ON STRUCTURE OF VALENCY BAND IN SEMICONDUCTOR MELTS $Bi_{1-x}Sb_x$

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On the base of the investigations of all independent galvanomagnetic coefficients in semiconductor melts $Bi_{1-x}Sb_x$ at 77-300K, the kinetic parameters of all types of charge carriers have been defined.

It is established, that new hole ellipsoids in the comparison with hole and electron ones in basis plane are less elliptic, than in binary and bisector planes.

The galvanomagnetic effects are easily measured already at fields of order of oersted parts because of very high mobility of charge carriers in $Bi_{1-x}Sb_x$. That's why in refs [1, 2], dedicated to the investigations of electron properties of these materials, the galvanomagnetic phenomenon were used for the development of the presentations about the character of their energetic spectrum. In the result of set theoretic [3,4] and experiment [5,6,7,8] refs the main characters of reconstruction of band structure of energetic spectrum in $Bi_{1-x}Sb_x$ at x composition change in $x \leq 30$ at.% region had been revealed. In some region $Bi_{1-x}Sb_x$ composition has the semiconductor properties. This region at T=4,2K longs from $x \leq 0.06$ at.% till 0.25 at.%, and at T=77K $0.07 \leq x \leq 0.20$; this region disappears totally at T>180 with temperature growth.

The band structure changes with the composition change so strongly, that melts, the compositions of which differ on 1at.%, it is need to consider as significantly different materials with different parameters, peculiar to them, so as effective mass, relaxation time of impulse and energy, the distribution of charge carriers on energetic data.

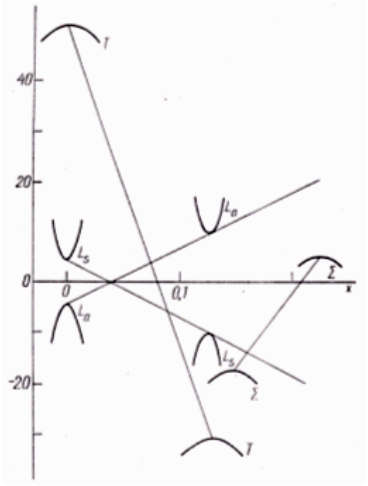

Fig.1. The scheme of reconstruction of energetic spectrum of bismuth-stibium melts at increase of stibium concentration.

From the reconstruction scheme of energetic spectrum of charge carriers of melt $Bi_{1-x}Sb_x$ on stibium [9] concentration of semiconductor melts of $0.15 \leq x \leq 0.22$ composition, presented on the fig.1., it is followed, that minimal energetic chink is defined by La and ∑ terms. However, La deposit of electrons in galvanomagnetic effects is so big in unalloyed melts, that it is difficult to study the structures of valency band. That's why, it is possible to obtain the information about structure of valency band of ∑ Brillouin, situating in formula, picking up the stibium content from the above mentioned interval and concentration of doped acceptor impurity of tin. The different parameters $Bi_{1-x}Sb_x$ were measured on the base of galvanomagnetic measurements at the temperature of liquid nitrogen [10, 11].

The new hole band, the extremum of which is in ∑ point, begins to play at further increase of stibium content.

Thus, in given ref the measurements of all independent galvanomagnetic coefficients at temperatures T=77-300K were carried out for the revealing of actuality of all these bands in transfers phenomenon and establishment of the form of isoenergetic surfaces in $Bi_{1-x}Sb_x$ melts with stibium content higher, than 15 at.%.

It is need to note, that above mentioned coefficients correspond to conditions of weak magnetic field. For the obtaining of such values the dependence of corresponding galvanomagnetic coefficient on the field is always taken. Moreover, the condition of weak magnetic field, i.e. the independence of coefficients R_{ikl} and $\rho_{ik,lm}$ on field, was checked. In many cases, however, the conditions of weak magnetic field are carried out at its tensity of order of one oersted and even, its parts because of very high values of mobility components and that's why it is need to take its value, obtained by extrapolation of the dependence to the zero field for the value of galvanomagnetic coefficient in weak field. The limit of weak magnetic field is different for different coefficients, and its change allows us to follow qualitatively for the change of energetic spectrum of charge carriers.

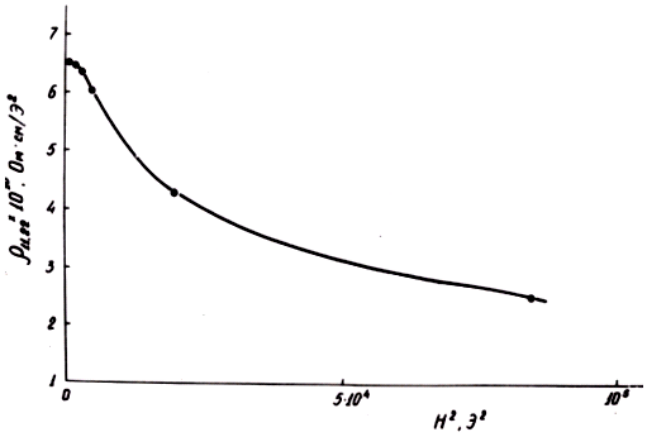

Fig.2. The dependence of magnetoresistance coefficient $\rho_{11,22}$ on H^2 for $Bi_{0,08}Sb_{0,20}$ melt at 77K.

The field dependences of coefficient of магнетосопротивление of $\rho_{11.22}$ on H^2 for $Bi_{0,08}Sb_{0,20}$ melt at 77K are shown on the fig.2.

The temperature dependencies of two components of specific resistance of $Bi_{1-x}Sb_x$ melts with different stibium content are shown on the figures 3 and 4.

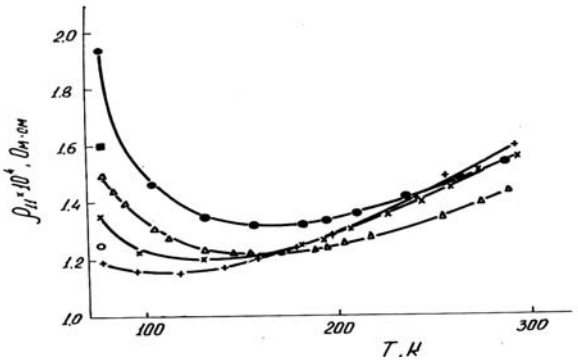

Fig.3. The temperature dependence of specific resistance ρ_{11}:Δ--$Bi_{0.92}Sb_{0..8}$
● $Bi_{0.84}Sb_{0.16}$ ⊕ $Bi_{0.82}Sb_{0.18}$
x -$Bi_{0.80}Sb_{0.20}$ ○ $Bi_{0.78}Sb_{0.22}$
\+ -$Bi_{0.75}Sb_{0.25}$.

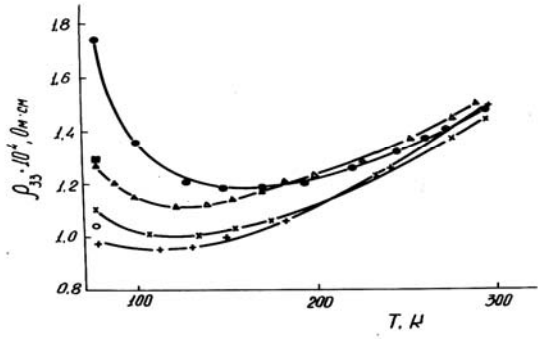

Fig.4. The temperature dependence of specific resistance . ρ_{33}: Δ--$Bi_{0.92}Sb_{0.08}$
● $Bi_{0.84}Sb_{0.16}$ $Bi_{0.82}Sb_{0.18}$
x -$Bi_{0.80}Sb_{0.20}$ ○ $Bi_{0.78}Sb_{0.22}$
\+ -$Bi_{0.75}Sb_{0.25}$

It is need to note, we can't judge about the value of width of forbidden band in $Bi_{1-x}Sb_x$ melts on the dependencies by type $ln\sigma \sim f(1/T)$, i.e. not only the width itself changes with temperature, but the participation in transfer of different actual extremums.

The temperature dependencies of components of Hall coefficient R_{231} and R_{123} for melts with 0,16%at are presented on the following figures 5 and 6.

As it is seen from the figures, both components of Hall coefficient for $Bi_{1-x}Sb_x$ melts of all investigated compositions significantly decrease with temperature. Such decrease evidences about concentration growth of current carriers. However, the conductivity of $Bi_{1-x}Sb_x$ melts in investigated temperature interval and changes of Hall coefficient can be connected with the change of ratio of mobility of electrons and holes. That's why the temperature change of components of Hall coefficients can't be quantitatively characterize the concentration change of charge carriers without calculations according to model of energetic spectrum. The carried out calculations will be in the next.

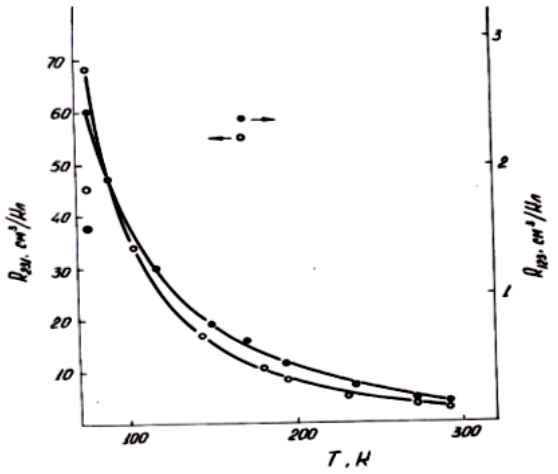

Fig.5. The temperature dependence of Hall R_{ijk} coefficients for $Bi_{0.84}Sb_{0.16}$ melt (separate points R_{ijk} at 77K for melt $Bi_{0.82}Sb_{0.18}$).

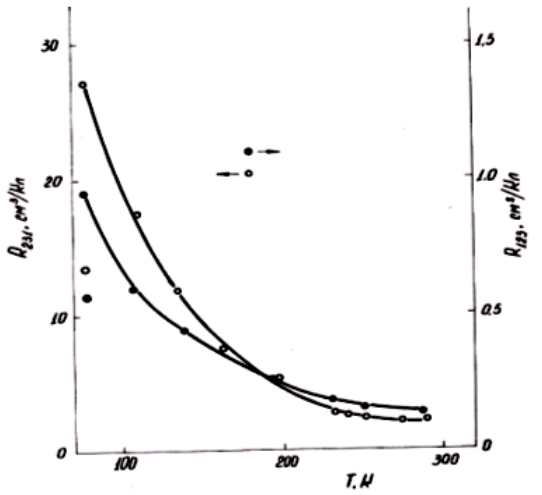

Fig.6. The temperature dependence of Hall R_{ijk} coefficients for $Bi_{0.80}Sb_{0.20}$ melt (separate points R_{ijk} at 77K for melt $Bi_{0.78}Sb_{0.22}$).

The temperature change of magnetoresistance $\rho_{11,22}$, $\rho_{11,33}$, $\rho_{11,11}$ and $\rho_{33,11}$ and $\rho_{33,33}$ for $Bi_{1-x}Sb_x$ melts with different stibium content are shown on the following figures 7,8,9.

The change character of all components of magnetoresistance with temperature stays constant.

It should be evidenced qualitatively about the saving of relations of mobility of electrons and holes. Indeed, the magnetoresistance is depended as on participation of different types of carriers in transfer phenomenon, so on ratios of components and their motilities in different crystallographic directions at participation of many-valley band structure. At the same time, if we propose, that ratios between components of mobility of separate groups of charge carriers don't change with temperature, the extremums of valency band and conduction band for transfer phenomena stay the same, and also the ratios of mobility of charge carriers don't change, so change dependencies with temperature of all components of magnetoresistance should be strongly similar.

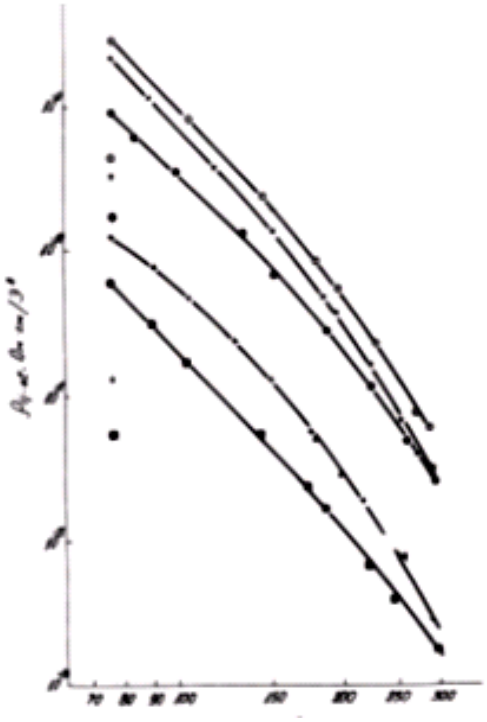

Fig.7. The temperature dependence of magnetoresistance coefficient $\rho_{ij,kl}$ of $Bi_{0.84}Sb_{0.16}$ melt (separate points $\rho_{ij,kl}$ at 77K for $Bi_{0.78}Sb_{0.22}$ melt) o- $\rho_{11.22}$, x -$\rho_{11.11}$, ●-$\rho_{33.11}$, + - $\rho_{11..33}$ ⊕ - $\rho_{33.33}$.

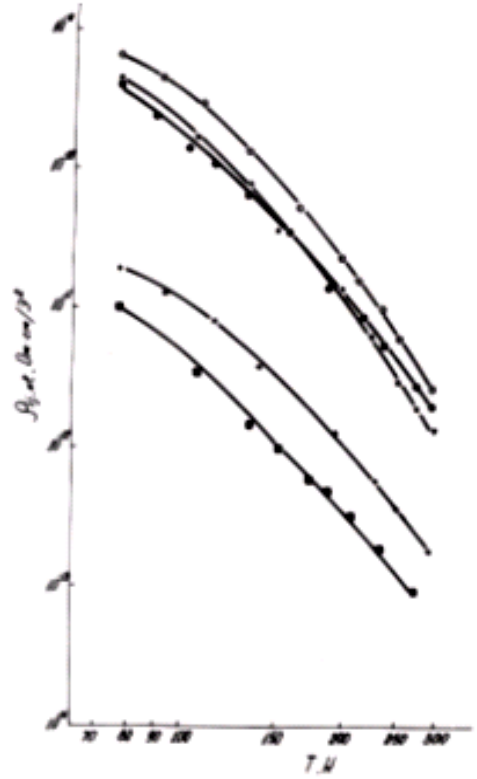

Fig.8. The temperature dependence of magnetoresistance coefficient $\rho_{ij,kl}$ of $Bi_{0.80}Sb_{0.20}$ melt, o - $\rho_{11.22}$, x -$\rho_{11.11}$, ●-$\rho_{33.11}$, +- $\rho_{11..33}$, ⊕ - $\rho_{33.33}$.

The components of Hall coefficients will be changed analogically to this. This gives the foundation on qualitative conclusion about weak change of all mentioned parameters in semiconductor melts $Bi_{1-x}Sb_x$ in interval 77-300K. The more detail data have been obtained on the base of quantitative calculations, which will be given further.

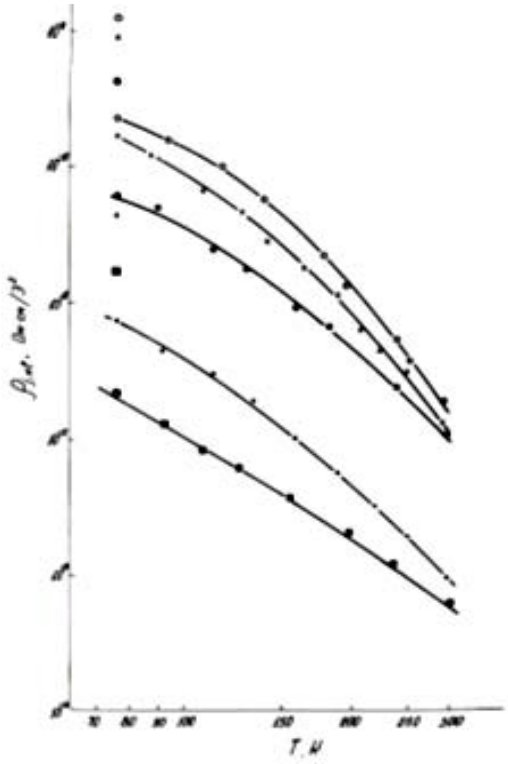

Fig.9. The temperature dependence of magnetoresistance coefficient $\rho_{ij,kl}$ of $Bi_{0.75}Sb_{0.25}$ melt (separate points $\rho_{ij,kl}$ at 77K for $Bi_{0.82}Sb_{0.18}$ melt) o- $\rho_{11.22}$, x -$\rho_{11.11}$, ●-$\rho_{33.11}$, + - $\rho_{11..33}$, ⊕ - $\rho_{33.33}$.

The ratios between components of tensors of galvanomagnetic coefficients of electron and hole mobilities, and also their concentrations, defined by model of energetic spectrum [12] were used for the quantitative interpretation of experimental results of galvanomagnetic properties $Bi_{1-x}Sb_x$ above mentioned. Such interpretation allows from the one side in the agreement of experimental and calculated values to judge about rightness of choice of energetic spectrum model and from another one to judge about change character of spectrum parameter, i.e. the component of tensor mobility is characterized by corresponding components of tensor effective mass with taking under consideration anisotropy of relaxation time or supposition of its anisotropy. From the above mentioned it is followed, that the model, presenting Fermi surface of electrons in three ellipsoids of common type, easily inclined relatively trigonal axis and transferring into each other at the turn on 120°C round this axis and situating in L in 3B point, was accepted by us for the interpretation of galvanomagnetic properties of $Bi_{1-x}Sb_x$ ($0.15 \le x \le 0.25$) melts. The Fermi surface of holes is presented by three or six ellipsoids of common type, inclined relatively trigonal axis and situated in ∑ and H 3B points.

Thus, for the actual phenomena of the phenomenon of transfer of carriers of all these bands and establishment of form of isoenergetic melt $Bi_{1-x}Sb_x$ (x=0,14-0,25)surface, measurements of all independent coefficients at temperatures T=77-300K were carried out.

The values of experimental and calculated values of galvanomagnetic coefficients for $Bi_{1-x}Sb_x$ melts with stibium content 0.16÷0.25 at.% at temperature 77K are given in table 1. As it is seen from the table, for all melt compositions the experimental and calculated values are in good state. The calculation was in such set of components of mobilites and concentrations, which supplied the best agreement of experimental and calculated values (table 2). As it is seen from the table 2 in the ration of hole components ∑ is equal to ν_2/ν_1=0,05, ν_3/ν_1=0,5 in all investigated melt compositions $Bi_{1-x}Sb_x$ (x=0.16, 0.25).

It is need to note, that analogical calculations were carried out in the refs [14,15].

In the ref [16] on the base of investigations of dispersion of electromagnetic magnetoplasma waves and galvanomagnetic effects it is established, that for L-electrons the ratios of mobility components is μ_2/μ_1=0,0001, μ_3/μ_1=0,7 and for L-holes one is ν_2/ν_1=0,009, ν_3/ν_1=0,7.

Table 1

The values of experimentally obtained and calculated galvanomagnetic coefficients in melts $Bi_{1-x}Sb_x$ at T=77K (ρ_{11}, ρ_{33} were measured with delicacy 3%, ρ_{123}, ρ_{231}-5%, $\rho_{11,22}$-10%, $\rho_{11,11}$ and $\rho_{33,11}$-15%, $\rho_{11,33}$ and $\rho_{33,33}$-20%; dimension is $\alpha_{ij.kl}$ –$\Omega^{-1}\cdot cm^{-1}$).

At,% Sb		σ_{11} 10^{-3}	σ_{33} 10^{-3}	σ_{231} 10^{-9}	σ_{123} 10^{-8}	
016	exp.	5,15	5,70	200	0,68	
	calc.	4,87	6,10	2,06	0,60	
018	exp.	6,25	7,80	2,20	0,58	
	calc.	6,03	7,70	2,26	0,59	
020	exp.	7,40	9,10	1,82	0,53	
	calc.	7,10	8,90	1,90	0,53	
022	exp.	7,94	9,60	1,28	0,34	
	calc.	7,53	9,38	1,38	0,31	
025	exp.	8,10	10,20	0,69	0,21	
	calc	7,27	9,10	0,86	0,19	
at,% Sb		$\sigma_{11,33}$ 10^{-12}	$\sigma_{33,11}$ 10^{-14}	$\sigma_{11,11}$ 10^{-14}	$\sigma_{11,22}$ 10^{-14}	$\sigma_{33,33}$ 10^{-12}
016	exp.	34,00	10,70	5,84	14,20	19,30
	calc.	39,00	14,30	5,10	15,6	20,00
018	exp.	17,50	10,30	3,55	11,1	10,50
	calc.	23,81	11,90	4,21	12,8	12,00
020	exp.	11,00	7,50	2,62	7,85	8,00
	calc.	23,17	7,20	2,60	7,85	7,00
022	exp.	8,60	2,90	1,74	4,30	5,72
	calc.	10,60	3,50	1,26	3,83	7,23
025	exp.	5,30	1,16	1,01	1,97	2,23
	calc	4,35	1,47	0,53	1,60	2,98

Table 2

The kinetic parameters of charge carriers for $Bi_{1-x}Sb_x$ melts at T=77K.

At.% Sb	016	018	020	022	025
φ_{oe}	5^0	$4^040'$	$4^010'$	$4^06'$	$4^06'$
φ_g	16^0	16^0	16^0	16^0	16^0
μ_1	9.00	7.15	5.20	3.44	2.32
(5)	(5)	(5)	(5)	(5)	
μ_2	8.10	6.43	6.48	3.09	2.09
(3)	(3)	(3)	(3)	(3)	
μ_3	6.30	5.00	3.64	2.41	1.62
(5)	(5)	(5)	(5)	(5)	
ν_1	3.00	1.80	1.3	9.10	5.80
(5)	(5)	(5)	(4)	(4)	
ν_2	1.50	0.9	0.65	4.55	2.90
(4)	(4)	(4)	(3)	(3)	
ν_3	1.50	0.9	0.65	4.55	2.90
(5)	(5)	(5)	(4)	(4)	
ν					
ν_2					
ν_3					
$N_э$	4,95	8,21	1,33	2,10	3,04
(16)	(16)	(17)	(17)	(17)	
N_g	4,95	8,21	1,33	2,10	3,04
(16)	(16)	(17)	(17)	(17)	

where N_e, N_g are concentrations of charge carriers measured in cm^{-3}.

μ_i and ν_i are tensor components of electron and hole mobilities correspondingly, measured in $cm^{-2}V^{-1}s^{-1}$.

We can make the following conclusions on obtained results:

1. The possibility of quantitative interpretation of galvanomagnetic effects in $Bi_{1-x}Sb_x$ ($0{,}16 \le x \le 0{,}25$) melts on base of model of Fermi electrons in the form of three ellipsoids of common type and holes, in form of three ellipsoids, situating in $\sum$ in 3B point is shown.

2. It is established, that new hole ellipsoids in the comparison with easy hole and electron ellipsoids are less elliptic ones in basis plane, than in binary and bisector planes.

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YARIMKEÇİRİCİ $Bi_{1-x}Sb_x$ BƏRK MƏHLULARININ VALENT ZONASININ QURULUŞU HAQQINDA

Yarımkeçirici $Bi_{1-x}Sb_x$ məhlularının T=77-300K temperatur intervalında qeyri-asılı qalvanomaqnit əmsallarının tətqiqi əsasında bütün növ yükdaşıyıcıların kinetik parametrləri təyin edilmişdir.

Müəyyənləşdirilmişdir ki, yeni deşik ellipsoidləri yüngül deşik və elektron ellipsoidləri ilə müqayisədə bazis müstəvisində binar və bissektris müstəvilərinə nisbətən daha kiçik elliptikliyə malikdir.

Б.А.Таиров, А.Г.Рагимов, С.З. Дамирова

О СТРУКТУРЕ ВАЛЕНТНОЙ ЗОНЫ В ПОЛУПРОВОДНИКОВЫХ СПЛАВАХ $Bi_{1-x}Sb_x$

На основе исследований всех независимых гальваномагнитных коэффициентов в полупроводниковых сплавах $Bi_{1-x}Sb_x$ при 77-300К определены кинетические параметры всех сортов носителей заряда.

Установлено, что новые дырочные эллипсоиды по сравнению с легкими дырочными и электронными эллипсоидами в базисной плоскости менее эллиптичны, чем в бинарных и биссектрисных плоскостях.

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