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The influence of heavy doping of TiCoSb intermetallic semiconductor with Cr atoms on structural, kinetic and energetic properties

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The structural, electrokinetic, and energetic properties of the TiCo₁₋ₓCrₓSb semiconductor obtained by doping TiCoSb with Cr atoms introduced into the structure by substituting Co atoms in the crystallographic position 4c were studied. It was shown that in TiCo₁₋ₓCrₓSb the structural defects of donor and acceptor nature are generated simultaneously in different ratios depending on the impurity concentration. At concentrations of x ≥ 0.02, the conductivity of TiCo₁₋ₓCrₓSb has a metallic character, and the contribution of current carrier scattering mechanisms to the value of electrical resistivity is of the same order as changes in the concentration of current carriers. It was established that at all temperatures in the range of concentrations x = 0–0.02, the rate of generation of donors exceeds the rate of generation of acceptors, and at concentrations x > 0.02, on the contrary, the rate of generation of acceptors is greater than that of donors. This is indicated by the positive values of thermopower coefficient a(x,T) of TiCo₁₋ₓCrₓSb for x > 0.03.

Keywords: semiconductor, electrical conductivity, thermopower coefficient, Fermi level.

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Introduction

The interest in semiconductor solid solutions based on half-Heusler phases (MgAgAs-type, space group F4̅3m [1]) is caused by the possibility, through appropriate doping of basic semiconductors, to smoothly change their values of electrical conductivity σ, thermopower coefficient α, and thermal conductivity κ and to obtain high values of thermoelectric factor Z (Z = α²σ/κ) [2, 3]. In this context, studies of the intermetallic semiconductor TiCoSb heavily doped with Cr impurity (3d⁶4s⁴), introduced into the structure by replacement of Co atoms (3d⁶4s²) in the crystallographic position 4c, are interesting. Since the Cr atom contains less 3d- electrons than the Co atom, the appearance of impurity acceptor states εₐ in the band gap εₘ was expected. In turn, by changing the concentration of such states, we can change the compensation degree of the semiconductor TiCo₁₋ₓCrₓSb [2, 4] and the mechanism of electrical conductivity. This makes it possible to optimize the kinetic properties of the thermoelectric material to increase the efficiency of converting thermal energy into electrical one [2, 3].

By comparing the results of experimental studies and calculated electronic structure of the TiCoSb semiconductor, the authors [5] established the defectiveness of its crystal structure. A model of such structure and a mechanism of simultaneous "a priori doping" of TiCoSb with donor and acceptor impurities was proposed, which now becomes heavily doped and highly compensated [5]. The model provides the presence of about ~1% vacancies (Vₐ) in the crystallographic position 4a of Ti atoms, and additional Co⁺⁺ atoms (~1%) are located in the tetrahedral voids of the structure. As a
The values of the unit cell parameter of the samples were calculated using the Fullprof Suite program of the EPMA. The characterization of the annealed samples, the as-cast titanium telluride, and the mechanism of electrical conductivity [7].

For the ordered variant of the TiCo$_1$Cr$_x$Sb crystal structure, the electronic structure was modeled by the KKR method (Korringa-Kohn-Rostocker method) in the approximation of the coherent potential of the CPA and the local density of the LDA [9] using the exchange-correlation potential Moruzzi-Janak-Williams (the licensed software AkaiKKR and SPR-KKR) [10]. To model the energy characteristics by calculating the DOS the Brillouin zone was divided into 1000 k-points. To capture all semi-core states of p-electrons the width of the energy window was chosen of 22 eV. The calculation accuracy of the Fermi level position is ± 4 meV. Measurements of the temperature and concentration dependences of the electrical resistivity $\rho(T,x)$ and the thermopower coefficient $\alpha(T,x)$ (relative to the copper) of TiCo$_1$Cr$_x$Sb samples were performed in the ranges: $T = 80$–400 K, $x = 0.01$–0.10. To reduce an influence of a possible p-n junction at the contact points measurements of the voltage drop on the samples were carried out in different current directions [2].

II. Study of structural properties of TiCo$_{1-x}$Cr$_x$Sb

According to the microprobe analysis data of the samples TiCo$_{1-x}$Cr$_x$Sb, $x = 0$–0.10, the concentration of atoms on the surface of the studied samples is in accordance with the composition of the charge. In turn, the X-ray phase analysis of TiCo$_{1-x}$Cr$_x$Sb samples did not reveal traces of impurity phases, and the main phase is indexed in the MgAgAs structure type [1]. Given that the concentration of impurity Cr atoms is insignificant, it was impossible to detect the fact of the ordering of the TiCo$_1$Cr$_x$Sb crystal structure by X-ray methods.

The calculated lattice parameter $a(x)$ of TiCo$_{1-x}$Cr$_x$Sb samples, $x = 0$–0.10 revealed a complex nature of behavior with changes in chromium content (Fig. 1). Thus, in the concentration range $x = 0$–0.02, the lattice parameter values $a(x)$ predictably increase since the atomic radius of Cr ($r_C = 0.128$ nm) is slightly greater than the atomic radius of Co ($r_C = 0.125$ nm). It is important to understand that the occupation of vacancies (Va) by Cr atoms in the 4a position of Ti atoms [5] can also cause an increase in the values of the unit cell parameter $a(x)$ of TiCo$_{1-x}$Cr$_x$Sb. However, the maximum observed on the dependence $a(x)$ of TiCo$_{1-x}$Cr$_x$Sb at $x \approx 0.02$ and the subsequent decrease of $a(x)$ values at $x > 0.02$ is unexpected. It appears that in TiCo$_{1-x}$Cr$_x$Sb simultaneous partial replacement by Cr atoms in position 4a of larger Ti atoms ($r_T = 0.146$ nm) is also possible. In the semiconductor solid solution TiCo$_{1-x}$Mn$_x$Sb, we observed a similar behavior of the unit cell parameter $a(x)$ with increasing concentration of Mn atoms (Fig. 1, inset) [7]. It was shown that doping of TiCoSb with Mn atoms simultaneously generates an acceptor band $\epsilon_A$ (substitution of Co atoms by Mn) and donor band $\epsilon_D$ of different nature.

Therefore, we can assume that alloying of TiCoSb with Cr atoms introduced into the structure by replacing Co atoms is accompanied by simultaneous changes in the crystallographic positions of Ti (4a) and Co (4c) atoms. This leads to the simultaneous appearance in the crystal structure of TiCo$_1$Cr$_x$Sb in different ratios of donor and
acceptor structural defects. It is clear that changes in the crystal structure of TiCo₁₋ₓCrₓSb will be reflected by changes in the electronic structure. Thus, in the case of substitution of Ti atoms (3d²4s²) for Cr atoms (3d⁶4s¹) in position 4a or their occupation of vacancies (Va) in TiCo₁₋ₓCrₓSb, structural defects of the donor nature will be generated (Cr atom contains more d-electrons than Ti). At the same time, partial occupation of vacancies by Cr atoms will simultaneously lead to a decrease by the same number of acceptor states that existed in TiCoSb. As a result, two kinds of donor states will appear in the band gap ε₁ of the TiCo₁₋ₓCrₓSb semiconductor near the donor band εD¹: when Ti atoms are replaced by Cr atoms (donor band εD¹) and when vacancies are occupied (donor band εD³).

**III. Modeling of the properties of TiCo₁₋ₓCrₓSb for an ordered version of the structure**

To predict the behavior of the Fermi level εF, the band gap ε₁, and the kinetic properties of TiCo₁₋ₓCrₓSb, the DOS (density of electronic states) was calculated for the ordered version of the crystal structure of the semiconductor (Fig. 2). This involves only substitution of Co atoms with Ti atoms in the 4c position.

**Fig. 2. DOS calculation for the ordered version of the TiCo₁₋ₓCrₓSb structure.**

Fig. 2 shows that in TiCoSb the Fermi level εF (dashed line) is located in the band gap ε₁ near the edge of the conduction band εC and electrons are the main current carriers. As mentioned above, the substitution of Co atoms for Cr atoms generates structural defects of an acceptor nature, then at the impurity concentration x = 0.01 in the TiCo₀.₉₉Cr₀.₀₁Sb semiconductor, the Fermi level εF will move away from the conduction band εC and will be located near the middle of the band gap ε₁. An increase in the concentration of impurity Cr atoms will be accompanied by an increase in the concentration of acceptors. At the same time, the Fermi level εF will approach, and later enter the valence band εV TiCo₁₋ₓCrₓSb: a dielectric-metal conduction transition will occur, which is the Anderson transition [11]. In the experiment, such a movement of the Fermi level εF will lead to a change in the sign of the thermopower coefficient α(x,T), and the holes will become the main current carriers. At the same time, the type of conductivity of the TiCo₁₋ₓCrₓSb semiconductor will also change from activation to metallic [2, 4], and the temperature dependences of the specific electrical resistivity will not contain activation areas. The electrical resistivity of TiCo₁₋ₓCrₓSb will increase with increasing temperature. It is important that the band gap ε₁ is preserved between the conduction band εC and the valence band εV of TiCo₁₋ₓCrₓSb.

DOS calculation for the ordered version of the TiCo₁₋ₓCrₓSb structure allows modeling the behavior of the kinetic properties of the semiconductor, in particular, ρ(x,T) and α(x,T) (Fig. 3). Modeling the behavior of the thermopower coefficient α(x,T), as expected, shows positive values at all temperatures for concentrations of...
TiCo$_1.x$Cr$_x$Sb, $x > 0.01$, and the maximum values of $\alpha(x, T)$ are reached at $x \approx 0.08$. Since the value of the specific electrical resistivity is inversely proportional to the density of states at the Fermi level, the 1/DOS($\epsilon_F$) dependence allows us to predict the behavior of the electrical resistivity of the TiCo$_1.x$Cr$_x$Sb semiconductor (Fig. 3b).

We can see that the dependence 1/DOS($\epsilon_F$) passes through a maximum at the concentration of Cr atoms, $x \approx 0.01$, and then rapidly decreases and reaches quasi-saturation at $x > 0.07$. This behavior of 1/DOS($\epsilon_F$) is understandable, because the growth of the dependence in the section $x = 0$−0.01 is associated with the crossing of the Fermi level $\epsilon_F$ of the middle of the band gap $\epsilon_g$, which will cause the smallest values of DOS($\epsilon_F$) and the maximum values of $\rho(x, T)$ TiCo$_1.x$Cr$_x$Sb. When the concentration of the Cr impurity increases, $x > 0.01$, the Fermi level $\epsilon_F$ will move in the direction of the valence band $\epsilon_v$. This will lead to an increase in both the concentration of holes and the density of states at the Fermi level of TiCo$_1.x$Cr$_x$Sb. Experimental studies of the properties of TiCo$_1.x$Cr$_x$Sb will show the degree of correctness of the modeling results.

IV. Study of kinetic and energetic properties of TiCo$_{1-x}$Cr$_x$Sb

The change in values with temperature of the specific electrical resistivity $\rho$ and the thermopower coefficient $\alpha$ of TiCo$_{1-x}$Cr$_x$Sb, $x = 0$−0.10, is shown in Fig. 4. For TiCo$_{1-x}$Cr$_x$Sb samples at compositions $x = 0$ and $x = 0.01$, we can see activation parts at high temperatures on the dependences ln($\rho(1/T, x)$) and $\alpha(1/T, x)$. This is evidence of the location of the Fermi level $\epsilon_F$ in the band gap $\epsilon_g$. Since at all temperatures the sign of the thermopower coefficient of TiCo$_{1-x}$Cr$_x$Sb samples at $x = 0$ and $x = 0.01$ is negative, the main carriers of electric current are electrons. At the same time, the Fermi level $\epsilon_F$ is close to the conduction band $\epsilon_c$. Therefore, TiCo$_{1-x}$Cr$_x$Sb samples with compositions $x = 0$ and $x = 0.01$ are doped and compensated semiconductors of the electronic conductivity type [4]. Their temperature dependence of the resistivity ln($\rho(1/T, x)$) (Fig. 4) can be described by the well-known expression (1) [4]:

$$\rho^{-1}(T) = \rho_1^{-1}e^x\left(\frac{\epsilon_1^{0}}{k_B T}\right) + \rho_3^{-1}e^x\left(\frac{\epsilon_3^{0}}{k_B T}\right), \tag{1}$$

where the first term describes the activation of current carriers $\epsilon_1^{0}(x)$ from the Fermi level $\epsilon_F$ into the conduction band $\epsilon_C$, and the second term describes the jump conduction $\epsilon_3^{0}(x)$ with energies close to the Fermi level $\epsilon_F$. For semiconductors TiCo$_{1-x}$Cr$_x$Sb with compositions $x = 0$ and $x = 0.01$, the thermopower coefficient $\alpha(1/T, x)$ (Fig. 4) changes with temperature according to expression (2) [11]:

$$\alpha = \frac{k_B}{e}\left(\frac{\epsilon_1^{0}}{k_B T} - \gamma + 1\right), \tag{2}$$

where $\gamma$ depends on the scattering mechanisms. Based on formula (2), the values of the activation energies $\epsilon_1^{0}(x)$ and $\epsilon_3^{0}(x)$ were calculated. The authors of [2] showed that in heavily doped compensated semiconductors, the values of the activation energies $\epsilon_1^{0}(x)$ are proportional to the amplitude of the large-scale fluctuation of the continuous energy bands. The amplitude of the band modulation is proportional to the compensation degree of the semiconductor [4].

Based on formulas (1) and (2), the depth of the Fermi level $\epsilon_F$ was calculated and the change in the degree of compensation of the semiconductor TiCo$_{1-x}$Cr$_x$Sb was estimated by calculating the values of $\epsilon_1^{0}(x)$. In the semiconductor TiCoSb, the depth of the Fermi level $\epsilon_F$ relative to the conduction band $\epsilon_C$ (negative values of the thermopower coefficient) is $\epsilon_F^{0} = 100.6$ meV, and the amplitude of the bands reaches $\epsilon_1^{0} = 214.1$ meV. The obtained results of activation energy values for TiCoSb coincide with literature data [2, 5].

Doping TiCoSb with the smallest concentration of Cr atoms in the experiment, $x = 0.01$, rapidly brought the Fermi level $\epsilon_F$ closer to the conduction band $\epsilon_C$ by a distance of $\epsilon_F^{0} = 7.3$ meV. This behavior of the Fermi level in TiCo$_{0.99}$Cr$_{0.01}$Sb is possible either under the condition of a rapid increase in the concentration of donor states or a rapid decrease in the band gap $\epsilon_g$ due to the redistribution of electronic states. We can assume that in TiCo$_{0.99}$Cr$_{0.01}$Sb, these phenomena occur simultaneously.
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Likewise, the amplitude of the fluctuation of the continuous energy bands of TiCo$_{0.99}$Cr$_{0.01}$Sb decreased rapidly to the value $\varepsilon_1 = 14.1$ meV, indicating a decrease in the compensation degree, and the semiconductor becomes weakly compensated when the concentration of donor states far exceeds that of acceptor states.

As mentioned above, in TiCo$_{1-x}$Cr$_x$Sb this is possible in cases of partial replacement of Ti atoms (3$d^2$4$s^2$) by Cr atoms (3$d^5$4$s^1$) in position 4$a$ or occupation of vacancies (Va) by Cr atoms. Considering that at concentrations of TiCo$_{0.5}$Cr$_{0.5}$Sb, $x = 0-0.01$, the lattice parameter $a(x)$ increases (Fig. 1), we can assume that vacancies (Va) in position 4$a$ are occupied by Cr atoms, which simultaneously generates donor states and decreases by the same number of acceptor states ($\varepsilon_A$ band) that existed in TiCoSb [5]. Let us recall that in the case of substitution of Ti atoms with Cr atoms in position 4$a$ in the semiconductor TiCo$_{1-x}$Cr$_x$Sb, donor states will also be generated, but in this case, the lattice parameter $a(x)$ should decrease ($r_T = 0.128$ nm and $r_T = 0.146$ nm). Therefore, the option of Cr atoms occupying vacancies (Va) in position 4$a$ at concentrations $x = 0-0.01$ looks more convincing.

At concentrations $x \geq 0.02$ at all investigated temperatures, the activation parts disappear on the dependences $\ln(\rho(T,x))$ of TiCo$_{1-x}$Cr$_x$Sb, and the resistivity values $\rho(T,x)$ tend to increase, which is characteristic of the metallic type of conductivity (Fig. 4). This can happen either if the Fermi level $\varepsilon_F$ leaves the band gap $\varepsilon_g$ and is located in the continuous energy bands, or the band gap itself $\varepsilon_g$ disappears when the continuous energy bands are overlapped due to the redistribution of electronic states. When TiCoSb is alloyed with Mn atoms by replacing Co atoms on the dependences $\ln(\rho(T,x))$ TiCo$_{1-x}$Mn$_x$Sb, $x = 0-0.10$, activation areas occurred at high temperatures and all concentrations. This experimental result indicated the location of the Fermi level $\varepsilon_F$ in the band gap $\varepsilon_g$ of the semiconductor TiCo$_{1-x}$Mn$_x$Sb [7].

The answer to the question about the location of the Fermi level $\varepsilon_F$ in TiCo$_{1-x}$Cr$_x$Sb for $x \geq 0.02$ is given by the analysis of the behavior of the thermopower coefficient $\alpha(T,x)$, which rapidly decreases, for example, at $T = 300$ K from $\alpha_{x=0.02} = -10$ $\mu$V/K to $\alpha_{x=0.05} = 0.04$ $\mu$V/K and $\alpha_{x=0.1} = 1.1$ $\mu$V/K (Fig. 4). Thus, in the concentration range $0.02 \leq x < 0.05$, the values of the thermopower coefficient...
\( \alpha(T,x) \) of TiCo\(_{1-x}\)CrSb are negative, and at concentrations 0.05 \(< x \) – positive. This behavior \( \alpha(T,x) \) is fundamentally consistent with the results of modeling the electronic structure for the ordered structure (Fig. 2). On the other hand, a slight increase in impurity concentration is sufficient for the transition of the Fermi level \( \varepsilon_F \) from the conduction band \( \varepsilon_C \) to the valence band \( \varepsilon_V \). This could indicate a rapid decrease in the band gap \( \varepsilon_g \) of the TiCo\(_{1-x}\)CrSb semiconductor.

The behavior \( \rho(x,T) \) and \( \alpha(x,T) \) of TiCo\(_{1-x}\)CrSb at different temperatures is interesting (Fig. 5). The analysis of the concentration dependences \( \rho(x,T) \) and \( \alpha(x,T) \) of TiCo\(_{1-x}\)CrSb complements the obtained results and conclusions. Doping by the smallest concentration of the Cr impurity in the experiment leads to a rapid decrease in the electrical resistivity, for example, at \( T = 80 \) K from the value \( \rho_{x=0.02} = 14170 \) \( \mu \Omega \cdot m \) to \( \rho_{x=0.01} = 139.3 \) \( \mu \Omega \cdot m \). A decrease in the electrical resistivity \( \rho(x,T) \) at concentrations \( x = 0.01 \) indicates a rapid increase in the electron concentration. This result correlates with the nature of the change in the Fermi level \( \varepsilon_F \) position which in TiCo\(_{0.95}\)Cr\(_{0.05}\)Sb approached the conduction band level \( \varepsilon_C \). We can also assume a rapid decrease in the width of the band gap \( \varepsilon_g \) of the semiconductor. The obtained experimental results of the change in specific electrical resistivity \( \rho(x,T) \) correspond to the results of calculations for an ordered version of the crystal structure of the semiconductor (Fig. 2).

At concentrations \( x > 0.01 \), when the Fermi level \( \varepsilon_F \) is located in the continuous energy band and the conductivity has a metallic character, we do not, however, observe a monotonous change of the \( \rho(x,T) \) and \( \alpha(x,T) \) values. Thus, at concentrations \( x = 0.01--0.02 \), the electrical resistivity \( \rho(x,T) \) increases. If the Fermi level \( \varepsilon_F \) is in the band gap \( \varepsilon_g \) of TiCo\(_{0.95}\)Cr\(_{0.05}\)Sb, then the change in the values of the resistivity would be associated exclusively with a decrease in the concentration of electrons (negative values of \( \alpha(x,T) \)). The reason for such a decrease would be the generation of acceptors that capture electrons. However, the insert in Fig. 5a shows that in the semiconductor TiCo\(_{0.95}\)Cr\(_{0.05}\)Sb, the values of resistivity \( \rho(x,T) \) are higher, the higher the temperature. It is in this order that the dependences of electrical resistivity \( \rho(x,T) \) are located for \( x > 0.02 \). This behavior of the electrical resistivity \( \rho(x,T) \) is characteristic of metals when the increase in resistivity is caused by the action of current carrier scattering mechanisms. Therefore, we cannot attribute the growth of the electrical resistivity of TiCo\(_{1-x}\)CrSb at concentrations \( x = 0.01--0.02 \) only to a decrease in the concentration of electrons, and the changes due to the scattering of current carriers in TiCo\(_{1-x}\)CrSb are of the same order as the changes which are associated with a change in the concentration of current carriers.

At concentration \( x = 0.02 \) at all investigated temperatures, an extremum appears in the \( \rho(x,T) \) dependence of TiCo\(_{1-x}\)CrSb. The appearance of an extremum on the \( \rho(x,T) \) dependence in a semiconductor of the electronic conductivity type is the result of a change in the ratio of ionized donor and acceptor states in favor of acceptors. Indeed, at concentrations of Cr impurity atoms, \( x > 0.03 \), the sign of \( \alpha(x,T) \) for TiCo\(_{1-x}\)CrSb becomes positive (Fig. 5b inset). This is possible, as mentioned above, only when Cr atoms occupy the 4c crystallographic position of Co atoms. However, this should lead to an increase in the lattice parameter \( a(x) \) of TiCo\(_{1-x}\)CrSb. In the experiment, we observe a monotonous decrease.

We can assume that in the TiCo\(_{1-x}\)CrSb semiconductor, both the substitution of Co atoms for Cr atoms in position 4c, which generates acceptor states, and the occupation of crystallographic position 4e by Cr atoms, which generates donor states, occur simultaneously at different rates. The given experimental results do not allow us to obtain numerical values of the rate of generation of acceptor and donor states, which can be done only by comparing the results of experimental measurements of structural and kinetic properties with modeling of these properties for different cases of arrangement of atoms in the unit cell. However, these results are beyond the scope of this paper.

**Conclusions**

According to the performed study of the structural, electrokinetic, and energy properties of the TiCo\(_{1-x}\)CrSb semiconductor obtained by doping TiCoSb with Cr atoms introduced into the structure by replacing Co atoms in the 4c crystallographic position, it was shown that in
TiCo$_1_\alpha$Cr$_x$Sb the structural defects of donor and acceptor nature are generated simultaneously. At concentrations $x \geq 0.02$, the conductivity of TiCo$_1_\alpha$Cr$_x$Sb has a metallic character, and the contribution of current carrier scattering mechanisms to the value of electrical resistivity is of the same order as changes in the concentration of current carriers. It was established that at all temperatures in the concentration range $x = 0.02$, the rate of generation of donors exceeds the rate of generation of acceptors, and at concentrations $x > 0.02$, on the contrary, the rate of generation of acceptors is greater than that of donors. This is indicated by the positive values of thermopower coefficient $\alpha(x,T)$ of TiCo$_1_\alpha$Cr$_x$Sb at $x > 0.03$. To understand the mechanism of structural and energy transformations in TiCo$_1_\alpha$Cr$_x$Sb, it is necessary to simulate these properties for different cases of atom arrangement in the unit cell.

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Вплив сильного легування інтерметалічного напівпровідника TiCoSb
атомами Cr на структурні, кінетичні та енергетичні властивості

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Досліджено структурні, електрокінетичні та енергетичні властивості напівпровідника TiCo₁₋ₓCrₓSb,
отриманого легуванням TiCoSb атомами Cr, уведенням у структуру шляхом заміщення у
кристалографічній позиції 4c атомів Co. Показано, що у TiCo₁₋ₓCrₓSb одночасно у різних співвідношеннях
залежно від концентрації домішки генеруються структурні дефекти донорної та акцепторної природи. За
концентрації х ≥ 0.02 провідність TiCo₁₋ₓCrₓSb носить металічний характер, а внесок від дії механізмів
розсіювання носіїв струму у значення електроопору є одного порядку зі змінами концентрації носіїв
струму. Встановлено, що за всіх температур на ділянці концентрацій х = 0–0.02 швидкість генерування
донорів переважає швидкість генерування акцепторів, а за концентрацій х > 0.02 навпаки, швидкість
genерування акцепторів є більшою, ніж донорів. На це вказують додатні значення термо-ерс
(TiCo₁₋ₓCrₓSb за х > 0.03. Для розуміння механізму структурних та енергетичних перетворень у
TiCo₁₋ₓCrₓSb необхідно провести моделюванням цих властивостей за різних варіантів просторового
розміщення атомів у вузлах комірки.

Ключові слова: напівпровідник, електропровідність, коєфіцієнт термо-ерс, рівень Фермі.