

# MEASURING TRANSDUCERS

## INVESTIGATION OF SENSITIVE ELEMENTS OF TEMPERATURE TRANSDUCERS BASED ON THERMOMETRIC MATERIAL $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$

*Volodymyr Pashkevych, Ph. Dr., As.-Prof., Volodymyr Krayovskyy, Dr. Sc., Prof., Petro Haranuk, Ph. Dr., As.-Prof., Volodymyr Romaka, Dr. Sc., Prof.,*  
*Lviv Polytechnic National University, Ukraine, e-mail: volodymyr.z.pashkevych@lpnu.ua*  
*Yuriy Stadnyk, Ph. Dr., Senior Scientist, Lyubov Romaka, Ph. Dr., Senior Scientist,*  
*Andriy Horyn, Ph. Dr., Senior Research,*  
*Ivan Franko National University of Lviv, Ukraine*

**Abstract.** The results of experimental studies of sensitive elements of temperature transducers based on semiconductor thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0.01-0.10$ , are presented. Thermometric materials  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  were made by fusing a mixture 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 hearth (anode). Heat treatment of alloys consisted of homogenizing annealing for 720 h in vacuum to 1.0 PA at a temperature of 1073 K. Arrays of diffraction data of X-ray diffraction studies were obtained on a powder diffractometer STOE STADI-P, and using the program Fullprof calculated structural characteristics. The chemical and phase compositions of the samples were monitored by metallographic analysis (scanning electron microscope Tescan Vega 3 LMU).

The basis of the sensitive element of the resistance thermometer on  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  materials is polycrystalline samples in the form of rectangular parallelepipeds with a size of  $0.5 \times 0.5 \times 5$  (mm<sup>3</sup>), to which the contacts are made of copper and/or platinum wire. Experimental measurements of electrical resistance values were performed using the four-contact method, and the values of the thermopower coefficient by the potentiometric method concerning copper and/or platinum. The thermoelectric pair platinum-thermometric material was the basis of the thermoelectric converter.

Modeling of thermometric characteristics of sensitive elements of the thermometer of resistance of the thermoelectric converter is carried out by a full potential method of linearized plane waves (Full Potential Linearized Augmented Plane Waves, Elk software package). The results of experimental measurements served as reference currents in modeling the characteristics.

X-ray phase analysis showed the homogeneity of the studied samples of thermometric materials  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ , as evidenced by the absence of traces of extraneous phases on the diffractograms. The dependences of the period of the unit cell  $a(x)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  are not linear, which indicates more complex structural changes than the one-act substitution of the Lu atom by Sc.

Measurements of the values of the specific magnetic susceptibility  $\chi(T, x)$  were performed by the relative Faraday method at  $T=273$  K using a thermogravimetric installation with an electronic microbalance EM-5-ZMP in magnetic fields up to 10 kGs. Experimental studies of the specific magnetic susceptibility of  $\chi(x)$  sensitive elements have shown that the samples at all concentrations are Pauli paramagnetics, and the value of  $\chi(x)$  is determined by the electron gas. In this case, the values of the magnetic susceptibility  $\chi(x)$  are proportional to the density of electronic states at the Fermi level  $g(\varepsilon_F)$ . In the area of concentrations  $x=0-0.02$ , the values of magnetic susceptibility  $\chi(x)$  undergo insignificant changes, which indicates small changes in the concentration of current carriers. At a concentration  $x>0.02$  there is a rapid increase in the density of electronic states at the Fermi level  $g(\varepsilon_F)$ , indicating an increase in the concentration of free current carriers.

The presence of high-temperature activation sites on the temperature dependences of the resistivity  $\ln(\rho(1/T))$  for all  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  samples indicates the location of the Fermi level  $\varepsilon_F$  in the band gap  $\varepsilon_g$  of the semiconductor, and positive values of the thermopower coefficient  $\alpha(T)$  specify its position - near the valence band  $\varepsilon_v$ . The main carriers of electric current are holes. The nature of the behavior of the resistivity  $\rho(x, T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  at all temperatures also corresponds to the results of modeling the kinetic properties. The fact that in the range of concentrations  $x=0-0.04$  the values of the resistivity  $\rho(x, T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  change slightly at all temperatures indicates a significant advantage of the concentration of holes over electrons. This is indicated by positive values of the thermopower coefficient  $\alpha(x, T)$ . At concentrations  $x \geq 0.04$ , the resistivity increases rapidly, which is due to the appearance of donors, which partially compensate for the acceptors, which reduces the concentration of free holes, and, as a result, we have an increase in the resistance.

The behavior of the thermopower coefficient  $\alpha(x, T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  is adequate. The appearance and increase in the electron concentration are accompanied by an increase in the thermopower coefficient  $\alpha(x, T)$ . At a concentration of  $x \approx 0.07$ , the dependence of the thermopower coefficient contains an extremum, and then the values of the thermopower coefficient rapidly decrease at a temperature of  $T=80$  K and concentrations at  $x \approx 0.1$ . Electrons are already the main current carriers. This is indicated by the negative values of the thermopower coefficient. It was experimentally established that at the concentration range  $x=0-0.07$  the Fermi level velocity  $\varepsilon_F$  from the valence band  $\varepsilon_v$  is  $\Delta\varepsilon_F/\Delta x=4.9$  meV /% Sc, and at the concentration,  $x \geq 0.07 - \Delta\varepsilon_F/\Delta x=11.2$  meV /% Sc. The presence of a difference in the velocities of the Fermi level  $\varepsilon_F$  indicates different rates of generation of acceptors and donors: at a concentration of  $x \geq 0.07$ , the concentration of donors increases  $\sim 2$  times faster than at the site  $x=0-0.07$ .

The functions of conversion of sensitive elements of resistance thermometer and thermoelectric transducers in the temperature range 4.2–1000 K are modeled. The ratio of the change in the values of the thermopower coefficient to the range of temperature measurements in thermocouples is greater than all known industrial thermocouples. In addition, the temperature coefficient of

resistance (TCR) of the obtained resistance thermometers is higher than the TCR of metals but is inferior to the value of TCR of sensitive elements made of traditional semiconductors. At the same time, none of the known resistance thermometers based on traditional semiconductors provides stable characteristics at temperatures of  $4.2 \div 1000$  K.

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

## 1. Introduction

The results of experimental studies of sensitive elements of temperature transducers based on a new semiconductor thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0.01-0.10$ , are presented. This study is a continuation of the modeling of structural, thermodynamic, kinetic and energy characteristics of the semiconductor thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  started in [1]. The simulation of the above-mentioned properties of  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  was performed by two methods: Koring-Kon-Rostocker (KKR method, AkaiKKR software package [2] in coherent potential approximation and full-potential linearized plane wave method (FLAPW 3), Elk software package. After all, the modeling of the electron density distribution and the electron localization function  $\text{Elf}$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  give an idea of the changes in the crystal and electronic structures. Based on the simulation results, a model of the structure of the thermometric material  $\text{Lu}_{1-x+y}\text{Sc}_x\text{Ni}_{1-2y}\text{Sb}$  was proposed, in which at position  $4a$  the Lu atoms are replaced by Sc atoms. In addition, the Lu atoms partially move to the  $4c$  position of the Ni atoms, and a vacancy (Vac) occurs simultaneously in this position. Moreover, the more Lu atoms additionally move to the  $4c$  position of Ni atoms, the more vacancies arise in this position. That is, if the Lu atoms at the number  $x=0.01$  move to position  $4c$  of Ni atoms, then there are additional vacancies with a concentration of  $x=0.01$ . Therefore, in position  $4c$  of Ni atoms is:  $\text{Ni} - x=0.98$ ,  $\text{Lu} - x=0.01$ ,  $\text{Vac} - x=0.01$ . In this model of the crystal structure  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ , the calculation of the density distribution of the electronic states of DOS shows the presence of the band gap  $\varepsilon_g$ , and the Fermi level  $\varepsilon_F$  lies near the valence band  $\varepsilon_V$ . This means that the values of the thermopower coefficient  $\alpha(T,x)$  at all investigated concentrations and temperatures will be positive in the experiment. The proposed model is correct only for a small number of Sc atoms because even partial occupation of the position of Ni atoms by Lu atoms deforms the structure with its subsequent decay. The disadvantage of this model is also the generation in the band gap  $\varepsilon_g$  a significant number of energy levels that intersect with the zones of continuous energies and fix the Fermi level  $\varepsilon_F$ , which complicates the determination of the band gap  $\varepsilon_g$  and the value of activation energy  $\varepsilon_1^p(x)$  from the Fermi level  $\varepsilon_F$  in valence zone  $\varepsilon_V$ .

The following results of structural, kinetic, energy, and magnetic properties of sensitive elements of thermocouples based on thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0-0.10$ , will establish the correctness of the used methods of modeling its properties [1], obtained by doping the basic semiconductor by LuNiSb Lu ( $4a$ ). The obtained results allow to specify the spatial arrangement

of atoms in the nodes of the unit cell, 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.

## 2. Disadvantages

Studies of the sensitive elements of resistance thermometers and thermoelectric temperature transducers based on the RNiSb semiconductor [4–6] have established their high sensitivity to heat treatment modes (temperature and duration of annealing).

## 3. Aim of the Paper

To establish the mechanisms of electrical conductivity of sensitive elements of thermocouples based on the thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ , 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  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0.01-0.10$ , were made by fusing a charge of components weighed with an accuracy of  $\pm 0.001$  g in an electric arc furnace with a tungsten electrode (cathode) in an atmosphere of purified argon at a pressure of 0.1 kPa on a copper water-cooled pod. Pre-alloyed spongy titanium was used as the hetero. To achieve homogeneity, the alloys were melted twice. Control of charge losses during melting was performed by repeated weighing. Heat treatment of alloys consisted of homogenizing annealing at a temperature of 1073 K. Annealing of samples was performed for 720 h in vacuum-packed up to 1.0 Pa ampoules of quartz glass in muffle electric furnaces with temperature control with an accuracy of  $\pm 10$  K. Diffraction data arrays obtained on powder diffraction STADI-P (Cu  $K\alpha_1$ -radiation), and with the help of the program Fullprof [7] the structural characteristics of  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  were calculated. The chemical and phase compositions of the samples were monitored by metallographic analysis (scanning electron microscope Tescan Vega 3 LMU).

The sensitive element of the resistance thermometer based on  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  is based on polycrystalline samples in the form of rectangular parallelepipeds with a size of  $0,5 \times 0,5 \times 5$  (mm<sup>3</sup>), to which the contacts are made of copper or platinum wire. Experimental measurements of electrical resistance values were performed using the four-contact method, and the values of the thermopower

coefficient by the potentiometric method concerning copper and platinum. To reduce the "parasitic" effects caused by the influence of thermo-emf at the points of contact, as well as the effects caused by the possible influence of the p-n junction, the voltage drop was measured in different directions of electric current. The thermoelectric pair platinum-thermometric material was the basis of the thermoelectric converter. Measurements of the values of the specific magnetic susceptibility  $\chi(T, x)$  were performed by the relative Faraday method at a temperature of 273 K using a thermogravimetric installation with an electronic microbalance EM-5-ZMP in magnetic fields up to 10 kGs.

Modeling of thermometric characteristics of sensitive elements of electro resistive and thermoelectric thermometers in the temperature range 4.2–1000 K was performed by the full potential method of linearized plane waves (Full Potential Linearized Augmented Plane Waves, Elk software package [3]). The results of experimental measurements served as reference currents in modeling the characteristics.

### 5. Study of Structural Characteristics of $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ samples

X-ray phase analysis showed the homogeneity of the studied samples of thermometric materials  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0.01-0.10$ , as evidenced by the absence of traces of extraneous phases on the diffractograms. Based on the fact that the atomic radius of Lu ( $r_{\text{Lu}}=0.173$  nm) is larger than Sc ( $r_{\text{Sc}}=0.164$  nm), it is expected to decrease the values of the period of the unit cell  $a(x)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  by substituting Lu atoms at position 4a for Sc atoms. As can be seen from Fig. 1, the course of the dependence  $a(x)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  confirms the assumption regarding the reduction of the period of the unit cell of the thermometric material. However, the dependence of  $a(x)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  is not completely linear and there are local extrema. The nonmonotonic change in the values of the period of the unit cell  $a(x)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  (Fig. 1) and the presence of local extrema depend on the dependence that more complex structural changes occur during the formation of thermometric material than the one-act substitution of the Lu atom by Sc.

The results of modeling the energy characteristics of the basic semiconductor LuNiSb [1] showed the existence of vacancies in position 4a of Lu atoms, which form a structural defect of acceptor nature and the appearance in the band gap  $\varepsilon_g$  acceptor level  $\varepsilon_A^1$ . In this case, the introduction of Sc atoms into the structure of LuNiSb will be accompanied by both the partial displacement of Lu atoms from position 4a and the occupation of vacancies in the same position. If Lu atoms are replaced by Sc atoms in position 4a, structural defects of neutral nature will be generated in the  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  thermometric material, since Lu and Sc atoms

are located in the same group of the Periodic Table of the Elements. When Sc atoms occupy vacancies in position 4a, it simultaneously eliminates the structural defect of acceptor nature and the corresponding acceptor level  $\varepsilon_A^1$  in the band gap  $\varepsilon_g$  of the semiconductor  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  and a structural defect of donor nature is formed with the appearance of band gap  $\varepsilon_g$  in the band  $\varepsilon_D^1$ .

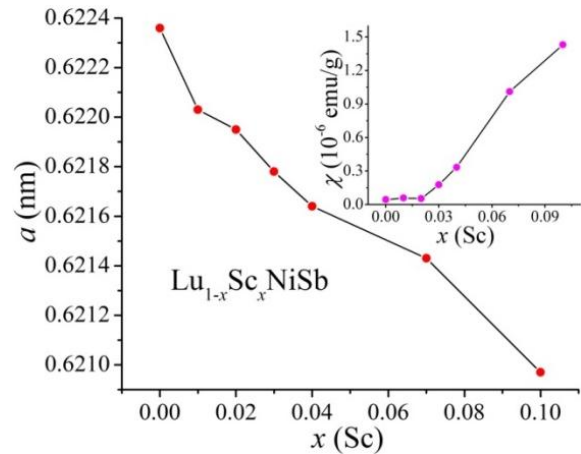


Fig. 1. Change in the values of the period of the unit cell  $a(x)$  and the specific magnetic susceptibility  $\chi(x)$  ( $x$ , 273 K) (insert)  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$

Therefore, the introduction of Sc atoms into the crystal structure of LuNiSb changes the electronic structure of the semiconductor thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  and redistributes the density of electronic states at the Fermi level  $g(\varepsilon_F)$ . Experimental studies of the specific magnetic susceptibility  $\chi(x)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  at  $T=273$  K showed that the samples at all concentrations are Pauli paramagnetics (Fig. 1, inset), and the value of the magnetic susceptibility is determined exclusively by the electron gas. In this case, the values of the magnetic susceptibility  $\chi(x)$  are proportional to the density of electronic states at the Fermi level  $g(\varepsilon_F)$ . We can see that in the area of concentrations  $x=0-0.02$  the values of magnetic susceptibility  $\chi(x)$  change insignificantly. This indicates slight changes in the concentration of current carriers in this range. And only at a concentration  $x>0.02$  there is a rapid increase in the density of electronic states at the Fermi level  $g(\varepsilon_F)$ , indicating an increase in the concentration of free current carriers. The results of magnetic studies of  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  are consistent with the conclusions of structural studies. The following results of the study of kinetic and energy characteristics of sensitive elements of thermocouples based on  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0-0.10$ , will identify the mechanisms of electrical conductivity and conditions for obtaining sensitive elements with high sensitivity and stability in the temperature range up to 1000 K.

## 6. Study of Kinetic and Energy Properties of Sensitive Elements Based on $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$

Temperature and concentration dependences of specific electrical resistance  $\rho$  and thermopower coefficient  $\alpha$  of sensitive elements of thermocouples based on thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  are shown in Fig. 2, 3. As can be seen from Fig. 2a, for all investigated cases, the temperature dependences of the resistivity  $\ln(\rho(1/T))$  are characteristic of semiconductors [8] and are described by relation (1):

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

here the first high-temperature term describes the activation of current carriers  $\varepsilon_1^\rho$  from the Fermi level  $\varepsilon_F$  to the level of continuous energy zones, and the second, low-temperature term, the hopping conductivity at impurity donor states  $\varepsilon_3^\rho$  with energies close to the Fermi level  $\varepsilon_F$ . In turn, the temperature dependences of the thermo-emf coefficient  $\alpha(1/T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  (Fig. 2b) can be described by the known expression (2):

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

here  $\gamma$  is a parameter that depends on the nature of the scattering mechanism [9]. From high- and low-temperature activation regions of the  $\alpha(1/T)$   $\text{LuNiSb}$  dependence, the values of activation energies  $\varepsilon_1^\alpha=35.3$  meV and  $\varepsilon_2^\alpha=1.9$  meV were calculated, respectively, which are proportional to the amplitude of large-scale fluctuations of zones of continuous energies and small-scale flux [8].

The presence of high-temperature activation sites on the temperature dependences of the resistivity  $\ln(\rho(1/T))$  for all  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  samples indicates the location of the Fermi level  $\varepsilon_F$  in the band gap  $\varepsilon_g$  of the

semiconductor, and positive values of the thermopower coefficient  $\alpha(T)$  specify its position - near the valence band  $\varepsilon_v$ . The main carriers of electric current are holes.

The nature of the behavior of the resistivity  $\rho(x, T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  at all temperatures (Fig. 3) also corresponds to the results of modeling the kinetic characteristics under conditions of vacancies at the positions of Lu and Ni atoms [1]. If the semiconductor simultaneously contains carriers of electric current of both types (electrons and holes), then the maximum depends on the resistivity  $\rho(x, T)$ , which shows that the concentrations of acceptors and donors are the same. The fact that in the range of concentrations  $x=0-0.04$  the values of the resistivity  $\rho(x, T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  change slightly at all temperatures, indicates a significant advantage of the concentration of holes over electrons. This is indicated by positive values of the thermopower coefficient  $\alpha(x, T)$ . And only at concentrations  $x \geq 0.04$  the values of resistivity begin to increase rapidly. We associate this increase in the values of  $\rho(x, T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  with the appearance of donors, which partially compensate for the acceptors, which reduces the concentration of free holes, and, as a result, we have an increase in the values of electrical resistance.

The behavior of the thermopower coefficient  $\alpha(x, T)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  is adequate (Fig. 3). The appearance and increase in the concentration of electrons are accompanied by an increase in the values of the thermopower coefficient. At a concentration of  $x \approx 0.07$ , the dependence of the thermopower coefficient  $\alpha(x, T)$  contains an extremum, and then the values of the thermopower coefficient decrease rapidly at a temperature of  $T=80$  K and concentrations at  $x \approx 0.1$ . Electrons are already the main current carriers. This is indicated by the negative values of the thermopower coefficient  $\alpha(x, T)$  (Fig. 3).

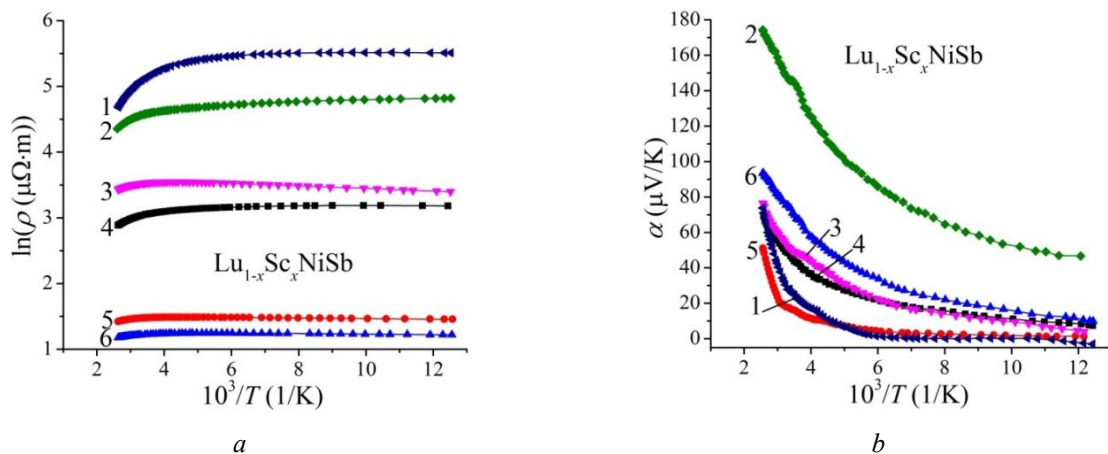


Fig. 2. Temperature dependences of specific electrical resistance  $\ln(\rho(1/T))$  (a) and thermopower coefficient  $\alpha(1/T)$  (b) of sensitive elements of thermocouples based on thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ : 1 –  $x=0.10$ ; 2 –  $x=0.07$ ; 3 –  $x=0.03$ ; 4 –  $x=0$ ; 5 –  $x=0.01$ ; 6 –  $x=0.02$

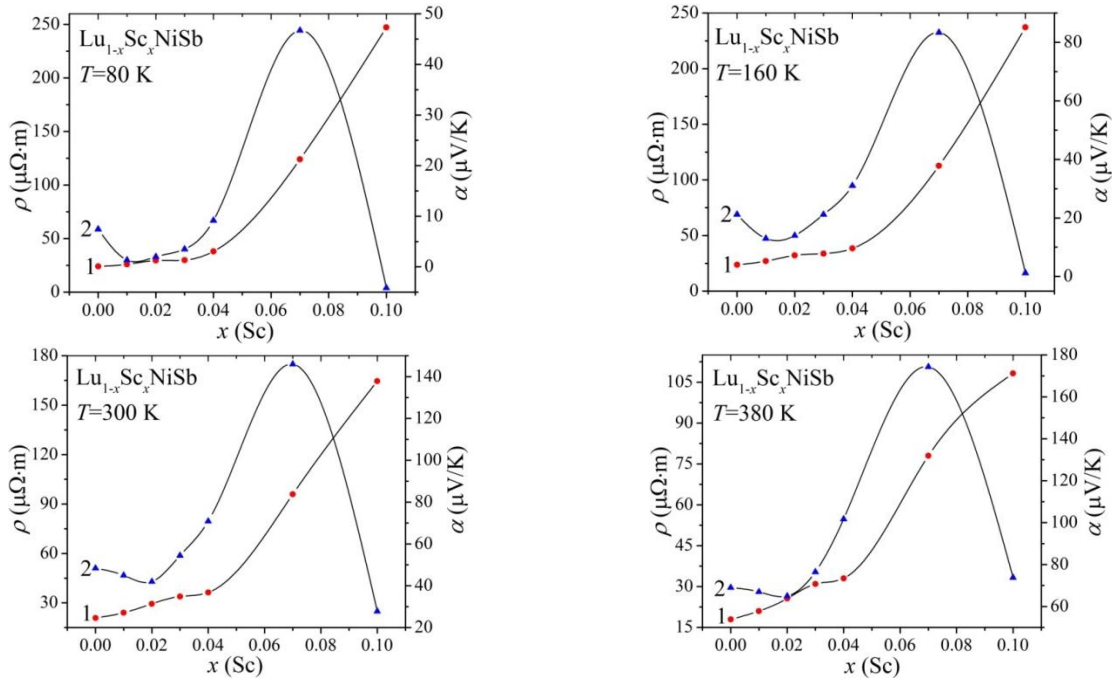


Fig. 3. Change in the values of resistivity  $\rho(x, T)$  (1) and the thermopower coefficient  $\alpha(x, T)$  (2)  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  at different temperatures

We can state that the substitution of Lu atoms by Sc atoms in  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  generates structural defects of neutral nature, and the occupation of vacancies by Sc atoms simultaneously eliminates the structural defect of acceptor nature and when Sc atoms are filled, the structural defect of acceptor nature and the corresponding acceptor zone  $\varepsilon_A^1$  are eliminated and a structural defect is formed. donor zone  $\varepsilon_D^1$ .

The analysis of energy characteristics of  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  turned out to be interesting. It is known that in  $p\text{-LuNiSb}$  the Fermi level  $\varepsilon_F$  is located at a distance of 10.2 meV from the edge of the valence band  $\varepsilon_V$ , and the amplitude of modulation of the zones of continuous energies is  $\varepsilon_1^\alpha = 35.3$  meV (Fig. 4). High values of the activation energy  $\varepsilon_1^\alpha$  indicate the presence of a significant number of uncontrolled donors in  $p\text{-LuNiSb}$ , and the position of the Fermi level  $\varepsilon_F$  is determined by the ratio of the concentrations of ionized acceptors and donors. And if the nature of the acceptors is related to the presence of structural defects of  $p\text{-LuNiSb}$  in the form of vacancies in positions 4a and 4c, the origin of the donors is related to the purity of the source components and the technology of obtaining materials.

Analysis of the behavior of  $\varepsilon_1^\rho(x)$   $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  shows (Fig. 4) that at the concentration range  $x=0-0.07$  the change in the activation energy values  $\varepsilon_1^\rho(x)$  is almost linear, and the velocity of the Fermi level  $\varepsilon_F$  from the valence band  $\varepsilon_V$  is constant and is  $\Delta\varepsilon_F/\Delta x = 4.9$  meV/% Sc. At a concentration,  $x \geq 0.07$ , the angle of inclination of the dependence  $\varepsilon_1^\rho(x)$  increases, which indicates an increase in the velocity of the Fermi level  $\varepsilon_F$

from the valence band to the values of  $\Delta\varepsilon_F/\Delta x = 11.2$  meV/% Sc. The presence of a difference in the velocities of the Fermi level  $\varepsilon_F$  from the valence band  $\varepsilon_V$  to the middle of the band gap  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  indicates different rates of generation of acceptors and donors. Thus, at the concentration  $x \geq 0.07$  the concentration of donors increases  $\sim 2$  times faster than at the site  $x=0-0.07$ . And this is caused by various changes in the crystal structure of  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  depending on the concentration of Sc atoms.

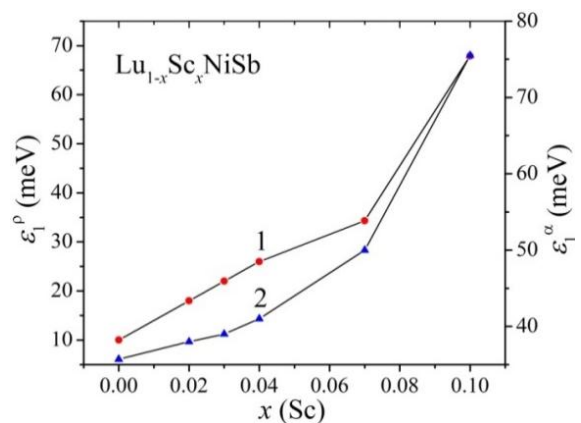


Fig. 4. Change in the values of activation energies  $\varepsilon_1^\rho(x)$  (1) and  $\varepsilon_1^\alpha(x)$  (2)  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$

Thus, the results of experimental studies of sensitive elements of temperature transducers based on  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  material completely coincide with the

results of modeling their kinetic characteristics under the presence of vacancies in the crystallographic positions 4a and 4c of Lu and Ni atoms, respectively [1]. Experimental studies of the electrokinetic, energy and magnetic properties of  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$  have revealed different rates of generation of structural defects of acceptor and donor nature at different concentrations, which is due to different mechanisms of Sc atoms entering the semiconductor matrix. The obtained results allow to specify the spatial arrangement of atoms in the nodes of the unit cell, 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.

### 7. Modeling of Function of Transformation of Sensitive Elements on Basis of Thermometric Material $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$

Simulation of the conversion functions of the sensitive elements of the resistance thermometer and thermoelectric transducer in the temperature range 4.2–1000 K was performed using the Full Potential Linearized Augmented Plane Waves method using the Elk software package [8]. The results of experimental measurements served as reference currents in modeling the characteristics.

In fig. 5, as an example, the conversion functions of the sensitive element of the resistance thermometer based on the thermometric material  $\text{Lu}_{0.99}\text{Sc}_{0.01}\text{NiSb}$  and the thermoelectric pair Pt-  $\text{Lu}_{0.99}\text{Sc}_{0.01}\text{NiSb}$  are given. We can see that the obtained sensitive elements of thermocouples based on the latest thermometric materials have a high sensitivity. The ratio of the change in the values of the thermopower coefficient to the range of temperature measurements in thermocouples is greater than all known industrial thermocouples. In addition, the

temperature coefficient of resistance (TCR) of the obtained resistance thermometers is higher than the TCR of metals but is inferior to the value of TCR of sensitive elements made of traditional semiconductors. At the same time, none of the known resistance thermometers based on traditional semiconductors provides stable characteristics at temperatures of  $4.2 \div 1000$  K.

### 8. Conclusions

Studies of structural, kinetic, energy, and magnetic properties of sensitive elements of thermotransducers based on the thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0-0.10$ , showed that the results of the experiment and modeling of characteristics are consistent [1]. The relationship between the spatial arrangement of atoms in the nodes of the unit cell (crystal structure) and the mechanisms of electrical conductivity of the thermometric material  $\text{Lu}_{1-x}\text{Sc}_x\text{NiSb}$ ,  $x=0-0.10$ . This allows us to determine the conditions of thermometric materials synthesis with the maximum efficiency of conversion of thermal into electrical energy. The regularities of the transformation functions of the sensitive element of the resistance thermometer based on the thermometric material  $\text{Lu}_{0.99}\text{Sc}_{0.01}\text{NiSb}$  and the thermoelectric pair Pt- $\text{Lu}_{0.99}\text{Sc}_{0.01}\text{NiSb}$  are established.

### 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.

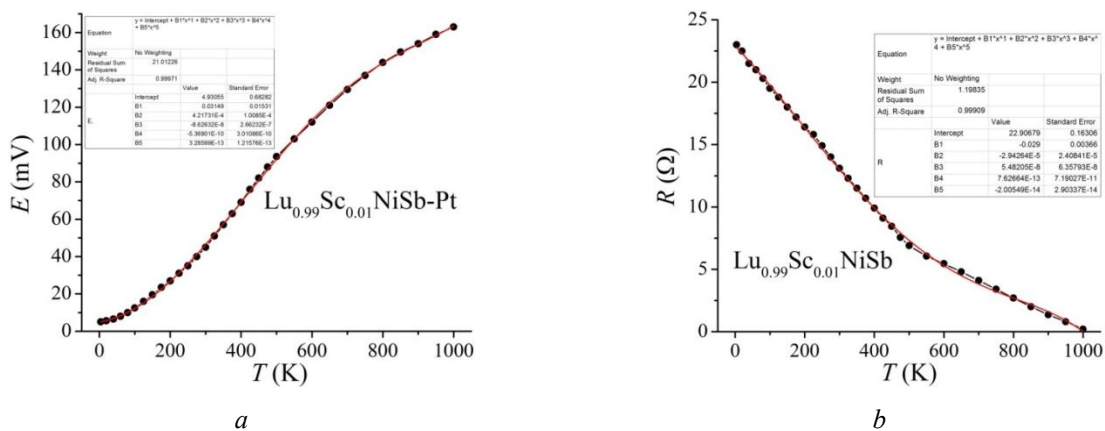


Fig. 5. Thermometric characteristics of resistance (a) and thermoelectric (b) thermometers based on thermometric material  $\text{Lu}_{0.99}\text{Sc}_{0.01}\text{NiSb}$

## References

- [1] V. Pashkevych, V. Krayovskyy, A. Horpenuk, V.A. Romaka, Yu. Stadnyk, L. Romaka, A. Horyn, V.V. Romaka. *Measuring Equipment and Metrology*, vol.83, no.2, p.21–25, 2022. (DOI: <https://doi.org/10.23939/istcmtm2022.02.021>).
- [2] M. Schruter, H. Ebert, H. Akai, P. Entel, E. Hoffmann, G.G. Reddy. *Phys. Rev. B*, vol.52, p.188–209, 1995. (<https://doi.org/10.1088/0953-8984/1/43/006>).
- [3] All-electron full-potential linearised augmented-plane wave (FP-LAPW) code – <http://elk.sourceforge.net>.
- [4] K. Wolanska, K. Synoradzki, K. Ciesielski, K. Zaleski, P. Skokowski, D. Kaczorowski. *Mater. Chem. Phys.*, vol.227, p. 29–36, 2019. (<https://doi.org/10.1016/j.matchemphys.2019.01.056>).
- [5] K. Synoradzki, K. Ciesielski, I. Veremchuk, H. Borrmann, P. Skokowski, D. Szymanski, Y. Grin, D. Kaczorowski. *Materials*, vol.12, p.1723–1730, 2019. (<https://doi.org/10.3390/ma12101723>).
- [6] B. Karla, J. Pierre, R. Skolozdra. *J. Alloys Compd.*, vol.265, p.42–50, 1998. ([https://doi.org/10.1016/S0925-8388\(97\)00419-2](https://doi.org/10.1016/S0925-8388(97)00419-2)).
- [7] T. Roisnel, J. Rodriguez-Carvajal. WinPLOTTR: a Windows Tool for Powder Diffraction Patterns analysis, *Mater. Sci. Forum, Proc. EPDIC7*, vol.378–381, p.118–123, 2001. (<https://doi.org/10.4028/www.scientific.net/MSF.378-381.118>).
- [8] B.I. Shklovskii, A.L. Efros. *Electronic Properties of Doped Semiconductors*. NY, Springer-Verlag, 1984. (<http://doi.org/10.1007/978-3-662-02403-4>).
- [9] N.F. Mott, E.A. Davis. *Electron processes in non-crystalline materials*. Oxford, Clarendon Press, 1979. [https://books.google.com.ua/books?hl=uk&lr=&id=P11b\\_yhKH-YC&oi=fnd&pg=PP1&dq=N.F.+Mott,+E.A.+Davis.+Electron+processes+in+non-crystalline+materials.&ots](https://books.google.com.ua/books?hl=uk&lr=&id=P11b_yhKH-YC&oi=fnd&pg=PP1&dq=N.F.+Mott,+E.A.+Davis.+Electron+processes+in+non-crystalline+materials.&ots)
- [10] V.A. Romaka, Yu. Stadnyk, V. Krayovskyy, L. Romaka, O. Guk, V.V. Romaka, M. Mykyuchuk, A. Horyn. *The latest heat-sensitive materials and temperature transducers*. Lviv Polytechnic Publishing House, Lviv, 2020. ISBN 978-966-941-478-6. [in Ukrainian]. (<https://opac.lpnu.ua/bib/1131184>).