THE CONDUCTION MECHANISMS IN n-ZrNiSn INTERMETALLIC SEMICONDUCTOR HEAVILY DOPED WITH A Cu DONOR IMPURITY

V.A. ROMAKA[1,2], M.G. SHELYAPINA[3], D. FRUSHART[4], YU.K. GORELENKO[5], YU.V. STADNYK[5], L.P. ROMAKA[5], V.F. CHEKURIN[1], A.M. HORIN[5]

[1]**Ya. Pidstryhach Institute of Applied Problems of Mechanics and Mathematics, Nat. Acad. Sci. of Ukraine**
(3b, Naukova Str., Lviv 79060, Ukraine),

[2]**National University "Lvivs'ka Politekhnika"**
(12, Bandera Str., Lviv 79013, Ukraine; e-mail: vromaka@polynet.lviv.ua),

[3]**V.A. Fock Institute of Physics of the St.-Petersburg National University**
(1, Ul'yanovskaya Str., Petrodvorets, St.-Petersburg 198504, Russia;
e-mail: marinashelyapinna@mail.ru),

[4]**Laboratoire de Cristallographie, CNRS**
(BP 166, Grenoble 38042, Cedex 9, France; e-mail: daniel.fruchart@grenoble.cnrs.fr),

[5]**Ivan Franko Lviv National University**
(6, Kyryl and Mefodii Str., Lviv 79005, Ukraine; e-mail: gorelenko_ yuriy@franko.lviv.ua)

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The calculations of the electronic structure for intermetallic semiconductor ZrNiSn heavily doped with donor impurities through a Cu substitution for Ni are performed. The conduction mechanisms for n-ZrNiSn with various concentrations of donor impurities are analyzed within the temperature region 80 — 380 K. The insulator-metal conduction transition (the Anderson-type transition), which is caused by a shift of the Fermi level from the impurity donor band to the conduction band upon an increase in the donor impurity concentration and was predicted by model calculations, is revealed in the $ZrNi_{1-x}Cu_xSn$ solid solution. The dependence of a thermoelectric power coefficient Z^* on the concentration of Cu donor impurities is specified for n-ZrNiSn in the temperature region 80 — 380 K.

1. Introduction

The calculations of the electronic structure as well as the experimental studies of the structural, kinetic, and magnetic characteristics of narrow-band intermetallic semiconductors n-ZrNiSn and n-TiNiSn upon their doping with the acceptor impurities of high concentrations ($N_A \sim 10^{18} \div 10^{21}$ cm^{-3}) through a substitution of Zr (Ti) ($4d^25s^2$) atoms by Sc ($3d^14s^2$) ones, or Ni ($3d^84s^2$) atoms by Co ($3d^74s^2$) ones, made it possible to (i) specify the electrical conduction mechanisms over wide concentration and temperature intervals, for the first time for the semiconductors of a given type, (ii) determine the role of acceptor bands in the conductivity of such semiconductors, (iii) suggest the models describing the rearrangement of acceptor bands, and (iv) observe the insulator-metal transition (the Anderson-type transition) predicted by calculations [1—5].

The topicality of the studies of intermetallic semiconductors of the MgAgAs structural type is associated with the peculiarities of their thermoelectric properties which have turned these semiconductors into the mostly studied and promising thermoelectric materials [6—11]. It is worth noting in this respect that, basing on the conductivity mechanisms suggested in [1—5, 11], the conditions for the appearance and thermal stability of a maximum of a thermoelectric power coefficient Z^* ($Z^* = \alpha^2\sigma$, where α is a thermoelectric coefficient and σ — specific conductivity) were determined in work [12] for the first time for ZrNiSn and TiCoSb intermetallic semiconductors.

In the above work, the effect of donor impurities of high concentrations on the changes in the electronic structure, the behavior of electrical resistivity ρ, the thermoelectric coefficient, and the spatial arrangement of atoms within a unit cell were studied for intermetallic semiconductors n-ZrNiSn upon their doping through a substitution of Ni by Cu ($3d^{10}4s^1$). In this case, the concentration of the donor impurities was changed from $N_D = 3.8\times10^{20}$ cm^{-3} ($x = 0.02$) to $N_D = 1.9\times10^{21}$ cm^{-3} ($x = 0.1$).

It is noteworthy that it is in this concentration range of donor impurities that the maximal values

of the thermoelectric power coefficient for such a material were observed [12]. On the other hand, for the semiconductors under study, the high values of donor impurity concentrations make it possible to specify the details of their kinetic characteristics at sufficiently high temperatures [13, 14].

The features of a specimens' fabrication method as well as the details of structural studies, measurements of resistivity and the thermoelectric coefficient (the latter — with respect to copper) over the temperature range 80—380 K are presented in [2].

Let' pay attention to the features of a fabrication technology, which will be of great importance, in our opinion, in discussing the results obtained for these semiconducting materials. As follows from the papers we know, the fabrication technology for the given semiconducting materials consists in a melting of the charge mixture of starting materials with a subsequent non-controlled cooling of the melt. It is noteworthy that, as a rule, such cooling, which is typical of the fabrication procedure for disordered solids [13], gives rise to the enhancement of structural disorder and local deformations in the crystallites of polycrystalline specimens. What is more, the modes of a homogenizing annealing (the annealing temperature, the duration and type of after-annealing cooling — quenching or tempering) also influence a degree of the crystalline structure perfection, and thus, a concentration of point and bulk defects [3]. On the other hand, the introduction of the donor impurities of high concentrations brings about an additional disorder which is caused by the fluctuations in charged impurity concentrations [14]. At the same time, as is shown in [12], it is the high values of impurity/defect concentration that serve as a necessary condition for the achievement of maximal values of Z^* in the intermetallic semiconductors of the MgAgAs structural type. Under these conditions, the conductivity state is realized where a material is no longer a semiconductor, but not yet a metal. It is this limit state by conductivity that is the object of investigations of the present work.

2. Calculations of Electronic Structure

The calculations of the electronic structure for $ZrNi_{1-x}Cu_xSn$ were carried out in the frames of the self-consistent Korringa—Kohn—Rostoker method combined with the coherent potential and local density approximations (KKR-CPA-LDA) [15]. The crystalline potential and electron charge density were chosen spherically symmetric inside a sphere and invariable within an intermediate region (muffin-tin method). In the intermetallic semiconductors of the MgAgAs structural type, only three of four possible atomic positions with the $\bar{4}3m$ symmetry type are filled [4]. To increase the packing density of a Wigner—Seitz cell, we introduced an additional empty sphere around the fourth, unoccupied position. For the non-overlapping spheres, the radii were chosen in such way that the maximal filling of a Wigner—Seitz cell would be achieved. The calculations of the total density of states (DOS) as well as individual partial contributions from various atoms and electronic shells with $l_{\max} = 2$ for all types of atoms were carried out. The procedure of self-consistency was performed until a difference between the potential values reached 10^{-4} Ry.

Fig. 1 shows the results of calculations of the electronic density distribution for each of the components of the $ZrNi_{1-x}Cu_xSn$ solid solution and the total distribution for various x values. As follows from the electronic structure calculations for a parent (undoped) semiconductor ZrNiSn, this material is a narrow-band semiconductor with the Fermi level (E_F) located within a band gap. The results obtained for ZrNiSn agree well with those calculated by the methods of pseudopotential [16], LDA [17], and CPA—LDA [4, 18] and also correlate with a number of experimental data (see, for example, [1—11]).

As is seen from Fig. 1, for $ZrNi_{1-x}Cu_xSn$, the electron density above the Fermi level is mainly determined by the Zr d-states, whereas the valence band is formed by the d-states of Ni or Cu which are overlapped with the d-states of Zr and p-states of Sn. The doping of ZrNiSn with donor impurities leads to a drift of the Fermi level towards the conduction band. As soon as x goes over 0.05, the Fermi level crosses the mobility edge of the conduction band. The further increase in N_D gives rise to the entering of E_F into the band of continuous energy levels and its drift into a depth of the conduction band. The calculations show that an abrupt change of the DOS at the Fermi level, $N(E_F)$, is observed at the concentrations of donor impurities corresponding to the compositions with $x \geq 0.05$. For the smaller x values (i.e. for the smaller concentrations of donor impurities), the DOS at the Fermi level is determined by the d-electrons of Zr with a substantial contribution from the d-states of Cu. At $x > 0.05$, a contribution of the Cu d-electrons becomes decisive. So, $N(E_F) = 1.085$ states/Ry for ZrNiSn, $N(E_F) = 4.87$ states/Ry for $ZrNi_{0.95}Cu_{0.05}Sn$, and $N(E_F) = 7.09$ states/Ry $ZrNi_{0.9}Cu_{0.1}Sn$.

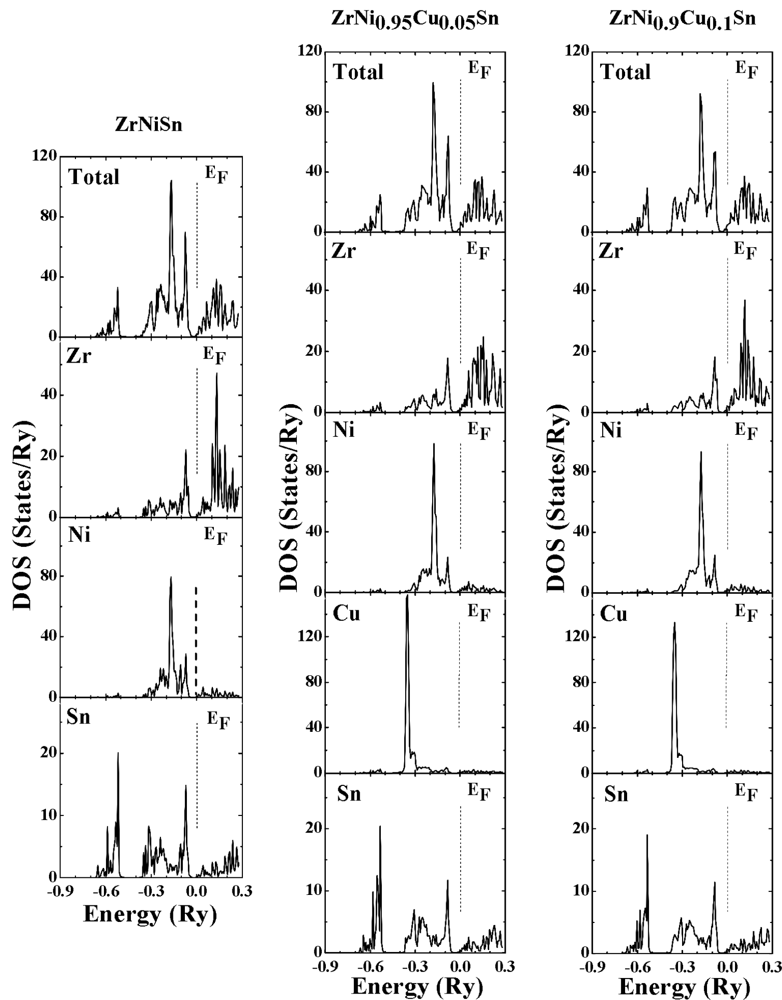

Fig. 1. Partial and total electron DOS for $ZrNi_{1-x}Cu_xSn$

The electronic structure calculations for ZrCuSn compound, which is at the opposite (with respect to ZrNiSn) end of $ZrNi_{1-x}Cu_xSn$ solid solution, show that E_F is located deep in the conduction band which is mainly formed by the states of Cu *d*-electrons [18].

The analysis of the results presented in Fig. 1 shows the following. Since the Fermi level of $ZrNi_{1-x}Cu_xSn$ lies within the band gap for the low-level doping ($x < 0.05$), the material is expected to demonstrate a semiconducting (activated) conductivity. What is more, it can be predicted that a hopping conductivity inside the donor impurity band (right up to the metallization of conductivity in the impurity band [13]) and the activation of electrons from E_F of the donor impurity band to the conduction band should be observed. For x exceeding 0.05, after the Fermi level crossed the mobility edge of the conduction band and drifts across it upon a growth in the donor impurity concentration (i.e. after the Anderson-type transition occurred [14]), $ZrNi_{1-x}Cu_xSn$ is expected to display the metallic conductivity rather than the activated one. Respectively, the conductivity of ZrCuSn will also have the metallic character.

Thus, it can be predicted that the doping of ZrNiSn with donor impurities by means of the substitution of Cu for Ni brings about a change in the conductivity mechanisms — from activated to metallic.

3. Experimental Results and Their Discussion

The X-ray phase and structure analyses confirmed that all the $ZrNi_{1-x}Cu_xSn$ specimens under investigation are single-phase, and the distribution of atoms in them corresponds to the MgAgAs structural type (space group

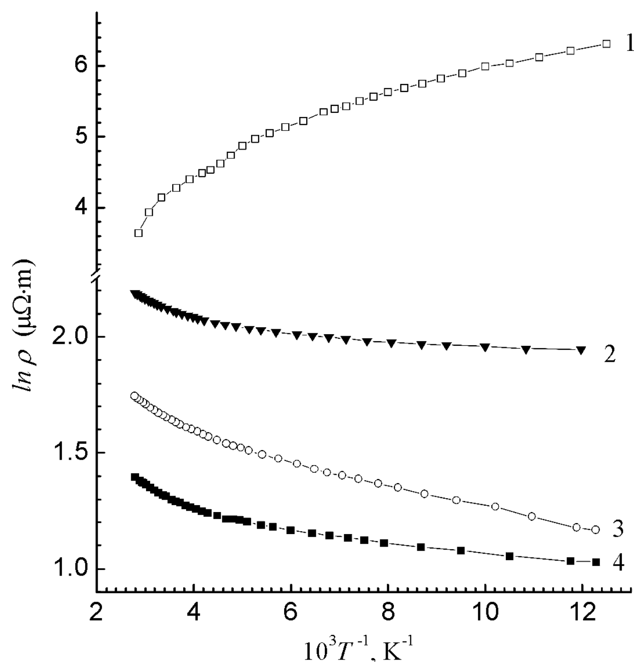

Fig. 2. Temperature dependences of resistivity for $ZrNi_{1-x}Cu_xSn$ with various values of x: *1* — 0; *2*- – 0.02; *3* — 0.05; *4* — 0.1. In these compounds, the values of x govern the contents of donor impurities

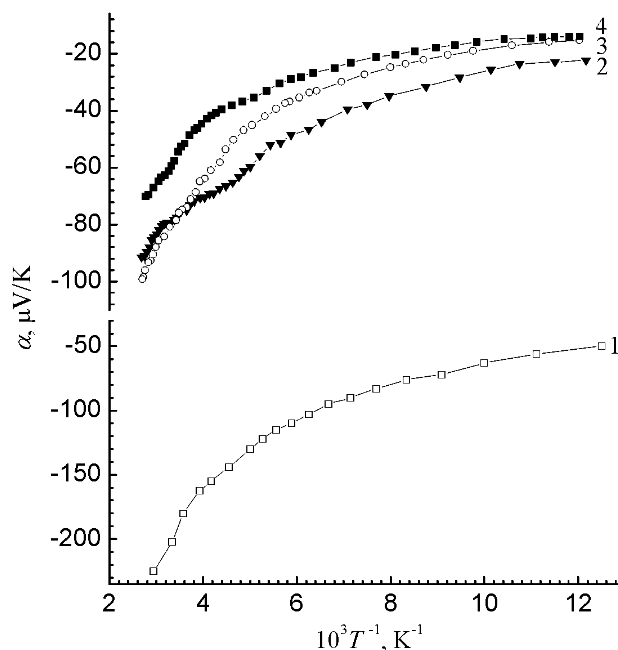

Fig. 3. Temperature dependences of the thermoelectric coefficient for $ZrNi_{1-x}Cu_xSn$ with various values of x. Designations are the same as in Fig. 2

$F\bar{4}3m$): 4Ni in 4(a) 0 0 0 (Ni+Cu); 4Sn in 4(c) 1/4 1/4 1/4; 4Zr in 4(d) 3/4 3/4 3/4.

The undoped n-ZrNiSn specimen displays activated conductivity (Fig. 2). The $\ln \rho$ vs $1/T$ dependence can be divided into three regions which are associated with different conductivity mechanisms: (i) the activation of electrons from E_F to nonlocalized states in the conduction band (a high temperature region, energy of activation ε_1), (ii) the activation of electrons from E_F to the mobility edge of the conduction band (an intermediate temperature region, the energy of activation ε_2), and (iii) a region of hopping conductivity (a low temperature region, the energy of activation ε_3) [13].

The conclusion about the semiconducting character of electrical conductivity in n-ZrNiSn is also confirmed by the temperature dependence of the thermoelectric coefficient (Fig. 3). At will, the α vs $1/T$ curve can also be divided into three different regions of activation. However, the temperature dependence of the thermoelectromotive force as a whole has a complicated ambiguous character. A negative sign, which is characteristic of the whole temperature region, of a thermoelectric coefficient for the undoped n-ZrNiSn semiconductor is the evidence for the presence of uncontrolled donor impurities of high concentrations. It should be noted that, according to the results of the phase and structure analyses, all the specimens are single-phase, i.e. these methods of analysis are incapable of controlling the impurity contents in full measure, although it is the presence of impurities that have a decisive influence on the kinetic properties of a semiconductor.

From the high temperature regions of the $\ln \rho(1/T)$ and $\alpha(1/T)$ dependences, the values of activation energies, ε_1^σ and ε_1^α, respectively, were determined for n-ZrNiSn. These quantities should give the value of an energy barrier between the conduction band bottom and a position of the Fermi level which is fixed by the Coulomb gap of the donor impurity band. The calculations give $\varepsilon_1^\sigma \approx 28.9$ meV and $\varepsilon_1^\alpha \approx 44.6$ meV. The result we obtained is non-trivial for classic semiconductors, where the energy of current carrier activation from the Fermi level of an impurity band to the band of continuous energy levels is invariable and independent of a method of its determination. Thus, two possibilities should be considered: either in the case of delocalized states and high temperatures, the behavior of $\alpha(1/T)$ is not determined in full measure by the

motion of electrons at the Fermi level and is described as

$$\alpha = k/e[(E_c - E_{\mathrm{F}})/k_{\mathrm{B}}T + 1],$$

and thus the determination of the activation energy ε_1 from this relation is not correct, or the obtained result is true and reflects the more complicated processes in a heavily doped semiconductor.

It is known that, in partially disordered semiconductors, there can be two reasons for the difference of the activation energies obtained from the temperature dependences of electrical conductivity and the thermoelectric coefficient. In the region of a hopping conductivity, the activation energies for ρ and α differ by a quantity w representing the energy necessary to perform a hop. Contrary to the case of $\alpha(1/T)$, the activation energy of mobility $w(T)$ contributes to the slope of $\ln\rho(1/T)$ line [13].

Another reason for the existence of a difference between ε_1^σ and ε_1^α lies in fluctuations, whose random fields lead to a change in the Fermi energy within the regions which can become so extensive, that a tunneling can occur [14]. According to [13], the energy difference δE between the maximum and the minimum of potential fluctuations (above we admitted the presence of considerable fluctuations of various nature in the specimens under study) can be estimated as $\varepsilon_1^\sigma - \varepsilon_1^\alpha \approx 1/6\ \delta E$. The obtained value $\delta E \approx 94$ meV, which is close to a half of the energy gap for ZrNiSn [6], is plausible for partially disordered solids. However, the anxiety about the validity of the determination of ε_1^α within a region of high temperatures make us abandon a deepening in this direction.

Besides a change in the carrier concentration, the doping of the n-ZrNiSn semiconductors with donor impurities gives rise also to changes in the impurity band structure, a Coulomb gap position, the electron localization radius, etc. This should lead, in turn, to changes in the activation energies, in particular in the hopping one with the variable hop length, and in the activation from the Fermi level either to the mobility edge of the conduction band or into the conduction band [1—5,11—14]. As shown in Fig. 2, the doping of n-ZrNiSn semiconductor with the donor impurities with the concentrations corresponding to $ZrNi_{1-x}Cu_xSn$ compositions with $x \geq 0.02$ results in the disappearance of the regions of activation on the $\ln\rho$ vs $1/T$ dependences. Over this concentrational region, the semiconductors acquire the typical features of metallic conductivity. On the other hand, for all the $ZrNi_{1-x}Cu_xSn$ specimens under investigation, the α vs $1/T$ dependences are similar to one another, have complicated character, and, as was noted above, are not adequately described in full measure by the known relations, especially within a region of high temperatures (in the heavily doped semiconductors, the thermoelectromotive force can change: $\alpha \to \infty$ as $1/T \to 0$, $\alpha \sim (T)^{1/2}$ [13], and the quasilinear behavior is observed [1,2,6,11]). Earlier, we have seen similar regularities in the behavior of $\rho(1/T)$ and $\alpha(1/T)$ dependences in intermetallic semiconductors with high levels of doping (N_D, $N_A \sim 10^{20}$ cm^{-3}), namely upon the doping of p-TiCoSb with the Ni donor impurities, n-ZrNiSn with the Sc acceptor impurities [1,2,11], and also in undoped n-ZrNiSn with the concentration of intrinsic donor impurities $N_D \sim 10^{20}$ cm^{-3} [6].

On the other hand, in the low-temperature region, the determination of the activation energy of a hopping conductivity ε_3 is correct for n-ZrNiSn heavily doped with donor impurities. For undoped n ZrNiSn, the activation energies determined from the low temperature regions of the $\ln\rho(1/T)$ and $\alpha(1/T)$ dependences are $\varepsilon_{3\ 0}^\sigma \approx 1.6$ meV and $\varepsilon_{30}^\alpha \approx 11.5$ meV, respectively. This result seems to be reasonable and offers the possibility to determine the energy value which is necessary for performing a hop between Anderson localized states in undoped n-ZrNiSn: $w(T) \approx 10$ meV.

For $ZrNi_{1-x}Cu_xSn$ with $x \neq 0$, the following values for the activation energy of a hopping conductivity are obtained from the α vs $1/T$ dependences: $\varepsilon_{3\ 0.02}^\alpha \approx 1.5$ meV, $\varepsilon_{3\ 0.05}^\alpha \approx 1.2$ meV, and $\varepsilon_{3\ 0.1}^\alpha \approx 0.6$ meV. Assume that the concentration of uncontrolled acceptors and donors and the conditions of a specimen fabrication are the same for all specimens. Then, in the case of heavily doped semiconductors, an increase in the donor impurity concentration gives rise to an increase in the Fermi energy (proportionally to $n^{2/3}$) as well as to a decrease in a potential relief (δE) due to the electron screening enhancement [13]. Since we actually deal with heavily doped semiconductors, the following relation is valid: $\varepsilon_3 \sim 1/R_D$ (i.e. $N_D^{1/3}$), where R_D is the mean distance between donor impurities [12]. In fact, the values of ε_3^α obtained by us for $ZrNi_{1-x}Cu_xSn$ decrease monotonically from 11.5 to 0.6 meV as x grows from 0 to 0.1. The decrease in ε_3^α is associated with the approach to the Anderson-type transition, at which the hopping conductivity is completely disappear. Although the conductivity has a metallic character for the $ZrNi_{1-x}Cu_xSn$ with the concentrations of donor impurities corresponding to the compositions with $x \geq 0.02$, the α vs $1/T$ dependences contain activated regions. The authors of

[2,11] associate such behavior with the mobility of free electrons which contribute to conductivity, but not to thermoelectromotive force; the $\alpha(T)$ dependence is less sensitive to changes in the semiconductor parameters than the $\rho(T)$ one [6].

The metallic character of conductivity characteristic of n-ZrNiSn doped with the Cu donor impurities testifies to the shift of E_F from the donor impurity band to the conduction band, which agrees with the results of calculations of the electronic structure of $ZrNi_{1-x}Cu_xSn$. In our opinion, this effect is similar to that observed in p-TiCoSb doped with Ni donor impurities [11].

It is known that the Anderson-type transition occurs when the composition of a solid solution is changed in such a way that $\Delta E = E_c - E_F$ changes its sign [13]. Thus, it follows from the results presented above that

a) n-ZrNiSn is a heavily doped semiconductor, whose characteristic features are (i) the activated character of conductivity, (ii) E_F is fixed by the impurity band, and (iii) $E_c - E_F > 0$;

b) the characteristic features of $ZrNi_{1-x}Cu_xSn$, especially for $x > 0.1$, are (i) the conductivity has metallic character and is governed by free electrons, (ii) the Fermi level lies within the conduction band, and (iii) $E_c - E_F < 0$.

Thus, the presented results show that the insulator-metal transition observed in ZrNiSn intermetallic semiconductor upon its doping with Cu donor impurities is the Anderson-type transition. This transition originates from the rearrangement of the impurity band of the heavily doped and compensated semiconductor, which is caused by the shift of E_F from the Coulomb gap of the donor impurity band through the mobility edge of the conduction band (or by the merging of the impurity band with the mobility edge of the conduction band) deep into the conduction band. A coincidence of the main results of theoretical calculations and experimental data is the evidence for the adequacy of the proposed model suggesting a rearrangement of the impurity band upon doping of n-ZrNiSn with Cu donor impurities.

Thermoelectric power coefficient Z^* for $ZrNi_{1-x}Cu_xSn$ as a function of temperature and x (in these compounds, the values of x govern the contents of donor impurities)

T, K	Z^*, μW K^{-2}cm^{-1}			
	$x = 0$	$x = 0.02$	$x = 0.05$	$x = 0.1$
80	0.04	0.70	0.73	0.69
150	0.41	2.62	2.41	2.00
200	1.28	4.65	4.55	3.82
250	3.22	5.96	8.19	5.59
300	6.53	7.55	12.10	9.56
350	13.52	8.50	15.70	12.22

4. Thermoelectric Power Coefficient for $ZrNi_{1-x}Cu_xSn$

It is shown in [12] that the condition for the appearance of maximal thermoelectric power in intermetallic semiconductors of the MgAgAs structural type is the high level of their doping with acceptor and/or donor impurities, so that E_F gets fixed by the mobility edge of one of the bands of continuous energy levels (depending on a type of impurities). What is more, it was shown that the donor impurity band for p-TiCoSb and n-ZrNiSn intermetallic semiconductors crosses the mobility edge of the conduction band at the concentrations of donor impurities corresponding to the compositions with $x \approx 0.03$. As follows from the above results, as well as from the data presented in the table, the conclusions made in [12] are completely fulfilled in the case where ZrNiSn is doped with Cu donor impurities.

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МЕХАНІЗМИ ПРОВІДНОСТІ ІНТЕРМЕТАЛІЧНОГО НАПІВПРОВІДНИКА n-ZrNiSn, СИЛЬНОЛЕГОВАНОГО ДОНОРНОЮ ДОМІШКОЮ Cu

В.А. Ромака, М.Г. Шеляпіна, Д. Фрушарт, Ю.К. Гореленко, Ю.В. Стадник, Л.П. Ромака, В.Ф. Чекурін, А.М. Горинь

Р е з ю м е

Здійснено розрахунок електронної структури інтерметалічного напівпровідника ZrNiSn, сильнолегованого донорними домішками шляхом заміщення атомів Ni на Cu. Проаналізовано механізми електропровідності n-ZrNiSn при різних концентрація донорних домішок у температурному інтервалі 80 — 380 K. Експериментально виявлено передбачений розрахунками перехід провідності діелектрик—метал в $ZrNi_{1-x}Cu_xSn$ (перехід Андерсона), зумовлений переходом рівня Фермі з домішкової донорної зони в зону провідності при збільшенні концентрації донорних домішок. Визначено залежність коефіцієнта термоелектричної потужності Z^* n-ZrNiSn від концентрації донорних домішок Cu в інтервалі температур 80—380 K