} = \frac{C_l/C_t+2}{6\,C_l/C_t} \left[a^2 + \frac{C_l}{C_t}\left(b^2+\frac{d^2}{2}\right)\right], \quad (9)$$

where a, b and d – the fundamental valence band deformation potentials; C_l and C_t – the spherically averaged elastic coefficients expressed in terms of elastic constants C_{ij}.

The calculation of the conductivity tensor components was made on the base of the formalism of a precise solution of the stationary Boltzmann equation [5]. Using this formalism one can obtain the additional fitting parameter $\gamma_{SS}N_{SS}$ (we put $\gamma_{SS}=1$) for SS- scattering mode. The parameters of indium antimonide used for calculation are listed in Table 1.

II. Comparison of theory and experiment

A comparison of the theoretical temperature dependences of the heavy-hole mobility $\mu_p(T)$ was made with the experimental data presented in [17, 18]. The Fermi level was calculated from the charge neutrality equation given by:

$$p - n = N_A,$$

where the value of acceptors concentration was defined from the relation $N_A = I/eR_{exp}$, R_{exp} – experimental value of Hall coefficient.

The theoretical $\mu_p(T)$ curves are presented in Fig. 1a-d. The solid lines represent the curves calculated on the basis of the short-range models within the framework of the exact solution of the Boltzmann equation. The obtained heavy-hole scattering parameters for different scattering modes are listed in Table 2. It is seen that the theoretical curves sufficiently well agree with experimental data in all investigated temperature and concentration range.

To estimate the role of the different scattering mechanisms in Fig. 2 the dashed lines represent the appropriate dependences for the sample with acceptor concentration $N_A = 5.0 \times 10^{13}\mathrm{cm}^{-3}$. It is seen that in the temperature range $T < 20K$ the main scattering mechanism are the static strain scattering and polar optical phonon scattering. At higher temperatures the contribution of the acoustic and piezoacoustic phonon scattering play the dominant role. Other scattering mechanisms such as ionized impurity scattering, nonpolar and piezooptic phonon scattering give negligibly small contributions. For the samples with high acceptor concentration ($\sim 10^{18} \div 10^{19}\mathrm{cm}^{-3}$) the contribution of the ionized impurity scattering become dominant in all investigated temperature range.

On the base of the obtained scattering parameters the temperature dependence of heavy-hole Hall factor was calculated (see Fig.3).

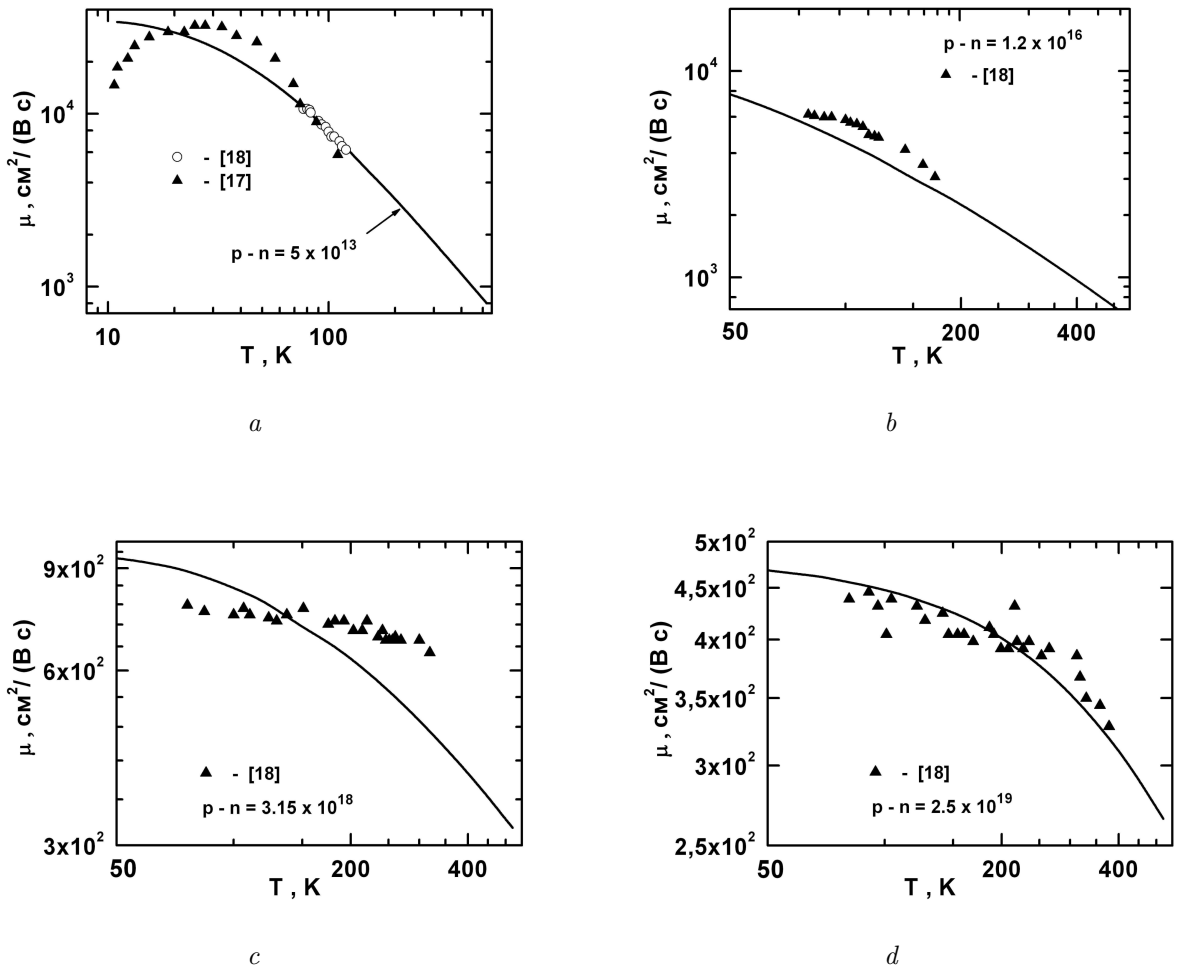

Fig. 1. The temperature dependence of the heavy-hole mobility in InSb crystals with different acceptor concentrations

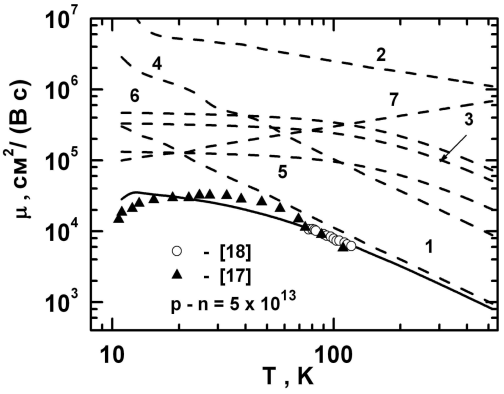

Fig. 2. The contribution of different scattering modes into heavy-hole mobility in InSb. Solid line – mixed scattering mechanism; 1,2,3,4,5,6,7 – AC-, II-, NPO-, PAC-, PO-, POP-, SS- scattering mechanism respectively

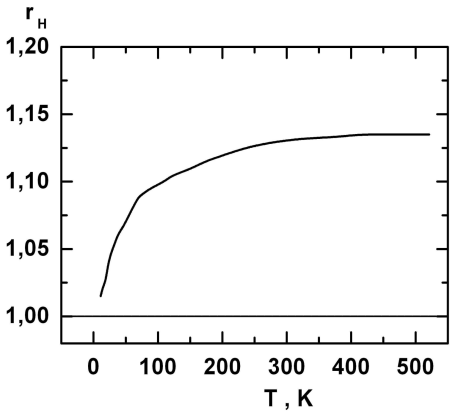

Fig. 3. The temperature dependence of Hall factor (heavy-holes) in InSb

Table 1

Parameters of wurtzite InSb used in calculations

Material parameter	Value	References
Lattice constant, a_0 (m)	6.47937×10^{-10}	
Energy gap, E_g (eV)	$0.235 - 0.27 \times 10^{-3} T^2/(T + 106)$	[6]
Heavy-hole effective mass, m_p/m_0	0.45	[8]
Density, ρ_0 ($\mathrm{gm \cdot cm^{-3}}$)	5.7746	[7]
Optical deformation potential, d_0 (eV)	26.8	[9]
Valence band deformation potentials:		
a (eV)	2.0	[10]
b (eV)	-2.0	[10]
d (eV)	-4.9	[10]
Elastic constants ($\times 10^{10}, \mathrm{N \cdot m^{-2}}$):		
C_{11}	6.665	[11]
C_{12}	3.645	[11]
C_{44}	3.020	[11]
Sound velosity, c ($\mathrm{m \cdot s^{-1}}$):		
$c_{\parallel}$	3.77×10^3	[12]
$c_{\perp}$	2.29×10^3	[12]
Optical phonon frequency:		
ω_{LO} ($\mathrm{rad \cdot s^{-1}}$)	3.59×10^{13}	[13]
ω_{TO} ($\mathrm{rad \cdot s^{-1}}$)	3.39×10^{13}	[13]
Piezoelectric tensor component, e_{14} ($\mathrm{C \cdot m^{-2}}$)	0.071	[14]

Table 2

Parameters γ for different scattering modes

N_A ($\mathrm{cm^{-3}}$)	γ_{PO}	γ_{PZ}	γ_{II}	$\gamma_{SS} \mathrm{N}_{SS} \times 10^{-14}$ ($\mathrm{cm^{-3}}$)
5×10^{13}	0.30	0.25	1.0	0.01
1.2×10^{16}	0.30	0.25	1.0	0.01
3.15×10^{18}	0.30	0.25	0.42	0.01
2.5×10^{19}	0.30	0.25	0.252	0.01

Conclusion

On the base of the short-range principle the heavy-hole scattering processes on the various types of crystal defects in p-InSb are considered. A sufficiently good agreement between theory and experiment in all investigated temperature and concentration range is established.

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ЛОКАЛЬНОЕ ВЗАИМОДЕЙСТВИЕ ТЯЖЕЛЫХ ДЫРОК С ДЕФЕКТАМИ КРИСТАЛЛИЧЕСКОЙ РЕШЕТКИ В АНТИМОНИДЕ ИНДИЯ

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Рассмотрены процессы рассеяния тяжелых дырок на близкодействующем потенциале, обусловленном взаимодействием с полярными и неполярными оптическими фононами, пьезоэлектрическими и акустическими фононами, полем статической деформации, заряженной примеси в образцах p-InSb с концентрацией носителей $\sim 5 \times 10^{13} \div 2 \times 10^{19}\,\text{см}^{-3}$. Рассчитаны температурные зависимости подвижности и Холл-фактора тяжелых дырок в интервале $11 - 520\,K$.

Ключевые слова: явления переноса, рассеяние носителей заряда, антимонид индия.

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ЛОКАЛЬНА ВЗАЄМОДІЯ ВАЖКИХ ДІРОК З ДЕФЕКТАМИ КРИСТАЛІЧНОЇ ГРАТКИ В АНТИМОНІДІ ІНДІЮ

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Розглянуто процеси розсіяння важких дірок на близькодіючому потенціалі, обумовленому взаємодією з полярними та неполярними оптичними фононами, п'єзоелектричними та акустичними фононами, полем статичної деформації, іонізованими домішками в зразках p-InSb з концентрацією носіїв $\sim 5 \times 10^{13} \div 2 \times 10^{19}\,\text{см}^{-3}$. Розраховано температурні залежності рухливості та Холл-фактора важких дірок в інтервалі $11 - 520\,K$.

Ключові слова: явища переносу, розсіяння носіїв заряду, антимонід індію.

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