MEASURING TRANSDUCERS

STUDY OF THERMOMETRIC MATERIAL Er$_{1-x}$Sc$_x$NiSb.
II. EXPERIMENTAL RESULTS

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Abstract. The results of a comprehensive study of the crystal and electronic structures, kinetic and energetic performances of the semiconductor thermometric material Er$_{1-x}$Sc$_x$NiSb, (x=0–0.1) are presented. Microprobe analysis of the concentration of atoms on the surface of Er$_{1-x}$Sc$_x$NiSb samples established their correspondence to the initial compositions of the charge, and the diffractograms of the samples are indexed in the structural type of MgAgAs. Because the atomic radius Sc (r_{Sc}=0.164 nm) is smaller than that of Er (r_{Er}=0.176 nm), it is logical to reduce the values of the unit cell's period $a(x)$ Er$_{1-x}$Sc$_x$NiSb, which correlate with the results of mathematical modeling.

The temperature dependences of the resistivity ln($\rho(1/T)$) contain high- and low-temperature activation regions, which are specific for semiconductors and indicate the location of the Fermi level ε_F in the bandgap, and positive values of the thermopower coefficient $\alpha(x, T)$ specify its position – near the valence band ε_V. This result does not agree with the results of modeling the electronic structure for its ordered version.

The presence of a low-temperature activation region on the ln($\rho(1/T)$) p-ErNiSb dependence with an activation energy ε_3^ρ=0.4 meV indicates the compensation of the sample provided by acceptors and donors of unknown origin. A decrease in the values of the resistivity $\rho(x, T)$ and the thermopower coefficient $\alpha(x, T)$ points to an increase in the concentration of holes in p-Er$_{1-x}$Sc$_x$NiSb in the area of concentrations x=0–0.03. This is possible in a p-type semiconductor only by increasing the concentration of the main current carriers, which are holes. The fact of increasing the concentration of acceptors in Er$_{1-x}$Sc$_x$NiSb at insignificant concentrations of impurity atoms is also indicated by the nature of the change in the values of the activation energy of holes ε_1^ρ from the Fermi level ε_F to the valence band ε_V. Consequently, if in p-ErNiSb the Fermi level ε_F was at a distance of 45.4 meV from the level of the valence band ε_V, then at the concentration Er$_{1-x}$Sc$_x$NiSb, x=0.01, the Fermi level ε_F shifted towards valence band ε_V and was located at a distance of 13.6. Since the Fermi level ε_F reflects the ratio of ionized acceptors and donors in the semiconductor, its movement by x=0.01 to the valence band ε_V is possible either with an increase in the number of acceptors or a rapid decrease in the concentration of ionized donors. At even higher concentrations of Sc impurity in p-Er$_{1-x}$Sc$_x$NiSb, x≥0.03, low-temperature activation sites appear on the ln($\rho(1/T)$) dependences, which is a sign of compensation and evidence of the simultaneous generation of acceptor and donor structural defects in the crystal nature. This is also indicated by the change in the position of the Fermi level ε_F in the bandgap of the semiconductor Er$_{1-x}$Sc$_x$NiSb, which is almost linearly removed from the level of the valence band ε_V: ε_1^ρ(x=0.05)=58.6 meV and ε_1^ρ(x=0.10)=88.1 meV. Such a movement of the Fermi level ε_F during doping of a p-type semiconductor is possible only if donors of unknown origin are generated. For a p-type semiconductor, this is possible only if the concentration of the main current carriers, which are free holes, is reduced, and donors are generated that compensate for the acceptor states. This conclusion is also confirmed by the behavior of the thermopower coefficient $\alpha(x, T)$ at concentrations x≥0.03.

The results of structural, kinetic, and energy studies of the thermometric material Er$_{1-x}$Sc$_x$NiSb allow us to speak about a complex mechanism of simultaneous generation of structural defects of acceptor and donor nature. However, the obtained array of experimental information does not allow us to unambiguously prove the existence of a mechanism for generating donors and acceptors. The research article offers a solution to this problem. Having the experimental results of the drift rate of the Fermi level ε_F as the activation energy $\varepsilon_1^\rho(x)$ from the Fermi level to the valence band ε_V by calculating the distribution of the density of electronic states (DOS) sought the degree of compensation, which sets the direction and velocity of the Fermi level ε_F as close as possible to the experimental results. DOS calculations are performed for all variants of the location of atoms in the nodes of the unit cell, and the degree of occupancy of all positions by their own and/or foreign atoms. It turned out that for ErNiSb the most acceptable option is one that assumes the presence of vacancies in positions 4a and 4c of the Er and Ni atoms, respectively. Moreover, the number of vacancies in the position Er (4a) is twice less than the number of vacancies in the position Ni (4c). This proportion is maintained for Er$_{1-x}$Sc$_x$NiSb.

Vacancies in the positions of Er (4a) and Ni (4c) atoms Er$_{1-x}$Sc$_x$NiSb are structural defects of acceptor nature, which generate two acceptor zones ε_A^{Er} and ε_A^{Ni} in the semiconductor. The introduction of impurity Sc atoms into the ErNiSb structure by substituting Er atoms in position 4a is also accompanied by the occupation of vacancies by Sc atoms and a reduction in their number. Occupying a vacancy, the Sc atom participates in the formation of the valence band and the conduction band of the semiconductor Er$_{1-x}$Sc$_x$NiSb, acting as a source of free electrons. We can also assume that the introduction of Sc atoms into the structure of the compound ErNiSb is accompanied by a process of ordering the structure of Er$_{1-x}$Sc$_x$NiSb and Ni atoms occupy vacancies in position 4c. This process also, however, 2 times slower, leads to a decrease in the concentration of structural defects of acceptor nature. In this case, Ni, giving valence electrons, now act as donors.

Key words: Electric conductivity, Thermopower coefficient, Fermi level.

1. Introduction

Modeling of structural, thermodynamic, energetic, and kinetic performances of the thermosensitive material $Er_{1-x}Sc_xNiSb$ for the case of ordered crystal structure allowed to establish [1] that structural defects of neutral nature are generated in the semiconductor, the concentration of which increases with increasing Sc atom content. The results of modeling the behavior of the Fermi level ε_F showed that it lies near the level of the conduction band and slightly change s its location. The obtained result does not agree with the experimental studies of the basic p-ScNiSb semiconductor [2], the authors of which established the hole type of its conductivity. According to the authors [2], vacancies in the Ni ($4c$) position are responsible for the hole type of ScNiSb conductivity, which generate structural defects of acceptor nature in the semiconductor.

The research article presents the results of experimental studies of structural, kinetic, and energetic thermometric material $Er_{1-x}Sc_xNiSb$ obtained by doping the basic semiconductor ErNiSb with Sc atoms by replacing Er atoms ($4a$). The obtained results allowed us to clarify the spatial arrangement of atoms in the nodes of the unit cell $Er_{1-x}Sc_xNiSb$, as well as to identify the mechanisms of electrical conductivity to determine the conditions for the synthesis of thermosensitive materials with maximum efficiency of thermal energy conversion into electricity. The investigated $Er_{1-x}Sc_xNiSb$ solid solution is a promising thermometric material but requires detailed experimental studies, which is supposed to be the subject of our next work.

2. Disadvantages

Studies of thermometric materials based on the basic semiconductor RNiSb have established their high sensitivity to heat treatment regimes (temperature and duration of annealing).

3. Research objective

To establish the mechanism of formation of structural defects in the thermometric material $Er_{1-x}Sc_xNiSb$, which let to identify the mechanisms of electrical conductivity and determine the conditions of their synthesis to obtain maximum efficiency of conversion of thermal energy into electricity.

4. Research methods

The synthesis of thermometric materials $Er_{1-x}Sc_xNiSb$, x=0–0.10, was performed by fusing the charge of the initial components in an electric arc furnace in an inert atmosphere. Heat treatment of alloys consisted of homogenizing annealing at 1070 K in vacuum quartz ampoules for a month. After annealing, the alloys were quenched in cold water without breaking the ampoule.

Diffraction arrays obtained on a DRON-4.0 diffractometer (Fe$K\alpha$ radiation) were used for X-ray phase analysis of the synthesized alloys and calculation of structural parameters. The distribution of components, chemical, and phase compositions of the samples was monitored by energy-dispersive X-ray spectral analysis (EDRS, scanning electron microscopes REMMA-102-02, Tescan Vega 3 LMU, used K- and L-spectral lines).

Modeling of the crystallographic characteristics of the thermometric material $Er_{1-x}Sc_xNiSb$ was performed using the program Fullprof Suite [3]. Modeling of the electronic structure of $Er_{1-x}Sc_xNiSb$ was performed by Coring-Kon-Rostocker (KKR) methods in the approximation of coherent potential (CPA) and local density (LDA) [4] using the exchange-correlation potential of Moruzzi-Janak-Williams [5] and LMTO Line Muffin-Tin Orbital) in the framework of the theory of DFT density functional. The Brillouin zone was divided into 1000 k-points, which were used to model energy characteristics by calculating DOS. The width of the energy window was 22 eV and was chosen to capture all semi-core states of p-elements. Full potential (FP) was used in the representation of the linear MT orbital in the representation of plane waves. The LDA approximation with MJW parameterization was also used as the exchange-correlation potential. The accuracy of calculating the position of the Fermi level $\varepsilon F \pm 6$ meV.

Temperature and concentration dependences of resistivity (ρ) and the thermopower coefficient (α) relative to copper of $Er_{1-x}Sc_xNiSb$ samples were measured in the ranges: T=80–400 K, x=0–0.10.

5. Structural studies of the thermometric material $Er_{1-x}Sc_xNiSb$

Microprobe analysis of the concentration of atoms on the surface of samples of semiconductor thermometric material $Er_{1-x}Sc_xNiSb$ established their correspondence to the initial compositions of the charge, and diffraction patterns of samples including the composition x=0–0.10 are indexed in the structural type MgAgAs [1] and do not contain traces(Fig. 1b). Because the atomic radius (r_{Sc}=0.164 nm) is smaller than that of Er (r_{Er}=0.176 nm),), it is logical to reduce the values of the period of the unit cell $a(x)$ $Er_{1-x}Sc_xNiSb$ (Fig. 1b). At concentrations, x>0.03, the angle of inclination of the dependence a (x) changes only slightly. This behavior of $a(x)$ $Er_{1-x}Sc_xNiSb$ is *one* of the arguments for obtaining a thermometric material in the form of a solid substitution solution when the Sc atoms occupy the crystallographic position $4a$ of the Er atoms. The experimental result of changing the values of the period of the unit cell $a(x)$ $Er_{1-x}Sc_xNiSb$ correlates with the results of mathematical modeling [1], and the calculated and experimentally obtained dependences of the period of the unit cell $a(x)$ are almost parallel (Fig. 1b), which confirms the correctness of the tool's modeling.
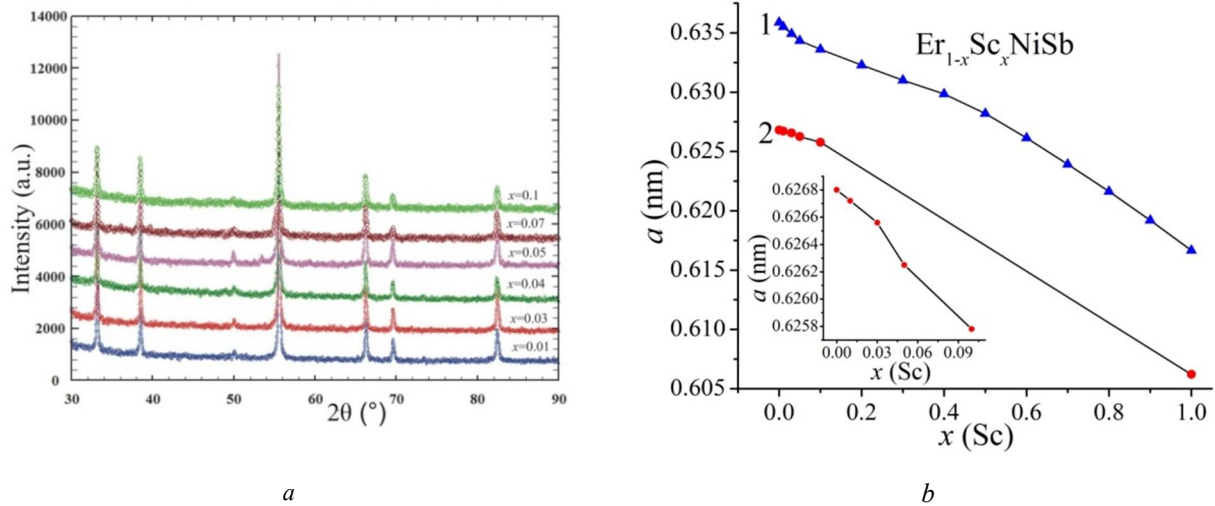
Fig. 1. Diffractograms of samples (a) and change of values of the period of the unit cell a (x) (b) Er$_{1-x}$Sc$_x$NiSb,
x=0–1.0: 1 – calculation [1], 2 - experimental results. Insert: change a(x) at concentrations x=0–0.10

The refinement of the crystal structure of the Er$_{1-x}$Sc$_x$NiSb thermometric material by the powder method with the simultaneous refinement of the isotropic parameters of atomic substitution and the occupancy of the crystallographic position 4*a* due to the low concentration of impurity Sc atoms did not reveal a structural disorder in which Sc atoms ∼ 24% of the volume of the unit cell. For this reason, in [1] to model the behavior of the Fermi level   , the bandgap   and the kinetic characteristics of Er$_{1-x}$Sc$_x$NiSb, have been calculated the distribution of the density of electronic states (DOS) for the case of an ordered variant of the structure.

The following results of experimental measurements of electrokinetic and energy characteristics of the thermometric material Er$_{1-x}$Sc$_x$NiSb show the correspondence of the simulation results to real processes in a semiconductor [1].

6. Investigation of electrokinetic and energetic performances of thermometric material Er$_{1-x}$Sc$_x$NiSb

Temperature and concentration dependences of resistivity ρ and Thermo-EMF coefficient α Er$_{1-x}$Sc$_x$NiSb are shown in Fig. 2 and 3. As we can see from Fig. 2*a*, for Er$_{1-x}$Sc$_x$NiSb samples, the dependences $\ln(\rho(1/T))$ contain high- and low-temperature activation regions that are characteristic of semiconductors and are approximated by the known relation (1):

$$ \qquad \qquad , \quad (1) $$

where the first high-temperature term describes the activation of current carriers   from the Fermi level   to the level of continuous energy bands, and the second, low-temperature term, the hopping conductivity   over impurity states with energies close to the Fermi level   .

In turn, the temperature dependences of the thermopower coefficient $\alpha(1/T)$ Er$_{1-x}$Sc$_x$NiSb (Fig. 2*b*) are described by the known expression (2):

$$ \qquad \qquad (2) $$

where γ is a parameter that depends on the nature of the scattering mechanisms. From the high-temperature region of the dependence $\alpha(1/T)$, the values of the activation energy   , are calculated, which are proportional to the amplitude of large-scale fluctuations of the zones of continuous energies of the strongly doped and compensated semiconductor.

The nature of the change in the values of resistivity $\ln(\rho(1/T))$ at high temperatures for all investigated samples Er$_{1-x}$Sc$_x$NiSb (the presence of high-temperature activation sites) (Fig. 2*a*) indicates the location of the Fermi level   in the bandgap of the semiconductor, and positive coefficient values thermopower coefficient $\alpha(x, T)$ (Figs. 2b and 3b) specify its position - near the level of the valence band   . The positive values of the thermopower coefficient $\alpha(x, T)$ for all Sc concentrations do not agree with the results of modeling the electronic structure of Er$_{1-x}$Sc$_x$NiSb for its ordered variant [1]. Consequently, in a real ErNiSb semiconductor, the main carriers of electricity are free holes of unknown nature.

The presence of a low-temperature activation region on the $\ln(\rho(1/T))$ *p*-ErNiSb dependence with an activation energy   =0.4 meV indicates the compensation of the sample provided by acceptors and donors of unknown origin. However, in the samples Er$_{1-x}$Sc$_x$NiSb, *x*=0.01 and *x*=0.03, there are no such activation sites, which indicates an increase in the concentration of acceptors when the radii of localization of holes (wave functions) intersect and there is metallization of conductivity in the impurity acceptor zone.
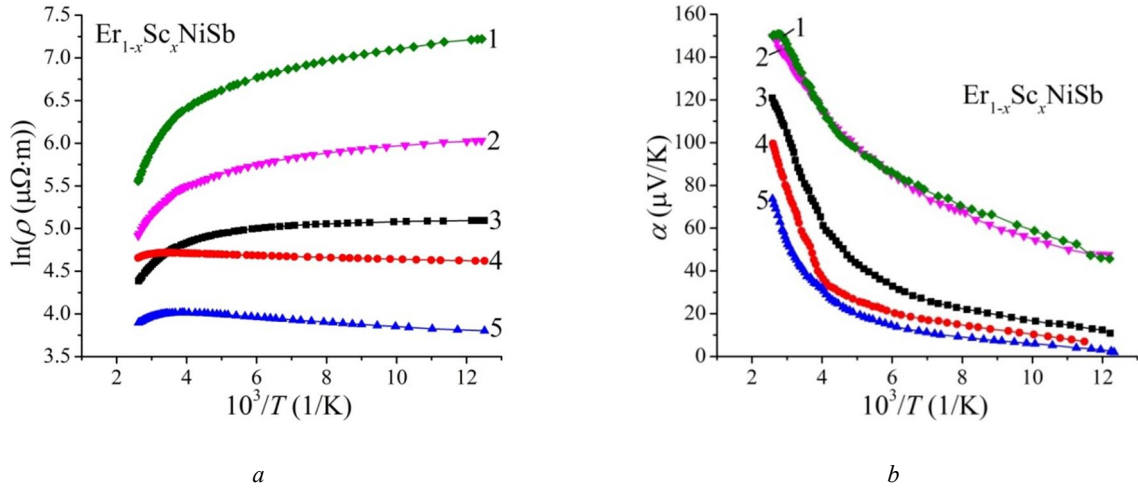
Fig. 2. Temperature dependences of specific electrical resistance ln(ρ(1/T))) (a) and thermopower coefficient α(1/T) (b) Er$_{1-x}$Sc$_x$NiSb: 1 – x=0.10, 2 – x=0. 05K, 3 – x=0, 4 – x=0.01, 5 – x=0.03
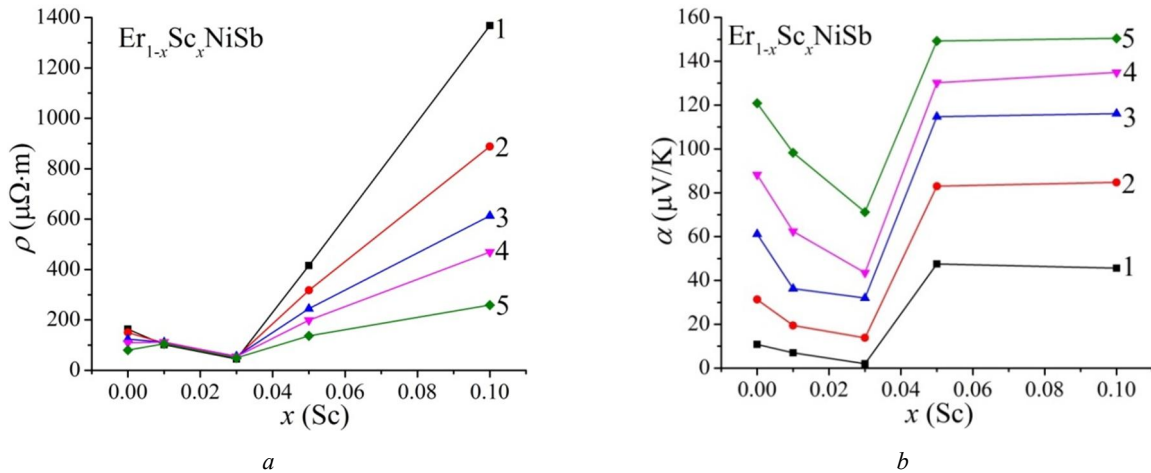
Fig. 3. Variation of electrical resistivity ρ(x,T) (a) and thermopower coefficient α(x,T) (b) for Er$_{1-x}$Sc$_x$NiSb at different temperatures: 1 – T=80 K, 2 – T=160 K 3 – T=250 K, 4 – T=300 K, 5 – T=380 K

An increase in the concentration of holes in *p*-Er$_{1-x}$Sc$_x$NiSb in the area of concentrations x=0–0.03 is indicated by a decrease in the values of the resistivity ρ(x, T) and the thermopower coefficient α(x, T) (Figs. 2, 3). Thus, the addition of the lowest in the experiment impurity concentrations Sc, for example, at a temperature *T* = 80 K, leads to a decrease of ~ 4 times the values of ρ(x, T): from ρ$_{x=0}$=163.3 μOhm to ρ$_{x=0.01}$=101.7 μOhm and ρ$_{x=0.03}$=44.8 μOhm. The values of the thermopower coefficient α(x,T) also decrease at all temperatures, for example, at temperatures *T* = 380 K, from α$_{x=0}$=120.9 μV/K to α$_{x=0.01}$=98.3 μV/K and α$_{x=0.03}$=71.2 μV/K. This is possible in a *p*-type semi-conductor only if the concentration of the main current carriers, which are holes, increases.

However, the nature of such an increase in the concentration of holes in Er$_{1-x}$Sc$_x$NiSb at concentrations x=0–0.03 is not completely clear. The assumption, by analogy with Er$_{1-x}$Zr$_x$NiSb, about the possible occupation by Sc atoms of the crystallographic position of 4c atoms Ni (3d^{8}4s^2) and the generation of structural defects of acceptor nature (Sc has fewer 3d electrons than Ni), is not confirmed by the behavior of the unit cell period a(x) Er$_{1-x}$Sc$_x$NiSb (Fig. 1a). If the Sc atoms (r$_{Sc}$ = 0.164 nm) at least partially occupied the position of 4c Ni atoms (r$_{Ni}$ = 0.124 nm), this would lead to an increase in the values of the period of the cell a(x) Er$_{1-x}$Sc$_x$NiSb, and we do not observe this.

The fact of increasing the concentration of acceptors in Er$_{1-x}$Sc$_x$NiSb at insignificant concentrations of impurity atoms is also indicated by the nature of the change in the values of the activation energy of holes from the Fermi level   to the valence band   (Fig. 4, curve 1).

If in *p*-ErNiSb the Fermi level   was at a distance of 45.4 meV from the level of the valence band   , then at the concentration Er$_{1-x}$Sc$_x$NiSb, x=0.01, the Fermi level   shifted towards the valence band   and

was located at a distance of 13.6 meV. Since the Fermi level reflects the ratio of ionized acceptors and donors in the semiconductor, its movement by $x = 0.01$ to the level of the valence band is possible either with an increase in the number of acceptors or a rapid decrease in the concentration of ionized donors.
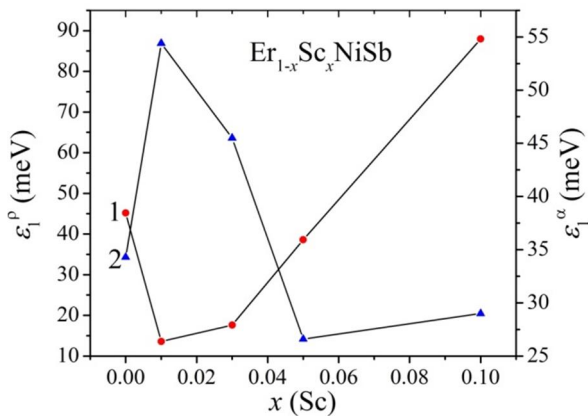

Fig. 4. Change of values of activation energies from Fermi level to the level of the valence band (1) and amplitude of modulation of large-scale fluctuation of continuous energy bands (2) $Er_{1-x}Sc_xNiSb$

At a higher concentration of acceptor impurity, $x = 0.03$, the Fermi level slightly deviated from the level of the valence band by a distance of 17.1 meV, indicating the appearance of a compensating impurity in the semiconductor, namely donors of unknown origin. At the same time, the concentration of donors is still insignificant, because at low temperatures in the semiconductor $Er_{0.97}Sc_{0.03}NiSb$ there is no jumping mechanism of electrical conductivity . We can say that in the region of concentrations $x = 0.03$ in the $Er_{1-x}Sc_xNiSb$ semiconductor, the number of generated acceptors far exceeds the donor concentration.

At even higher concentrations of Sc impurities in p-$Er_{1-x}Sc_xNiSb$, $x \geq 0.03$, the characteristics of the semiconductor undergo significant changes. Low-temperature activation regions appear on the $\ln(\rho(1/T))$ dependences, which is a sign of compensation and evidence of the simultaneous generation of structural defects of acceptor and donor nature in the crystal: the semiconductor becomes strongly doped and compensated. This is also indicated by the nature of the change in the position of the Fermi level in the bandgap of the semiconductor $Er_{1-x}Sc_xNiSb$, which practically by a linear law (Fig. 4, curve 1) moves away from the valence band : $(x=0.05)=58.6$ meV and $(x=0.10)=88.1$ meV. Such a movement of the Fermi level during doping of a p-type semiconductor is possible only if donors of unknown origin are generated.

The behavior of the dependences of the resistivity $\rho(x, T)$ and the coefficient of Thermo-EMF $\alpha(x, T)$ in p-$Er_{1-x}Sc_xNiSb$, $x \geq 0.03$, (Fig. 3) also indicates the

appearance of donors of unknown origin in the semiconductor. Thus, in the area of concentrations $Er_{1-x}Sc_xNiSb$, $x=0.03$–0.10, the values of the resistivity $\rho(x, T)$ increase rapidly, for example, at a temperature of $T = 80$ K from the values of $\rho_{x=0.03}=44.8$ μOhm to $\rho_{x=0.10}=1367.8$ μOhm. For a p-type semiconductor, this is possible only if the concentration of the main current carriers, which are free holes, is reduced, as well as the generation of donors that compensate for the acceptor states. This conclusion is also confirmed by the behavior of the thermopower coefficient $\alpha(x, T)$ at concentrations $x \geq 0.03$.

The appearance of donors of unknown nature in the p-$Er_{0.90}Sc_{0.10}NiSb$ semiconductor is indicated by the nature of the change in the values of the thermopower coefficient $\alpha(x, T)$ (Fig. 2b), in particular, the change in the slope of the dependence and the appearance of an extremum at high temperatures. We can predict that at higher temperatures it is possible to change the sign of the thermopower coefficient.

Thus, the results of structural, electrokinetic, and energy studies of the semiconductor solid solution $Er_{1-x}Sc_xNiSb$ allow us to speak about the complex mechanism of simultaneous generation in the crystal of structural defects of acceptor and donor nature. However, the obtained array of information does not allow to unambiguously prove the existence of a mechanism for generating donors and acceptors. The following mechanism is proposed.

7. Clarification of energy and structural parameters $Er_{1-x}Sc_xNiSb$

Based on the fact that the results of $Er_{1-x}Sc_xNiSb$ studies did not provide answers to the mechanisms of generating structural defects of different nature, we use the method of optimizing the crystal structure model based on the results of calculating the electronic spectrum and physical properties of the semiconductor. It is known that to calculate the energy of an electron in the first Brillouin zone, it is necessary to know the spatial arrangement of atoms (or their absence - vacancies) in the nodes of the unit cell. On the other hand, the smallest structural changes change the local symmetry and density distribution of DOS electronic states. Therefore, the adequacy of DOS results and experimental studies suggests that the model of its structure is as close as possible to the real one.

Having the experimental results of the drift rate of the Fermi level as the activation energy (x) from the Fermi level to the level of the valence band (Fig. 4, curve 1), we looked for the degree of compensation (ratio of structural defects of donor and acceptor nature). the direction and velocity of the Fermi level is as close as possible to (x). Calculations of the density distribution of electronic states of DOS are performed for almost all variants of the location of atoms in the

nodes of the unit cell, and the degree of employment of all positions by their own and/or foreign atoms, as well as the availability of vacancies. It turned out that the most acceptable variant for the ErNiSb compound is one that assumes the presence of vacancies in the crystallographic positions 4a and 4c of the Er and Ni atoms, respectively. Moreover, the number of vacancies in the

position Er (4a) is twice less than the number of vacancies in the position Ni (4c) (Fig. 5a). This proportion is maintained for a solid solution of $Er_{1-x}Sc_xNiSb$. We can note that the change in the values of the resistivity $\rho(x, T)$ $Er_{1-x}Sc_xNiSb$ at the lowest temperature in the experiment (Fig. 3a, curve 1) varies according to the same law as obtained by modeling in [1].
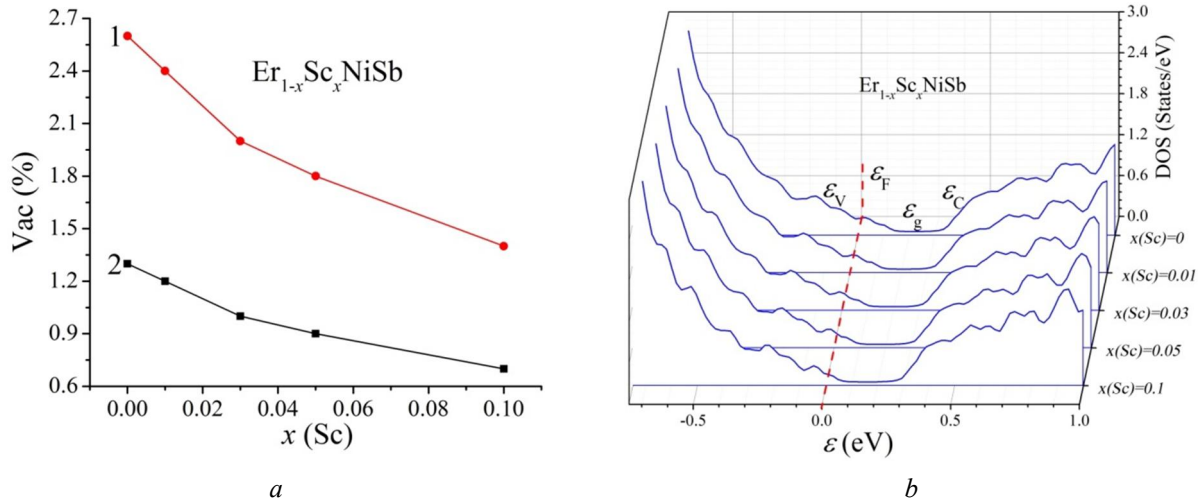

a

b

Fig. 5. Dynamics of change of vacancy concentration in crystallographic positions of Ni (4c) (1) and Er (4a) (2) (a) atoms and calculation of DOS $Er_{1-x}Sc_xNiSb$ in the presence of vacancies

Therefore, the results of experimental studies of the electrokinetic and energetic performances of the semiconductor solid solution $Er_{1-x}Sc_xNiSb$ are consistent with the results of modeling these characteristics under the simultaneous existence of vacancies in the crystallographic positions of Er (4a) and Ni (4c) atoms. Moreover, the number of vacancies in position 4a is twice less than the number of vacancies in position 4c.

In turn, vacancies in the crystallographic positions of Er (4a) and Ni (4c) atoms $Er_{1-x}Sc_xNiSb$ are structural defects of acceptor nature, which generate in the semiconductor at least two acceptor zones   and of different power and with different depths. the level of the valence band   . The introduction of impurity Sc atoms into the structure of the ErNiSb compound by replacing the Er atoms in position 4a is also accompanied by the occupation of vacancies by Sc atoms and a reduction in their number. Occupying a vacancy, the Sc atom participates in the formation of the valence band and the conduction band of the semiconductor $Er_{1-x}Sc_xNiSb$, acting as a source of free electrons. We can also assume that the introduction of Sc atoms into the structure of the compound ErNiSb is accompanied by a process of ordering the structure of $Er_{1-x}Sc_xNiSb$ and Ni atoms occupy vacancies in position 4c. This process also, however, 2 times slower, leads to a decrease in the concentration of structural defects of acceptor nature. In this case, Ni, giving valence electrons, now act as donors.

In fig. 5b presents the results of calculations of the density distribution of electronic states DOS of the semiconductor $Er_{1-x}Sc_xNiSb$, which adequately reflect the degree of its compensation. From fig. 5b also shows that the Fermi level $Er_{1-x}Sc_xNiSb$ at all impurity concentrations Sc slightly changes its location relative to the level of the valence band   , which corresponds to positive values of the $\alpha(x,T)$ (Fig. 2b, 3b).

8. Conclusions

Thus, as a result of a comprehensive study of the crystal and electronic structures, kinetic and energy characteristics of the semiconductor thermometric material $Er_{1-x}Sc_xNiSb$, ($x=0–0.1$) it is shown that there are vacancies in the structure of ErNiSb compounds at positions 4a and 4c of Er and Ni atoms, respectively. structural defects of acceptor nature. The number of vacancies in position 4a is twice less than in position 4c. This proportion is preserved for $Er_{1-x}Sc_xNiSb$. The introduction of impurity Sc atoms into the structure of the ErNiSb compound by substituting Er atoms is accompanied by both the substitution of Er atoms and the filling of vacancies in position 4a. In this case, Ni atoms occupy vacancies in position 4c, which may be accompanied by the process of ordering the structure of $Er_{1-x}Sc_xNiSb$. Occupation of vacancies by Sc and Ni atoms leads to an increase in the concentration of free electrons, an increase in the degree of compensation of the semiconductor, which changes the position of the Fermi level   and the mechanisms of electrical conductivity.

9. Gratitude

10. Conflict of interest

The authors declare that there is no financial or other possible conflict related to this work.

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