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SIMULATION OF CHARACTERISTICS OF SENSITIVE ELEMENTS OF TEMPERATURE CONVERTERS BASED ON $TiCo_{1-x}Cr_xSb$

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Abstract. The results of modeling the thermodynamic, structural, and kinetic properties of the thermometric material $TiCo_{1-x}Cr_xSb$, x=0–0.10, as well as the conversion functions of sensitive elements of a thermoelectric converter based on it in the temperature range of 4.2–1000 K are presented. The results presented continue the research of sensitive elements of temperature converters based on basic semiconductor thermometric material TiCoSb. Previous studies of the structural, energetic, and kinetic properties of TiCoSb showed that its crystal structure is disordered, and there are vacancies in the crystallographic positions of the 4*c* Co atoms and 4*a* Ti atoms. In the semiconductor TiCoSb, the Fermi level ε_F is located in the band gap εg, the width of which is $\varepsilon_g \approx 257$ meV.

The sensitive elements of the temperature transducers are made of thermometric material $TiCo_{1-x}Cr_xSb$, obtained by doping the base semiconductor TiCoSb with Cr atoms ($3d^54s^1$), introduced into the structure by substitution of Co atoms ($3d^74s^2$) in the crystallographic position 4*c*. Since the Cr atom has fewer 3*d*-electrons than Co, such doping should have generated impurity acceptor states in the band gap ε_g. In this way, it is planned to change the degree of compensation of $TiCo_{1-x}Cr_xSb$ and the mechanisms of electrical conductivity. In turn, having a mechanism for changing the concentration of energy states, we can predictably optimize the kinetic properties of the $TiCo_{1-x}Cr_xSb$ thermometric material. This will increase the sensitivity and accuracy of sensitive elements of resistance thermometers and thermoelectric converters.

Thermometric materials $TiCo_{1-x}Cr_xSb$, 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). Titanium was used as a getter. Heat treatment of alloys consisted of homogenizing annealing at a temperature of 1073 K for 720 hours. in vacuumed quartz ampoules (up to 1.0 Pa) with temperature control with an accuracy of ±10 K. Arrays of diffraction data were obtained on a STOE STADI-P powder diffractometer (Cu $K\alpha_1$-radiation), and structural characteristics of $TiCo_{1-x}Cr_xSb$ 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).

DFT calculations were performed using the Vienna Ab initio Simulation Package VASP v. 5.4.4 with potentials of the PAW type. The Perdew-Burke-Enzerhoff exchange-correlation functional in the Monkhorst-Pack generalized gradient approximation (GGA) for the 11×11×11 *k*-grid was used. In all calculations, the plane wave cutoff was set to 400 eV. A supercell approach was used for mixed-arrangement crystal structures. In this case, lattice symmetry was reduced and all unique atom distributions were generated using a combinatorial approach. The lattice parameters for such structures were optimized by varying the lattice volume, which was then fitted by the universal equation of state. The electronic kinetic coefficients were calculated using the Exciting code (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 performed using the Korringa-Kohn-Rostoker (KKR) method (AkaiKKR software package) in the Coherent Potential Approximation (CPA) and Local Density Approximation (LDA) for the exchange-correlation potential with by the Moruzzi-Janak-Williams (MJW) parameterization]. The accuracy of calculating the position of the Fermi level ε_F is ±6 meV. 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 FLAPW method, Elk software package.

Modeling of the cell period change $a(x)$ for the ordered version of the $TiCo_{1-x}Cr_xSb$ structure, x=0–0.1, showed a linear increase in the cell period, since the atomic radius of Cr (r_{Cr}=0.128 nm) is greater than the atomic radius of Co (r_{Co}=0.125 nm) . Experimental studies of the structure of samples $TiCo_{1-x}Cr_xSb$, x=0–0.1, established that the change in the period $a(x)$ does not correspond to the simulation results. In the concentration range x=0–0.02, the values of the period $a(x)$ increase, which was expected when replacing Co atoms ($3d^74s^2$) with Cr atoms ($3d^54s^1$), because the atomic radius of Cr is larger than the atomic radius of Co. Such changes will lead to a redistribution of the electron density and the appearance of defects of an acceptor nature, since the Cr atom contains fewer *d*-electrons than the Co atom. Occupancy by Cr atoms of vacancies in the 4*a* position of Ti atoms and 4*c* of Co atoms, which are present in TiCoSb, can also cause an increase in the values of the cell period $a(x)$ of $TiCo_{1-x}Cr_xSb$. The presence of vacancies gives rise to structural defects of an acceptor nature, and acceptor states will appear in the band gap ε_g. If Ti atoms ($3d^24s^2$) are replaced by Cr atoms in position 4*a* or they occupy vacancies in $TiCo_{1-x}Cr_xSb$, structural defects of the donor nature will be generated (Cr has more *d*-electrons than Ti).

For the ordered version of the structure of the hypothetical thermometric material $TiCo_{1-x}Cr_xSb$, x=0–1.0, the calculation of thermodynamic characteristics in the approximation of harmonic oscillations of atoms was carried out within the framework of the DFT density functional theory. The results of calculating the change in the values of the Gibbs thermodynamic potential $\Delta G_{mix}(x)$ of the thermometric material $TiCo_{1-x}Cr_xSb$ show a negligible solubility of Cr atoms.

Calculation of the electronic structure of the semiconductor thermometric material $TiCo_{1-x}Cr_xSb$, x=0–0.10, for the ordered variant of the crystal structure showed that in the basic thermometric material TiCoSb the Fermi level ε_F lies in the band gap ε_g near its middle. Doping TiCoSb with the lowest concentration of Cr atoms (x=0.005) leads to the appearance of defects of an acceptor nature (Cr has fewer d-electrons than Co). As a result, corresponding acceptor states ε_A will appear in the band gap ε_g, which are located near the valence band ε_V. The Fermi level ε_F in $TiCo_{0,995}Cr_{0,005}Sb$ will move from the middle of the band gap ε_g to the valence band ε_V. In the experiment, we will obtain a thermometric material with positive values of the thermopower coefficient $\alpha(T,x)$, which will serve as one branch of the thermoelectric temperature converter.

When the concentration of Cr admixture increases, for example in $TiCo_{0,98}Cr_{0,02}Sb$, the concentration of acceptor states will increase, which will force the Fermi level ε_F to cross the edge of the valence band ε_V and be located in the zone of continuous energies. Finding the Fermi level ε_F in the valence band ε_V will change the type of electrical conductivity of the thermometric material $TiCo_{1-x}Cr_xSb$ from activation to metallic.

Having calculated the electronic structure of $TiCo_{1-x}Cr_xSb$, we will obtain a tool for modeling the behavior of the resistivity $\rho(x,T)$ and the thermopower coefficient $\alpha(T,x)$ when acceptor states appear in the band gap ε_g. At the lowest concentration of the acceptor impurity Cr, x=0.002, the electrical conductivity has a metallic character, and the values of $\rho(T,x)$ are the highest. The increase in the values of the specific resistance $\rho(x,T)$ $TiCo_{1-x}Cr_xSb$ with increasing temperature is due to the mechanisms of scattering of current carriers. High values of the thermopower coefficient $\alpha(T,x)$ at temperatures T=40–800 K show that the thermometric material $TiCo_{1-x}Cr_xSb$ remains a highly doped semiconductor, whose Fermi level ε_F lies in the valence band ε_V. This is indicated by the positive values of the thermopower coefficient $\alpha(T,x)$. An increase in the concentration of the acceptor impurity Cr is accompanied by an increase in the concentration of holes, and this leads to a decrease in the values of the specific resistance $\rho(x,T)$, and the holes continue to be the main current carriers of the thermometric material $TiCo_{1-x}Cr_xSb$. The simulation showed that the introduction of Cr atoms into the TicoSb structure changes its electronic structure and redistributes the density of electronic states at the Fermi level $g(\varepsilon_F)$.

The transformation functions of the Pt-$TiCo_{0.99}Cr_{0.01}Sb$ thermoelectric pair are presented. 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 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 $TiCo_{1-x}Cr_xSb$, x>0.005, the temperature coefficient of resistance (TCR) of the obtained resistance thermometers is greater than the TCR of metals, but it 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 modeling the thermodynamic, structural, and kinetic properties of the thermometric material $TiCo_{1-x}Cr_xSb$, x=0.01–0.10, as well as the conversion functions of the sensitive elements of the resistance thermometer and the thermoelectric converter in the temperature range of 4.2–1000 K are presented. The results presented continue the research of the sensitive elements of temperature converters based on base semiconductor material TiCoSb. Previous studies of the structural, energy, and kinetic properties of the base material TiCoSb showed that its crystal structure is disordered, and there are vacancies in the crystallographic positions of 4c atoms of Coand 4a of Ti atoms [1]. In the semiconductor TiCoSb, the Fermi level ε_F is located in the band gap εg, the width of which is $\varepsilon_g \approx 257$ meV.

The sensitive elements of the temperature transducers are made of thermometric material $TiCo_{1-x}Cr_xSb$, obtained by doping the base semiconductor TiCoSb with Cr atoms ($3d^5 4s^1$), introduced into the structure by substitution of Co atoms ($3d^7 4s^2$) in the crystallographic position 4c. Since the Cr atom has fewer 3d-electrons than Co, such doping should have generated impurity acceptor states in the band gap ε_g of the semiconductor. In this way, it is planned to change the degree of compensation of the thermometric material $TiCo_{1-x}Cr_xSb$ and the mechanisms of electrical conductivity. In turn, having a mechanism for changing the concentration of impurity states of the thermometric material, we can predictably optimize the kinetic properties of $TiCo_{1-x}Cr_xSb$. This will increase the sensitivity and accuracy of sensitive elements of resistance thermometers and thermoelectric converters [2]. The results of theoretical studies of the structural, thermodynamic, kinetic and energy properties of $TiCo_{1-x}Cr_xSb$ presented below will allow to identify the structural changes that cause the transformation of the electronic structure and the mechanisms of electrical conductivity, the knowledge of which is a condition for the successful optimization of the properties of thermometric materials and sensitive elements of thermotransducers based on them.

2. Disadvantages

Studies of sensitive elements of resistance thermometers and thermoelectric temperature converters based on the basic semiconductor TiCoSb [1] established

their high sensitivity to thermal treatment modes (temperature and duration of annealing).

3. Research objective

To determine the area of existence of thermometric material $TiCo_{1-x}Cr_xSb$ to determine the limit concentration of Cr admixture while optimizing kinetic properties, which will increase the sensitivity and accuracy of sensitive elements of electroresistance and thermoelectric thermometers. Establishing the mechanisms of electrical conductivity of sensitive elements of thermal converters based on thermometric material $TiCo_{1-x}Cr_xSb$ will allow to 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 $TiCo_{1-x}Cr_xSb$, x=0.01–0.10, for the manufacture of sensitive elements of thermotransducers 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). Pre-alloyed spongy titanium was used as a getter. Heat treatment of the alloys consisted of homogenizing annealing at a temperature of 1073 K. The samples were annealed for 720 hours. in vacuum ampoules (up to 1.0 Pa) made of quartz glass in muffle electric furnaces with temperature control with an accuracy of ±10 K. Arrays of diffraction data were obtained on a STOE STADI-P powder diffractometer (Cu $K\alpha_1$-radiation), and with the help of the Fullprof program [3] calculated the structural characteristics of $TiCo_{1-x}Cr_xSb$. The chemical and phase compositions of the samples were monitored using metallographic analysis (scanning electron microscope Tescan Vega 3 LMU).

DFT calculations were performed using the Vienna Ab initio Simulation Package VASP v. 5.4.4 with potentials of the PAW type [4]. The Perdew-Burke-Enzerhoff exchange-correlation functional was used in the Monkhorst-Pack generalized gradient approximation (GGA) for the k-grid 11×11×11 [5]. In all calculations, the plane wave cutoff was set to 400 eV. A supercell approach was used for mixed-arrangement crystal structures. 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 varying the lattice volume, which was then fitted by the universal equation of state. The electronic kinetic coefficients were calculated using the Exciting code [7] (FLAPW – Full Potential Linearized Augmented Plane Waves method) by solving the linearized Boltzmann equation in the approximation of a constant relaxation time [8]. The modeling of the distribution of the density of electronic states (DOS) was carried out using 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 [10]. The accuracy of calculating the position of the Fermi level ε_F is ±6 meV. 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 FLAPW method, Elk software package [7, 8]. The results of experimental measurements served as reference currents for modeling characteristics.

5. Modeling of structural and thermodynamic properties of thermometric material $TiCo_{1-x}Cr_xSb$

A priori, we understood that in the thermometric material $TiCo_{1-x}Cr_xSb$ will have a small extent due to the limited solubility of Cr atoms in the matrix of the base semiconductor TiCoSb. After all, according to the crystal-chemical concept of E. Zintl [2], the formation of a chemical compound with the MgAgAs structure is possible if it has 18 valence electrons. Understanding all the limitations of this concept, which does not take into account the non-monotonic change in atomic radii, electronegativities, ionization potentials of atoms within the same group, etc., it allows to qualitatively predict the formation of solid solutions with the MgAgAs structure, as well as the possible area of their existence.

The basic thermometric material TiCoSb has 18 valence electrons, and the introduction of Cr atoms with 6 valence electrons instead of Co atoms with 9 valence electrons into its structure can limit the area of existence of the thermometric material $TiCo_{1-x}Cr_xSb$. However, taking into account the disorder of the crystal structure of TiCoSb and the presence of vacancies in positions 4*a* and 4*c*, it seems to us that the real area of existence of the thermometric material $TiCo_{1-x}Cr_xSb$ will be larger than can be predicted by calculations for an ordered version of the structure.

Modeling of the change in the unit cell period $a(x)$ for the ordered version of the structure of the thermometric material $TiCo_{1-x}Cr_xSb$, x=0–0.1, showed a linear increase in the cell period, which is understandable because the atomic radius of Cr (r_{Cr}=0.128 nm) is greater than the atomic radius Co (r_{Co}=0.125 nm) (Fig. 1*a*).

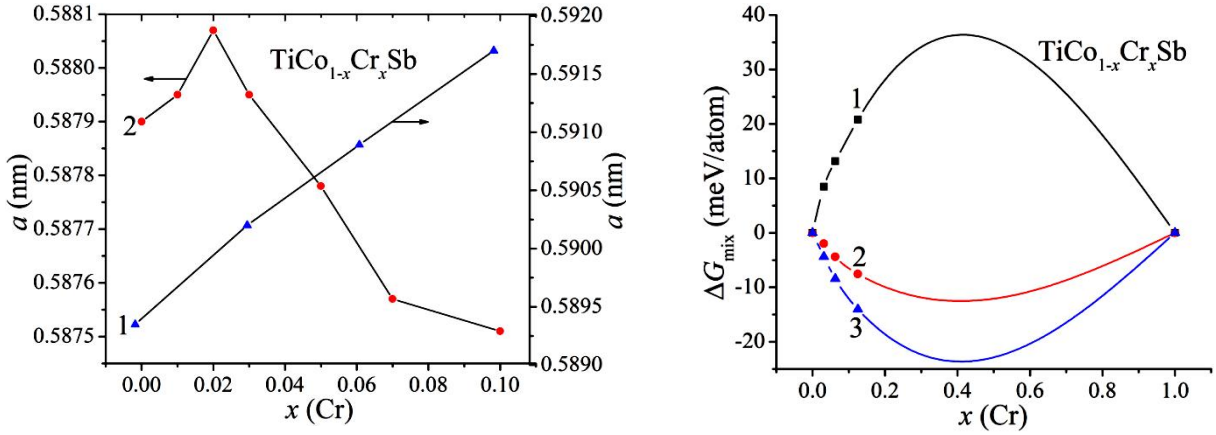
In turn, experimental studies of the structure of samples of the thermometric material $TiCo_{1-x}Cr_xSb$, x=0–0.1, established that the diffractograms are indexed in the MgAgAs structural type [1], however, the change in the period of the cell $a(x)$ does not agree with the simulation

results and is of a complex nature (Fig. 1). In the concentration range x=0–0.02, the cell period values $a(x)$ predictably increase, which was expected when Co atoms ($3d^7 4s^2$ were replaced by Cr atoms ($3d^5 4s^1$) in crystallographic position 4*c*, because the atomic radius of Cr is greater than the atomic radius of Co. Such changes in the structure will lead to a redistribution of the electron density and the appearance of structural defects of an acceptor nature in the 4*c* position, since the Cr atom contains fewer *d*-electrons than the Co atom.

On the other hand, the occupation by Cr atoms of vacancies in the position 4*a* of Ti atoms and 4*c* of Co atoms, which are present in TiCoSb [1], can also cause an increase in the values of the cell period a(x) of the $TiCo_{1-x}Cr_xSb$ thermometric material. The presence of vacancies in the TiCoSb structure gives rise to structural defects of an acceptor nature, and corresponding acceptor states will appear in the band gap ε_g. If Ti atoms ($3d^2 4s^2$) are replaced by Cr atoms in position 4*a* or they occupy vacancies in $TiCo_{1-x}Cr_xSb$, structural defects of the donor nature will be generated (Cr has more *d*-electrons than Ti).

At a concentration of x≈0.02, there is a maximum on the $a(x)$ dependence of $TiCo_{1-x}Cr_xSb$, and at higher concentrations, the values of the cell period decrease. Under the condition of the existence of a solid solution, such a substitution can occur only in the case of partial substitution of Ti atoms (r_{Ti}=0.146 nm) with smaller Cr atoms (r_{Cr}=0.128 nm) in position 4*a*. In the case of substitution of Ti atoms ($3d^2 4s^2$) for Cr atoms ($3d^5 4s^1$) in position 4*a*, as well as in the case of vacancies being occupied by them, defects of a donor nature will be generated in $TiCo_{1-x}Cr_xSb$ (Cr contains more *d*-electrons than Ti). As a result, acceptor and donor states will simultaneously appear in the band gap ε_g of the $TiCo_{1-x}Cr_xSb$ thermometric material, and the semiconductor material will be heavily doped and compensated [11].

It is important to understand within what limits the existence of thermometric material $TiCo_{1-x}Cr_xSb$ is energetically appropriate. For this purpose, for the ordered variant of the crystal structure of the hypothetical thermometric material $TiCo_{1-x}Cr_xSb$, x=0–1.0, when only in the 4*c* position the substitution of Co atoms for Cr atoms occurs, the calculation of thermodynamic characteristics in the approximation of harmonic oscillations of atoms was carried out within the framework of the DFT density functional theory. The results of calculating the change in the values of the Gibbs potential $\Delta G_{mix}(x)$ (Fig. 1*b*) of the thermometric material $TiCo_{1-x}Cr_xSb$ show a negligible solubility of Cr atoms.



a b

Fig. 1. Modeling (1) and experimental values (2) of changes in the cell period a(x) (a) and the results of calculating the Gibbs thermodynamic potential ΔG_{mix} (b) of $TiCo_{1-x}Cr_xSb$ for the ordered of the structure: 1 – ΔH_{mix}, 2 – T=873 K , 3 – T=1073 K

6. Modeling of energy and kinetic properties of sensitive elements based on thermometric material $TiCo_{1-x}Cr_xSb$

The calculation of the electronic structure of the semiconductor thermometric material $TiCo_{1-x}Cr_xSb$, x=0–0.10, for the ordered variant of the crystal structure was performed to model the behavior of the Fermi level ε_F, the band gap ε_g, and kinetic properties (fig. 2). From fig. 2 we can see that in the basic thermometric material TiCoSb the Fermi level ε_F lies in the band gap ε_g ear its middle. Doping the semiconductor material TiCoSb with the lowest concentration of Cr atoms (x=0.005) leads to the appearance of structural defects of an acceptor nature (Cr has fewer *d*-electrons than Co). As a result, corresponding acceptor states ε_A will appear in the band gap ε_g, which are located near the valence band ε_V. The Fermi level ε_F in $TiCo_{0,995}Cr_{0,005}Sb$ will move from the middle of the band gap ε_g to the valence band ε_V. In the experiment, we will obtain a thermometric material with positive values of the thermopower coefficient $\alpha(T,x)$, which will serve as one branch of the thermoelectric temperature converter.

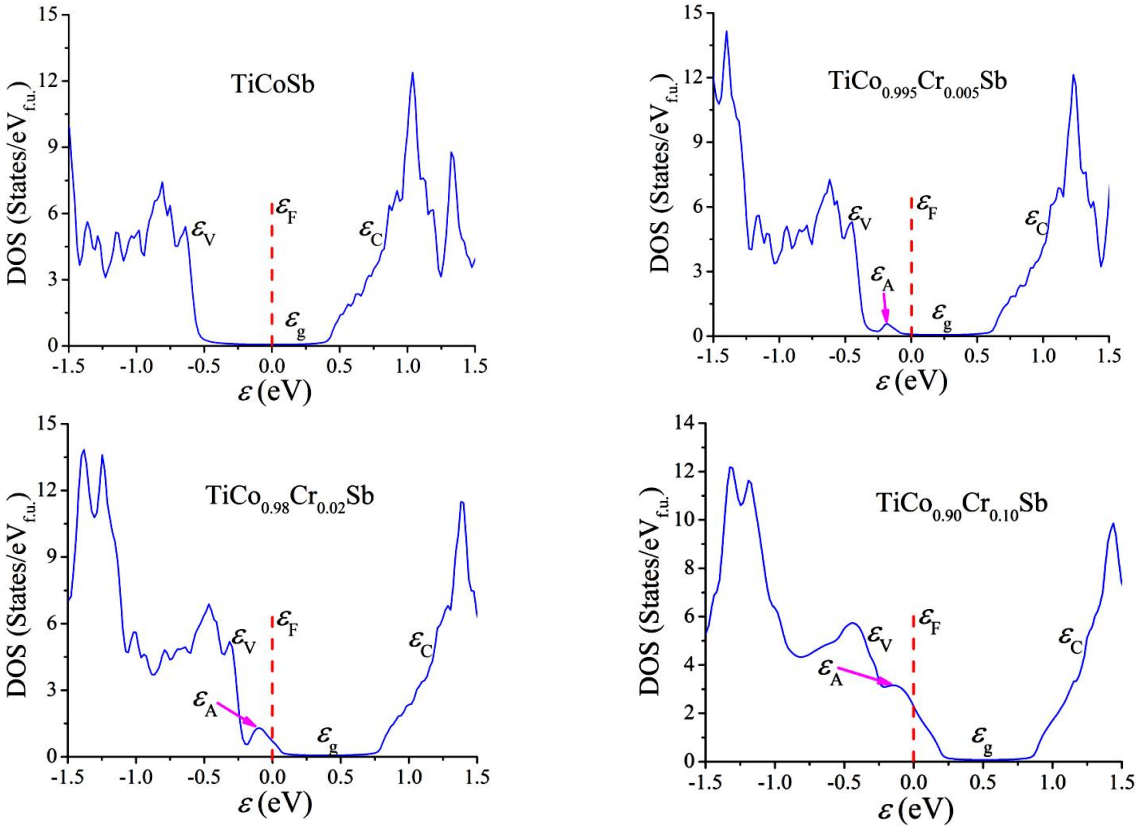
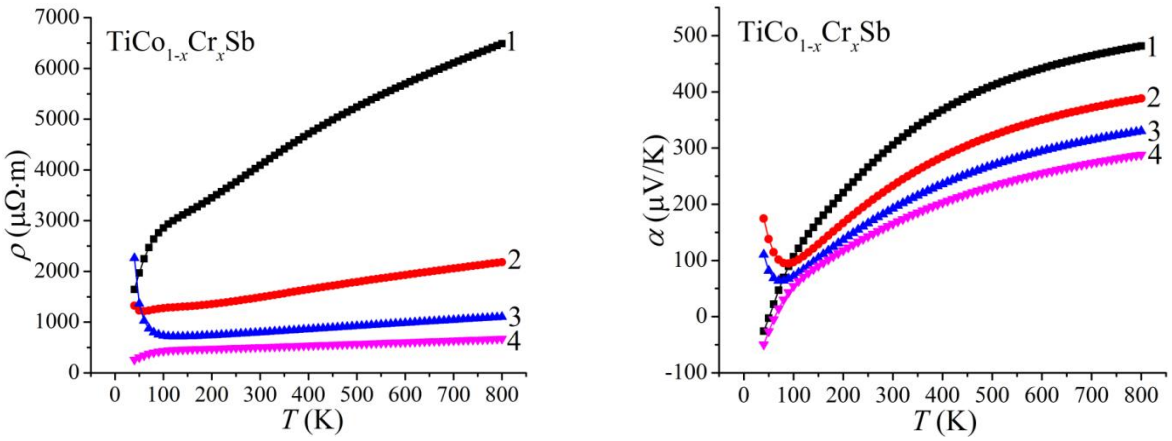


Fig. 2. Calculation of the distribution of the density of electronic states (DOS) of the thermometric material $TiCo_{1-x}Cr_xSb$ for the ordered variant of its structure

When the concentration of Cr admixture increases, for example in $TiCo_{0,98}Cr_{0,02}Sb$, the concentration of acceptor states will increase, which will force the Fermi level ε_F to cross the edge of the valence band ε_V and be located in the zone of continuous energies. A dielectric-metal conductivity transition will occur, which is an Anderson transition [11]. Finding the Fermi level ε_F in the valence band ε_V will change the type of electrical conductivity of the $TiCo_{1-x}Cr_xSb$ thermometric material from activation to metallic [11]. In experimental studies, the values of electrical resistance will increase due to the action of scattering mechanisms and the activation areas will disappear on the temperature dependences $\ln(\rho(1/T))$. However, in the thermometric material $TiCo_{1-x}Cr_xSb$, the forbidden band ε_g still exists.

After calculating the electronic structure of the thermometric material $TiCo_{1-x}Cr_xSb$ for the ordered variant of the crystal structure (Fig. 2), we will obtain a tool for modeling the behavior of the specific electrical resistance $\rho(x,T)$ and the thermopower coefficient $\alpha(T,x)$ (Fig. 3). During the analysis of possible changes in the crystal structure of the thermometric material $TiCo_{1-x}Cr_xSb$, it was concluded that acceptor and donor states can be generated simultaneously in the band gap ε_g of the semiconductor. However, in the case of the ordered structure, when Co atoms are replaced by Cr atoms, acceptor states are generated in the thermometric material. And therefore, when modeling the electroinetic properties of the thermometric material $TiCo_{1-x}Cr_xSb$, it is advisable to first investigate the case of the appearance of acceptor states in the band gap ε_g.

From fig. 3, we can see that at the lowest concentration of the acceptor impurity Cr, x=0.002, the electrical conductivity has a metallic character, and the values of the specific electrical resistance $\rho(x,T)$ are the highest. It is quite clear that the values of the specific resistance $\rho(x,T)$ of the thermometric material $TiCo_{1-x}Cr_xSb$ increase with increasing temperature, which is due to the existing mechanisms of dispersion of current carriers. High values of the thermopower coefficient $\alpha(T,x)$ at temperatures T=40–800 K show that the thermometric material $TiCo_{1-x}Cr_xSb$ remains a highly doped semiconductor, whose Fermi level ε_F lies in the valence band ε_V. This is indicated by the positive values of the thermopower coefficient $\alpha(T,x)$. An increase in the concentration of the acceptor impurity Cr is accompanied by an increase in the concentration of holes, and this leads to a decrease in the values of the specific resistance $\rho(x,T)$, and the holes continue to be the main current carriers of the thermometric material $TiCo_{1-x}Cr_xSb$.



a b

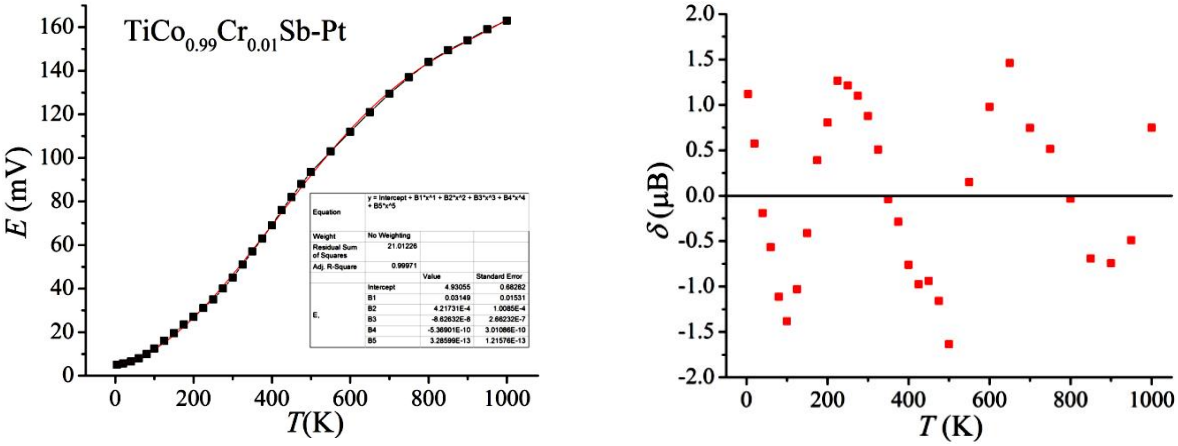
Fig. 3. Modeling of the temperature dependences of the specific resistance ρ(T,x) (**a**) and the thermopower coefficient α(T,x) (**b**) of the sensitive elements of thermotransducers based on the thermometric material $TiCo_{1-x}Cr_xSb$

Therefore, the introduction of Cr atoms into the crystal structure of the basic thermometric material TiCoSb changes its electronic structure and redistributes the density of electronic states at the Fermi level $g(\varepsilon_F)$. The following results of research on the conversion functions of sensitive elements of thermotransducers based on thermometric material $TiCo_{1-x}Cr_xSb$ will show the prospects of its use in the manufacture of sensitive elements with high sensitivity and stability in the temperature range up to 1000 K.

7. Modeling of the transformation funcions of sensitive elements based on the thermometric material $TiCo_{1-x}Cr_xSb$

Modeling of the conversion functions of the sensitive elements of the resistance thermometer and the thermoelectric converter based on the thermometric material $TiCo_{1-x}Cr_xSb$ in the temperature range 4.2–1000 K was carried out using the FLAPW method, the Elk software package [7, 8].

In fig. 4, as an example, the conversion functions of the Pt-$TiCo_{0.99}Cr_{0.01}Sb$ 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 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 $TiCo_{1-x}Cr_xSb$, x>0.005, the temperature coefficient of resistance (TCR) of the obtained resistance thermometers is greater than the TCR of metals, but it is inferior to the value of TCR of sensitive elements made of semiconductor materials.



a b

Fig. 4. Conversion functions of the thermoelectric converter E(T) $TiCo_{0.99}Cr_{0.01}Sb$-Pt (a) and regular deviations δ (b)

8. Conclusions

Modeling of the structural, thermodynamic, energetic and kinetic properties of the thermometric material $TiCo_{1-x}Cr_xSb$ for the case of an ordered crystal structure showed that structural defects of the acceptor nature of nature are generated in the semiconductor, the concentration of which increases with an increase in the content of Cr atoms. The studied thermometric material $TiCo_{1-x}Cr_xSb$ is promising for the manufacture of sensitive elements of electroresistive and thermoelectric temperature transducers. The dependence between the spatial arrangement of atoms in the nodes of the elementary cell (crystalline structure) and the mechanisms of electrical conductivity of the thermometric material has been revealed, which allows determining the conditions for the synthesis of materials with the maximum efficiency of converting thermal energy into electrical energy. The regularities of the conversion functions of the Pt-$TiCoo_{0.99}Cr_{0.01}Sb$ thermoelectric pair were studied.

9. Gratitude

The authors express their gratitude to the members of the scientific seminar of the Department of Information and Measurement Technologies of Lviv Polytechnic National University for an interesting and meaningful discussion on the results of these studies.

10. Conflict of interest

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

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