MEASURING TRANSDUCERS

SENSITIVE ELEMENTS OF TEMPERATURE CONVERTERS BASED ON $HfNi_{1-x}Cu_xSn$ THERMOMETRICAL MATERIAL

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Abstract. The results of experimental studies of sensitive elements of temperature transducers based on semiconductor thermometric material $HfNi_{1-x}Cu_xSn$ are presented. Thermometric materials $HfNi_{1-x}Cu_xSn$, x=0.01–0.10, were produced by fusing a charge of components in an electric arc furnace with a tungsten electrode (cathode) in an atmosphere of purified argon under a pressure of 0.1 kPa on a copper water-cooled base (anode). Heat treatment of the alloys consisted of homogenizing annealing at a temperature of 1073 K. The samples were annealed for 720 hours. in quartz glass ampoules vacuumed to 1.0 Pa in muffle electric furnaces with temperature control with an accuracy of ±10 K. Diffraction data arrays were obtained on a STOE STADI-P powder diffractometer (Cu $K\alpha_1$ radiation), and the structural characteristics of $HfNi_{1-x}Cu_xSn$ were calculated using the Fullprof program. The chemical and phase compositions of the samples were monitored using metallographic analysis (scanning electron microscope Tescan Vega 3 LMU).

The thermoelectric pair platinum-thermometric material Pt-$HfNi_{0.99}Cu_{0.01}Sn$ was the basis of the thermoelectric converter.

Modeling of thermometric characteristics of sensitive elements of thermotransducers in the temperature range of 4.2–1000 K was carried out by the full potential linearized plane wave method (Full Potential Linearized Augmented Plane Waves, Elk software package). The results of experimental measurements served as reference currents for modeling characteristics.

X-ray phase analysis showed the absence of traces of extraneous phases in the diffractograms of the studied samples of $HfNi_{1-x}Cu_xSn$ thermometric materials, and the microprobe analysis of the concentration of atoms on their surface established the correspondence to the original composition of the charge.

Refinement of the crystal structure of $HfNi_{1-x}Cu_xSn$ showed that the introduction of Cu atoms orders the structure, which makes it stable, and the kinetic characteristics are reproducible during thermocycling at temperatures T=4.2–1000 K. Ordering the structure of the thermometric material $HfNi_{1-x}Cu_xSn$ leads to changes in the electronic structure. At the same time, the number of donors decreases – Ni leaves the Hf position, and the substitution of Ni atoms for Cu leads to the generation of structural defects of the donor nature (Cu atoms contain more 3*d*-electrons), and another donor band ε^D_{Cu} will appear in the band gap ε_g.

For the sensitive elements of thermoconverters at Cu impurity concentrations x=0.005 and x=0.01, the temperature dependences of the specific electrical resistance $\ln(\rho(1/T))$ contain activation areas, which is consistent with the results of electronic structure modeling. This indicates the location of the Fermi level ε_F in the band gap ε_g, and the negative value of the thermopower coefficient $\alpha(T)$ at these temperatures specifies its position – near the conduction band ε_C. The value of the activation energy from the Fermi level ε_F to the bottom of the conduction band ε_C was calculated. For the base semiconductor *n*-HfNiSn, the Fermi level ε_F lies at a distance of ε_F=81 meV from the co ε_C conduction band ε_C, and in the sensitive elements of thermoconverters with concentrations of $HfNi_{0.995}Cu_{0.005}Sn$ and $HfNi_{0.99}Cu_{0.01}Sn$ – at distances of ε_F=1 meV and ε_F=0.3 meV respectively. Therefore, an increase in the concentration of the Cu donor impurity leads to a rapid movement of the Fermi level ε_F to the bottom of the conduction band at a rate of $\Delta\varepsilon_F/\Delta x\approx 81$ meV/%Cu.

The impurity concentration x=0.01 is sufficient for the metallization of the conductivity of sensitive elements of $HfNi_{1-x}Cu_xSn$ converters at low temperatures. This is possible if the Fermi energy ε_F is close to the conduction band ε_C (ε_F=0.3 meV), which simplifies the thermal ionization of donors and the appearance of a significant number of free electrons. However, this impurity donor zone still does not intersect with the bottom of the conduction band ε_C.

At concentrations of the Cu donor impurity in $HfNi_{1-x}Cu_xSn$, x=0.2–0.07, the high-temperature activation regions disappear on the temperature dependences of the resistivity $\ln(\rho(1/T,x))$, which indicates the movement of the Fermi level ε_F from the band gap ε_g to the conductivity ε_C. At the same time, the values of specific electrical resistance $\rho(T,x)$ increase monotonically with increasing temperature), and the scattering of electrons by phonons determines the conductivity of sensitive elements of thermotransducers based on the thermometric material $HfNi_{1-x}Cu_xSn$. The metallization of the electrical conductivity of the thermometric material $HfNi_{1-x}Cu_xSn$ at concentrations x>0.01 is accompanied by a rapid decrease in the values of the thermopower coefficient $\alpha(x, T)$. Thus, if in *n*-HfNiSn at a temperature of T=80 K, the value of the thermal erst coefficient was $\alpha_{x=0}$=-178 μV/K, then in the $HfNi_{0.93}Cu_{0.07}Sn$ material $\alpha_{x=0.07}$=-24 μV/K. The results of the kinetic properties of $HfNi_{1-x}Cu_xSn$ are consistent with the conclusions of structural and energetic studies.

The simulation of the conversion functions of the sensitive elements of the resistance thermometer and the thermoelectric converter in the temperature range of 4.2–1000 K was carried out. As an example, the conversion functions of the thermoelectric pair Pt-$HfNi_{0.99}Cu_{0.01}Sn$ are given. The ratio of change of thermo-emf values to the range of temperature measurements in thermocouples is greater than all known industrial thermocouples. However, due to the metallization of the conductivity of the thermometric material $HfNi_{1-x}Cu_xSn$, x>0.01, the temperature coefficient of resistance (TCR) of the obtained resistance thermometers is greater than the TCR of metals, but is inferior to the value of TCR of sensitive elements made of semiconductor materials.

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

1. Introduction

The results of research on sensitive elements of temperature transducers based on the new semiconductor thermometric material $HfNi_{1-x}Cu_xSn$, x=0.01–0.10, are presented. This research is a continuation of the work on the research of sensitive elements of temperature converters based on the base semiconductor *n*-HfNiSn, which we started for the first time in [1].

The results of the structural, kinetic, and energy properties of the sensitive elements of thermotransducers based on the thermometric material $HfNi_{1-x}Cu_xSn$, x=0.01–0.10, presented below will allow us to establish the correctness of the used methods of modeling its properties obtained by doping the base semiconductor HfNiSn with Cu atoms by replacing Ni atoms (4*c*). The obtained results will make it possible to clarify the spatial arrangement of atoms in the nodes of the elementary cell, as well as to identify the mechanisms of electrical conductivity to determine the conditions for the synthesis of thermosensitive materials with the maximum efficiency of converting thermal energy into electrical energy.

2. Disadvantage

Studies of the sensitive elements of resistance thermometers and thermoelectric temperature transducers based on the HfNiSn semiconductor have established their high sensitivity to heat treatment modes (temperature and duration of annealing).

3. Goal

To establish the mechanisms of electrical conductivity of sensitive elements of thermocouples based on the thermometric material $HfNi_{1-x}Cu_xSn$, which will determine the conditions for obtaining sensitive elements with high sensitivity and stability in the temperature range up to 1000 K.

4. Research methods

Thermometric materials $HfNi_{1-x}Cu_xSn$, x=0.01–0.10, were produced by fusing a charge of components weighed with an accuracy of ±0.001 g in an electric arc furnace with a tungsten electrode (cathode) in an atmosphere of purified argon under a pressure of 0.1 kPa on a copper water-cooled base (anode). Pre-alloyed spongy titanium was used as a getter. To achieve homogeneity, the alloys were remelted twice. Control of losses of the charge during melting was carried out by repeated weighing. Heat treatment of the alloys consisted of homogenizing annealing at a temperature of 1073 K. The samples were annealed for 720 hours. in ampoules made of quartz glass vacuumed to 1.0 Pa in muffle electric furnaces with temperature control with an accuracy of ±10 K. Diffraction data arrays were obtained on an STOE STADI-P powder diffractometer ($CuK\alpha_1$-radiation), and calculated using the Fullprof program [2] structural characteristics of $HfNi_{1-x}Cu_xSn$. The chemical and phase compositions of the samples were monitored using metallographic analysis (scanning electron microscope Tescan Vega 3 LMU).

DFT calculations were performed with help of the Vienna Ab initio Simulation Package VASP v. 5.4.4 with potentials of the PAW type [3]. The Perdew-Burke-Enzerhoff exchange-correlation function was used in the Monkhorst-Pack generalized gradient approximation (GGA) for the k-grid 11×11×11 [4]. In all calculations, the plane wave cutoff was set to 400 eV. For crystal structures with the mixed arrangement, the supercell approach was applied [5]. In this case, lattice symmetry was reduced and all unique distributions of atoms were generated using a combinatorial approach [6]. The lattice parameters for such structures were optimized by a variable lattice volume, which was then selected by the universal equation of state [7]. The electronic kinetic coefficients were calculated using the Exciting code [8] (FLAPW - Full Potential Linearized Augmented Plane Waves method) by solving the linearized Boltzmann equation in the approximation of a constant relaxation time. The modeling of the distribution of the density of electronic states (DOS) was carried out by the Korringa-Kohn-Rostoker (KKR) method (AkaiKKR program package [9]) in the Coherent Potential Approximation (CPA) and Local Density Approximation (LDA) for exchange-correlation potential with the Moruzzi-Janak-Williams (MJW) parameterization. The accuracy of calculating the position of the Fermi level ε_F is ±6 meV. The basis of the sensitive element of the resistance thermometer based on $HfNi_{1-x}Cu_xSn$ is polycrystalline samples in the form of rectangular parallelepipeds of size 0.5×0.5×5 (mm^3), to which copper or platinum wire contacts were connected. Experimental measurements of the electrical resistance values were carried out using the four-contact method, and the values of the thermopower coefficient were measured by applying the potentiometric method relative to copper and platinum. To reduce the "parasitic" effects caused by the influence of the thermopower coefficient at the contact points, as well as the effects caused by the possible influence of the *p-n* transition, the voltage drop was measured in different directions of the electric current. A thermoelectric pair of platinum-thermometric material was the basis of a thermoelectric transducer. Modeling of thermometric characteristics of sensitive elements of electroresistive and thermoelectric thermometers in the temperature range of 4.2–1000 K was carried out using the full potential linearized plane wave method (Full Potential Linearized Augmented Plane Waves, Elk program package [8]). The results of experimental measurements served as reference currents for modeling characteristics.

5. Investigation of structural characteristics of thermometric material $HfNi_{1-x}Cu_xSn$

X-ray phase analysis showed the absence of traces of extraneous phases in the diffractograms of the studied samples of thermometric materials $HfNi_{1-x}Cu_xSn$, x=0.01–0.10, and the microprobe analysis of the concentration of the atoms on the surface of the samples established correspondence with the original composition of the charge. This allows us to state that the obtained thermometric material was homogeneous in composition, and its crystal structure corresponded to the structural type of MgAgAs [1].

Since the atomic radius of Cu (r_{Cu}=0.128 nm) is greater than that of the Ni atom (r_{Ni}=0.124 nm), it is logical to increase the values of the period of the unit cell $a(x)$ of the thermometric material $HfNi_{1-x}Cu_xSn$ at concentrations x=0–0.07 under the condition of substitution in positions 4*c* of Ni atoms to Cu atoms. However, experimental studies of changes in the values of the cell period $a(x)$ of $HfNi_{1-x}Cu_xSn$ established that at concentrations of x>0.07 the values of the cell period $a(x)$ decrease. This may indicate the solubility limit of Cu atoms in the matrix of the HfNiSn compound.

Refinement of the crystal structure of $HfNi_{1-x}Cu_xSn$ samples, x=0.01–0.07, showed that the introduction of Cu atoms orders the crystal structure ("heals" structural defects) and Ni atoms leave the position of Hf atoms (4*a*). In turn, the ordering of the $HfNi_{1-x}Cu_xSn$ structure makes it stable, and the kinetic characteristics are reproducible during thermal cycling in the temperature range T=4.2–1000 K.

The ordering of the crystal structure of the semiconductor thermometric material $HfNi_{1-x}Cu_xSn$ is accompanied by changes in its electronic structure. If in *n*-HfNiSn there are structural defects of the donor nature as a result of displacement of up to ~1% of Hf atoms by Ni atoms [1], then the ordering of the $HfNi_{1-x}Cu_xSn$ structure is accompanied, on the one hand, by a decrease in the number of donors – Ni leaves the Hf position. On the other hand, the substitution of Ni atoms ($3d^84s^2$) for Cu atoms ($3d^{10}4s^1$) leads to the generation of structural defects of the donor nature (Cu atoms contain more 3*d*-electrons). At the same time, another donor band ε^D_{Cu} will appear in the band gap ε_g of the semiconductor thermometric material $HfNi_{1-x}Cu_xSn$, and the semiconductor will become heavily doped [10]. Changes in the electronic structure will be reflected in the kinetic characteristics of the sensitive elements of thermotransducers based on the thermometric material $HfNi_{1-x}Cu_xSn$.

6. Modeling of energy characteristics of sensitive elements based on thermometric material $HfNi_{1-x}Cu_xSn$

The calculation of the electronic structure of the semiconductor thermometric material $HfNi_{1-x}Cu_xSn$ was carried out to model the mechanisms of electrical conductivity, the behavior of the Fermi level ε_F, and the band gap ε_g. Since the doping of the base semiconductor *n*-HfNiSn with Cu atoms orders its crystal structure, the calculation of the distribution of the density of electronic states (DOS) was carried out for the ordered version of the structure (Fig. 1a).

The results of modeling the energy characteristics of the base semiconductor *n*-HfNiSn are consistent with the results of previous studies [1]. As mentioned above, the irregularity of the crystal structure of the HfNiSn compound is associated with the partial occupation by Ni atoms (~1%) of the crystallographic position 4a of Hf atoms ($5d^26s^2$), which generates energy states of the donor band ε_D^1 in the band gap ε_g of the semiconductor (the Cu atom contains more than 3*d*-electrons than the Hf atom).

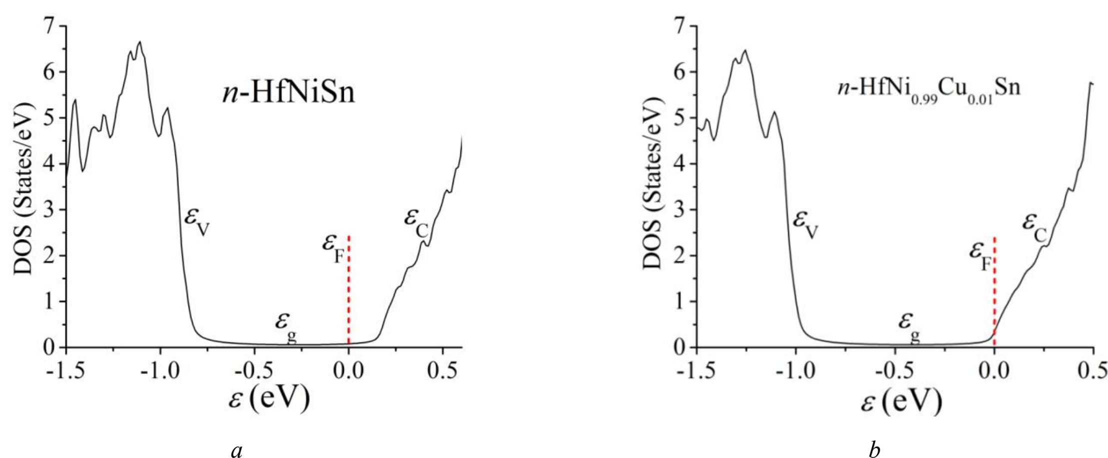

Fig. 1. Calculation of the distribution of the density of electronic states (DOS) of n-HfNiSn (a) and n-HiNi$_{0.99}$Cu$_{0.01}$Sn (b) for an ordered version of the structure of the thermometric material

From fig. 1a shows that the base semiconductor n-HfNiSn has a band gap with a width of $\varepsilon_g\approx360$ meV, the Fermi level ε_F is fixed by the generated donor band ε_D^1, located near the edge of the conduction band ε_C. At the same time, free electrons are the main carriers of electric current, which will be reflected in the experiment by negative values of the thermopower coefficient $\alpha(T)$. At high and low temperatures, there will be high- and low-temperature activation areas on the temperature dependence of the specific electrical resistance $\ln(\rho(1/T))$ n-HfNiSn.

Modeling of the electronic structure shows that introducing into the n-HfNiSn base semiconductor the lowest experimentally achievable Cu impurity concentrations (x=0.005 and x=0.01) causes a drift of the Fermi level ε_F to the conduction band ε_C (Fig. 1b) since structural defects are generated in the crystal donor nature and another donor zone ε^D_{Cu} appears. From the simulation results, we can predict that at concentrations of Cu atoms x=0.005 and x=0.01, activation regions will be present on the temperature dependences of the specific electrical resistance $\ln(\rho(1/T))$ $HfNi_{1-x}Cu_xSn$, since the admixture of Cu atoms is not sufficient for the Fermi level ε_F crossed the bottom of the conduction zone ε_C. The high-temperature activation region reflects the activation of electrons from the Fermi level ε_F to the edge of the conduction band ε_C, and the low-temperature region represents the hopping affinity for impurity donor states with energies close to the Fermi level ε_F.

Therefore, the introduction of Cu atoms into the crystal structure of the HfNiSn compound changes the electronic structure of the semiconductor thermometric material $HfNi_{1-x}Cu_xSn$ and redistributes the density of electronic states at the Fermi level $g(\varepsilon_F)$.

The following results of the study of the kinetic characteristics of sensitive elements of thermotransducers based on $HfNi_{1-x}Cu_xSn$, x=0.01–0.10, will allow us to identify the mechanisms of electrical conductivity and the conditions for obtaining sensitive elements with high sensitivity and stability in the temperature range up to 1000 K.

7. Investigation of kinetic and energy properties of sensitive elements

The temperature and concentration dependences of the specific electrical resistance ρ and the thermopower coefficient α of the sensitive elements of thermotransducers based on the thermometric material $HfNi_{1-x}Cu_xSn$ are shown in Fig. 2 and 3. As can be seen from fig. 2, for the sensitive elements of thermotransducers at Cu impurity concentrations x=0.005 and x=0.01, the temperature dependences of the specific electrical resistance $\ln(\rho(1/T))$ contain activation areas, which is consistent with the results of modeling the electronic structure (Fig. 1). In this case, the temperature dependence of specific electrical resistance is described by relation (1) [10]:

$$\rho^{-1}(T)=\rho_1^{-1}\exp\left(-\frac{\varepsilon_1^{\rho}}{k_BT}\right)+\rho_3^{-1}\exp\left(-\frac{\varepsilon_3^{\rho}}{k_BT}\right), \quad (1)$$

here the first high-temperature term describes the activation of current carriers ε_1^{ρ} from the Fermi level ε_F to the edge of the conduction band ε_C, and the second, low-temperature term, describes the jump conduction through impurity donor states ε_3^{ρ} with energies close to the Fermi level ε_F.

In turn, the temperature dependence of the thermopower coefficient $\alpha(1/T)$ $HfNi_{1-x}Cu_xSn$ (Fig. 2) can be described by the well-known expression (2):

$$\alpha=\frac{k_B}{e}\left(\frac{\varepsilon_i^{\alpha}}{k_BT}-\gamma+1\right), \quad (2)$$

here γ is a parameter that depends on the nature of the scattering mechanism [11]. The values of the activation energy ε_1^{α}, which are proportional to the amplitude of the large-scale fluctuation of continuous energy zones, and the values of the activation energy ε_3^{α}, which are proportional to the amplitude of the modulation of the small-scale fluctuation of a heavily doped and compensated semiconductor, were calculated from the high-temperature section of the dependence $\alpha(1/T)$ [10].

The presence of high-temperature activation regions on the temperature dependences of the resistivity $\ln(\rho(1/T))$ for $HfNi_{1-x}Cu_xSn$ samples, x=0–0.01, indicates the location of the Fermi level ε_F in the band gap ε_g, and the negative values of the thermopower coefficient $\alpha(T)$ at these temperatures specify its position – near the conduction zone ε_C. At the same time, electrons are the main carriers of electric current. The behavior of the resistivity $\rho(x, T)$ of $HfNi_{1-x}Cu_xSn$, x=0–0.01, at all temperatures (Fig. 2) also corresponds to the results of modeling the electronic structure under the condition that Ni atoms are replaced by Cu atoms in the crystallographic position 4*a*.

From the high-temperature dependences of the resistivity $\ln(\rho(1/T))$ $HfNi_{1-x}Cu_xSn$ of samples with concentrations x=0, x=0.005, and x=0.01, the value of the activation energy from the Fermi level ε_F to the bottom of the conduction band ε_C was calculated. For the base semiconductor n-HfNiSn, the Fermi level ε_F lies at a distance of ε_F=81 meV from the conduction band ε_C, and in the sensitive elements of thermoconverters with concentrations of $HfNi_{0.995}Cu_{0.005}Sn$ and $HfNi_{0.99}Cu_{0.01}Sn$ – at distances of ε_F=1 meV and ε_F=0.3 meV respectively. Therefore, an increase in the concentration of the Cu donor impurity leads to a rapid movement of the Fermi level ε_F to the bottom of the conduction band at a rate of $\Delta\varepsilon_F/\Delta x\approx81$ meV/%Cu.

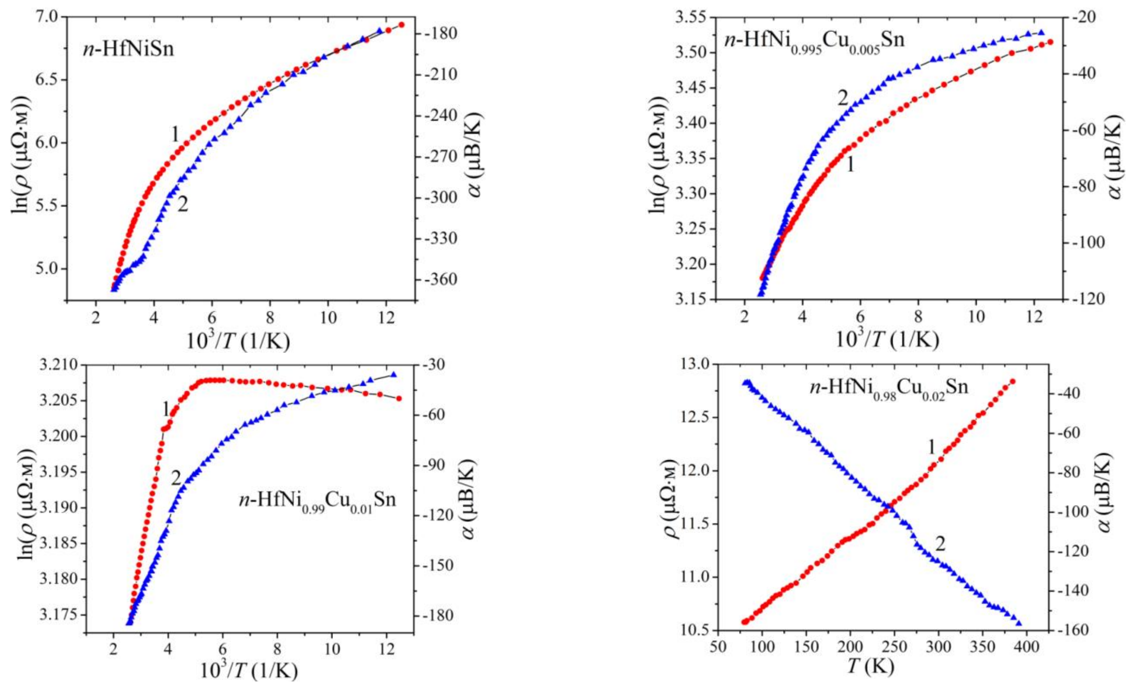

Fig. 2. Temperature dependences of the specific electrical resistance ln(ρ(1/T)) (1) and the thermopower coefficient α(1/T) (2) of the sensitive elements of thermotransducers based on the $HfNi_{1-x}Cu_xSn$ thermometric material

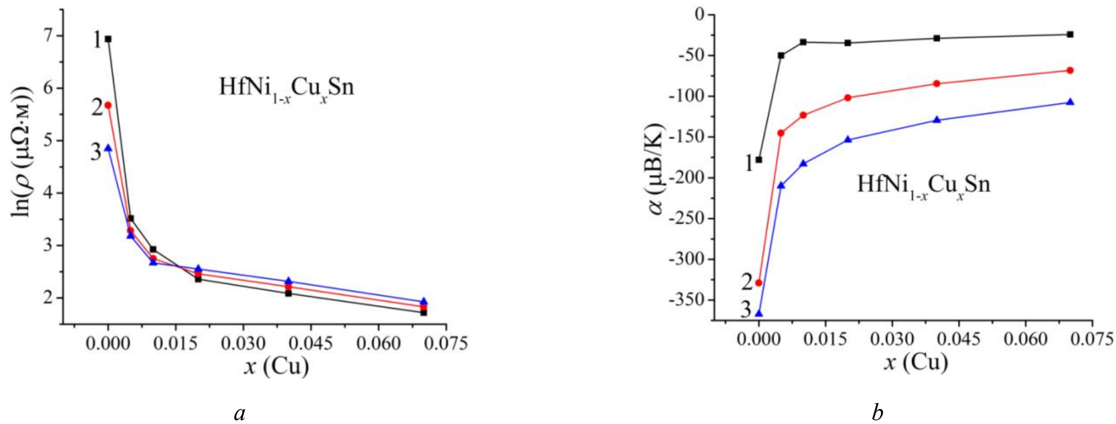

Fig. 3. Change in the values of the specific electrical resistance ρ(x, T) (a) and the thermo-emf coefficient α(x, T) (b) $HiNi_{1-x}Cu_xSn$ at different temperatures: 1 – T=80 K, 2 – T=250 K, 3 – T=380 K

At low temperatures, the electrical conductivity of sensitive elements of thermotransducers with $HfNi_{1-x}Cu_xSn$ compositions, $x \leq 0.005$, is determined by jumps of carriers in localized states in the vicinity of the Fermi energy ε_F. The presence of a jumping mechanism of electrical conductivity for $HfNi_{1-x}Cu_xSn$, $x \leq 0.005$, indicates an insufficient concentration of impurity Cu atoms to overlap the wave functions of impurity states near the Fermi energy ε_F and metallization of conductivity.

The impurity concentration x=0.01 is sufficient for the metallization of the conductivity of the sensitive elements of thermotransducers at low temperatures of $HfNi_{1-x}Cu_xSn$. This is possible if the Fermi energy ε_F is close to the conduction band ε_C (ε_F=0.3 meV), which simplifies the thermal ionization of donors and the appearance of a significant number of free electrons. However, this impurity donor zone still does not intersect with the bottom of the conduction band ε_C.

At concentrations of the Cu donor impurity in $HfNi_{1-x}Cu_xSn$, x=0.2–0.07, the high-temperature activation regions disappear on the temperature dependences of the resistivity ln(ρ(1/T,x)) (Fig. 2). This nature of the change in the specific resistance values indicates the movement of the Fermi level ε_F from the band gap ε_g to the conduction band ε_C. Therefore, at concentrations x=0.2–0.07, the Fermi level ε_F crosses the edge of the conduction band ε_C and locates in the band of continuous energies. At the same time, the values of specific electri-

cal resistance $\rho(T,x)$ monotonically increase with temperature (Fig. 2), and the scattering of electrons by phonons determines the conductivity of the sensitive elements of thermotransducers based on the thermometric material $HfNi_{1-x}Cu_xSn$.

To understand the mechanisms of electrical conductivity and the type of main electric current carriers of sensitive elements of thermotransducers based on the thermometric material $HfNi_{1-x}Cu_xSn$, the behavior of the dependences of the specific electrical resistance $\rho(x, T)$ and the thermopower coefficient $\alpha(x, T)$ at different concentrations and temperatures is considered (Fig. 3). Thus, in the area of concentrations of $HfNi_{1-x}Cu_xSn$, x=0–0.01, specific electrical resistance $\rho(x, T)$ rapidly decreases. This is possible in a semiconductor material of the electronic conductivity type only if the concentration of free electrons increases rapidly. This reason, as mentioned above, is the generation of an additional donor zone ε^{D}_{Cu} in the semiconductor thermometric material of n-type conductivity, formed by structural defects of the donor nature when Ni atoms are replaced by Cu atoms.

The metallization of the electrical conductivity of the thermometric material based on $HfNi_{1-x}Cu_xSn$ at concentrations $x>0.01$ is expected to be accompanied by a rapid decrease in the values of the thermopower coefficient $\alpha(x, T)$. So, if in the base semiconductor n-HfNiSn at a temperature of T=80 K, the value of the thermopower coefficient was $\alpha_{x=0}$=-178 μV/K, then in the thermometric material $HfNi_{0.93}Cu_{0.07}Sn$ $\alpha_{x=0.07}$=-24 μV/K. We can see that the results of the kinetic properties of $HfNi_{1-x}Cu_xSn$ agree with the conclusions of structural and energy studies. An increase in the period of the unit cell a(x) can only be caused by the replacement of Ni atoms with Cu atoms. At the same time, another donor zone ε^{D}_{Cu} is formed in the thermometric material.

Therefore, the results of studies of sensitive elements of thermos convertors based on $HfNi_{1-x}Cu_xSn$ are consistent with the results of the simulation of their energy characteristics under the condition of substitution of Ni atoms by Cu in the crystallographic position 4*c*. The obtained results make it possible to clarify the spatial arrangement of atoms in the nodes of the elementary cell, as well as to identify the mechanisms of electrical conductivity to determine the conditions for the synthesis of thermosensitive materials with the maximum efficiency of converting thermal energy into electrical energy.

8. Modeling of the function of transformation of sensitive elements on basis of $HfNi_{1-x}Cu_xSn$

The simulation of the conversion functions of the sensitive elements of the resistance thermometer and the thermoelectric converter in the temperature range of 4.2–1000 K was carried out with help of the Full Potential Linearized Augmented Plane Waves method using the Elk software package [8]. The results of measurements served as reference currents for modeling characteristics.

In Fig. 4, as an example, the conversion functions of the Pt-$HfNi_{0.99}Cu_{0.01}Sn$ thermoelectric pair are given. We can see that the obtained sensitive elements of thermotransducers based on the latest thermometric materials have high sensitivity. The ratio of change of thermopower coefficient values to the range of temperature measurements in thermocouples is greater than in industrial thermocouples. However, due to the metallization of the conductivity of the thermometric material $HfNi_{1-x}Cu_xSn$, $x>0.01$, the temperature coefficient of resistance (TCR) of the obtained resistance thermometers is greater than the TCR of metals, but is inferior to the value of TCR of sensitive elements made of semiconductor materials.

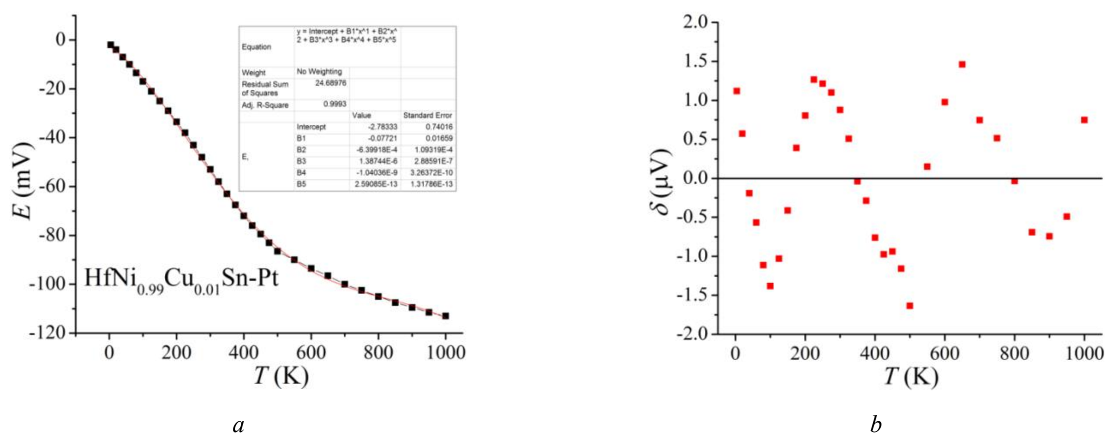

Fig. 4. Transformation function of the thermoelectric converter E(T) Pt-$HfNi_{0.99}Cu_{0.01}Sn$ (a) and regular deviations δ (b)

9. Conclusions

Based on the results of the studies of the structural, kinetic, and energy properties of thermometric materials $HfNi_{1-x}Cu_xSn$, the area of their existence with an unchanged crystal structure, which is limited to concentrations of x=0.01–0.10, was established. The introduction of modeling methods of crystal and electronic structures made it possible to establish the relationship between the spatial arrangement of atoms in the nodes of the elementary cell (crystal structure) and the mechanisms of electrical conductivity of the thermometric material. This clarifies the conditions for the synthesis of thermometric materials with given kinetic properties and the maximum efficiency of converting thermal energy into electrical energy. The regularities of the transformation functions of the Pt-$HfNi_{0.99}Cu_{0.01}Sn$ thermocouple have been established.

10. Gratitude

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11. Conflict of interest

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

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