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The Character of Phaseformation in the In_2Te_3-$Cu_2Ga_4Te_7$ System and Some Electrophysikal Properties in the Solid Solutions $(Cu_2Ga_4Te_7)_{1-X}$ - $(In_2Te_3)_X$

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Abstract **– By the methods of the character of physical-chemical interaction analysis, determination of density and by measurement of microhardness the character of chemical interaction in the In_2Te_3-$Cu_2Ga_4Te_7$ has been investigated and its faze diagram has been plotted. It is established that the system is quasibinary, of eutectic type. In the system the chemical combination of $CuGa_2InTe_7$ composition melting congruently at 855^{0}C is generated. There have been revealed solid solutions boundary of which based on $Cu_2Ga_4Te_7$ - 7mol%. at room temperatures.**

Keywords **– Qnasibinary System, Faze Diagram, Solid Solutions, Dispersion of Phonons, Thermoelectric Efficiency, Electronic Structures.**

I. INTRODUCTION

Chalcogenides of copper, gallium and indium, as well solid solutions on their base are widely used in semiconducting electronics [1-3]. Therefore, obtaining the new complicated homogeneons phases based on them presents actuality for science and technics.

The triple chalcogenides with participation of copper and elements of III subgroup crystallized in a structure of chalcopyrites were earlier synthesized by khan and collaborators [3]. It is established that compounds of $A^1B^{III}C_2^{VI}$ type mainly holey conductivity, high coefficient of thermo e.m.f., high photoconductivity and possess rectification on dotted contact [4,5]. The complex system In_2Te_3-$Cu_2Ga_4Te_7$ has not been investigated yet up to preset.

The aim of the present work is revealing the character of physical-chemical interaction in the In_2Te_3-$Cu_2Ga_4Te_7$ system with plotting a state diagram.

Compounds In_2Te_3 melts congruently at 667^{0}C and crystallizes in cubic syngony with a parameter of lattice a=6,146A^0 (F43m-T_d^2). Picknometric density is equal to d=5,78g/sm^3 and microhardnese $H\mu$ =1660 MPa [6]. It is semiconductor with thickness of the prohibited zone equal to~0,96eV.

Compound $Cu_2Ga_4Te_7$ also melts congruently at 874^{0}C and crystallizes in cubic syngony of ZnS type, lattice parameter $a = 5.93\,\overset{0}{A}(T_d^2 - F43m)$. It has a density d=5.84q/sm^3 and microhardness H_μ =3100 MPa [7].

Temperature dependences of electric conductivity [6]., the coefficient of thermoelectric power of general heat conductivity (degen.) Halls mobility of charge carriers (u_x) of solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$, where x=0.03; 0.05 have been investigated. Simultaneously, by using the data of temperature dependence of general heat conductivity, temperature dependences of phonon heat resistance and bipolar constituent of heat conductivity have been calculated and constructed. The mechanisms of dispersion of electrons and phonons in the alloys of solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$, have been revealed. For the purpose of determining suitableness of synthesized alloys for preparation of thermoelectric of energy at different temperatures there has been calculated thermoelectric efficiency of the composition $(Cu_2Ga_4Te_7)_{0.95}(In_2Te_3)_{0.05}$.

II. EXPERIMENTAL PART

The alloys of the In_2Te_3-$Cu_2Ga_4Te_7$ system have been synthesized from the components In_2Te_3 and $Cu_2Ga_4Te_7$ in the vacuum quarts ampules at temperature 900-925^{0}C, while crystallization cycle was carried out in the mode of turned off above. The they carried out thermo homogenous annealing of the samples at 600 and 820^{0}C within 350h. The conditions of thermal treatment of alloys were chosen on the basis of preliminarily plotted diagram of fusibility.

At plotting a state diagram there were used the data received by the methods of differential-thermal (DTA), x-ray phase (x-ray A), microstructural (MSA) analyses, as well measurement of micro hardness and determination of picknometric density. DTA was conducted on low frequency thermorester of "HTP-73" mark with chromel-alumel thermocouples , x-ray was made by the method of powder on z-ray diffractometer of "DPOH-3 " mark (CuK α -radiation with Ni filter). Microstructure was determined with the use of the microscope "MUM-8". To etch the grinding and polished surfaces of alloys they used diluted mixture HNO_3+H_2O=1:1. Microhardness of the samples of investigated system was determined picknometrically where toluene served as a filler. Measurements of heat physical parameters were made on polycrystalline samples of a parallelepiped form in analogy with methods [8].

III. RESULTS AND DISCUSSION

The alloys of the In_2Te_3-$Cu_2Ga_4Te_7$ system were received in a form of solid bars. The composition rich in In_2Te_3 were of dark grey color and the alloys rich in $Cu_2Ga_4Te_7$ of more dark color. All the alloys are steady to

moisture and oxygen of air at room temperature. Organic dissolvent's don`t effect them. Alkalines and mineral acids, on the contrary, decompose their structure.

On the basis of the results of the above-mentioned methods of physical-chemical analysis the fragment faze diagram of In_2Te_3-$Cu_2Ga_4Te_7$ has been plotted (Fig1).

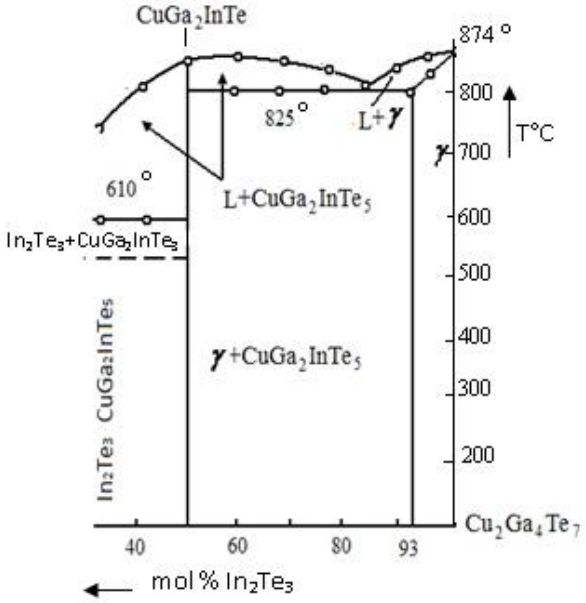

Fig.1. The fragment faze diagram of the In_2Te_3-$Cu_2Ga_4Te_7$ system

On thermograms of alloys two-three end thermal effects. In particular, on the side of In_2Te_3 the compositions had three temperature effects.

Faze diagram of the system turned to be of eutectic type with the formation of the complex chemical compound of $CuGa_2InTe_5$ composition. This compound is of congruently melting character, temperature of which corresponds to 855^0

On the basis of both initial compositions the regions of solid solutions are discovered, the boundaries of which at room temperature reach 7 mol% on side of $Cu_2Ga_4Te_7$.

The microstructural analysis has shown that compositions close to the initial components and the alloy containing 50 mol% $Cu_2Ga_4Te_7$ are one-phase.

The rest alloys are tow-phase what corresponds to quasibinary character of the system. In_2Te_3-$Cu_2Ga_4Te_7$ some physical-chemical properties of the alloys of the In_2Te_3-$Cu_2Ga_4Te_7$ system are cited in a table 1. By the results of x-ray A there were plotted steak x-ray grams of the initial compounds and received new phases (Fig.2). As is seen, arrangement and values of intensities of diffraction maxima of compounds $CuGa_2InTe_5$ a differed from such ones for the initial components, i.e. the results of DTA and MSA are in qualitative agreement with the results of x-ray A.

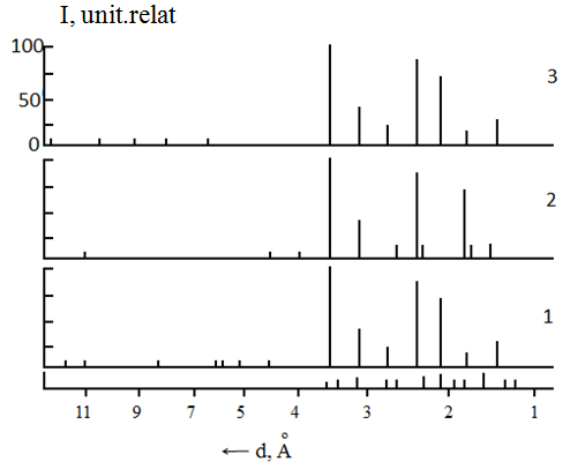

Fig.2. Schemes of steak X-rayograms of the alloys of system In_2Te_3-$Cu_2Ga_4Te_7$ (1-50 mol% $Cu_2Ga_4Te_7$, 2-70 mol% $Cu_2Ga_4Te_7$, 3 - $Cu_2Ga_4Te_7$)

Table 1: The physico-chemical properties the some alloys in the In_2Te_3-$Cu_2Ga_4Te_7$ system.

Composition, mol %		Thermal effect of heating, ^0C	Density 10^3kq/m^3	Microharness phase, MPa		
In_2Te_3	$Cu_2Ga_4Te_7$			I (α)	II $CuGa_2InTe_5$	III (γ)
				P=0,2 H (load)		P = 0,25 H (load)
60	40	610,810	5,95	1740	2300	-
50	50	855	5,98	1740	2350	-
40	60	825,850	5,92	-	2400	3500
30	70	825,845	5,90	-	2500	3300
20	80	830	5,88	-	-	-
15	85	825	5,88	-	eutec	eutec
10	90	825,850	5,87	-	-	3500
5	95	850,870	5,87	-	-	3500
3	97	860,870	5,86	-	-	3200
0	100	874	5,84	-	-	3100

At measurement of micro-hardness of the alloys of In_2Te_3-$Cu_2Ga_4Te_7$ system there received three rows of values, which characterize micro hardness of In_2Te_3 base, a new phase $CuGa_2InTe_5$ and γ solid solutions on $Cu_2Ga_4Te_7$ base.

Density of alloys remains almost constant excluding the alloy of composition 50 mol% $Cu_2Ga_4Te_7$, corresponding to a new phase $CuGa_2InTe_5$. On discussing the results of carried out studies it is possible to note that liquidus of the In_2Te_3-$Cu_2Ga_4Te_7$ system consists of three branches of a

primary isolation form liquid of α -phase, a new complicated phase $CuGa_2InTe_7$ and γ phase. In the interval of concentrations 20-25 mol% $Cu_2Ga_4Te_7$ lower than liquidus line two phases (L +$CuGa_2InTe_5$) are present. With decrease in temperature the liquid gradually dissolves and lower than solidus line two-phase alloys containing (In_2Te_3+$CuGa_2InTe_5$) and (γ +$CuGa_2InTe_5$) crystallize. In_2Te_3 and $CuGa_2InTe_5$ form eutectic between themselves, composition of which corresponds to 20 mol% $CuGa_2Te_7$ and temperature 610^0C. In this non-variant point three-phase equilibrium L↔γ+$CuGa_2InTe_5$ occurs. Composition in 85 mol% $Cu_2Ga_4Te_7$ and temperature ~825^0C meet the second eutectic of the system arranged between In_2Te_3 and $Cu_2Ga_4Te_7$.

In Fig.3 temperature dependence of electric conductivity of the alloys of composition $(Cu_2Ga_4Te_7)_{0.97}(In_2Te_3)_{0.03}$ and $(Cu_2Ga_4Te_7)_{0.95}(In_2Te_3)_{0.05}$

is cited. The course of curves of dependence lgσ~f(10^3/T,K) is semi conducting with a wide mixture field. Beginning with 513K for the first composition and with 573K for the second composition a sharp increase in electro conductivity is observed what is obviously connected with approximation of own conductivity. According to incline of the curves in this field a value of thermal width of prohibited zone has been calculated. At riper part of Fig.1 the graph of dependence values of this parameter on composition of examined solutions is presented. As is seen, addition of In_2Te_3 into $Cu_2Ga_4Te_7$ is accompanied by increasing thermal of prohibited zone. Increase in ΔE_g in solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$ most probably is connected with physical and chemical peculiarities of the chemical elements entering the composition. Thus, in particular is seen that width of prohibited zone depends on chemical bond [8] and one may suppose that at forming the crystalline structure of investigated materials a degree of ion-covalent share of chemical bond increases what con stimulate increase of ΔE_g.

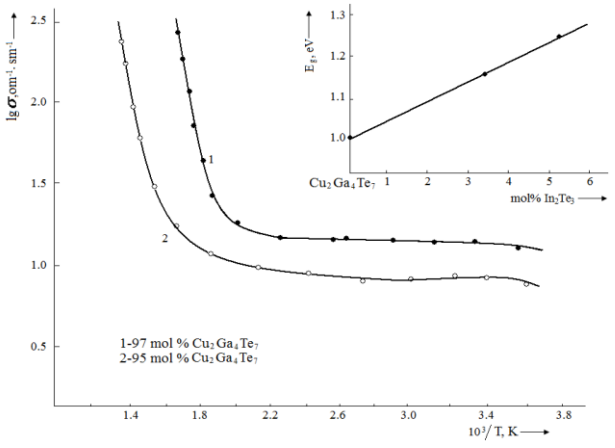

Fig.3. Temperature dependence of electric conductivity of the alloys of solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$ dependence values of width of prohibited zone on a composition of solid solutions (upper graph).

Figure 4 reflects temperature dependence of thermal – e.m.f. coefficient of investigated solid solutions. The coefficient of thermal e.m.f. in both compositions increases first in straight-line, passing through maximum, then displays tendency to decrease. The straight-line increase in the coefficient of thermal - e.m.f. at relatively law temperatures is typical for semi conductors with complex zone structure [10], of which experimentally found thermal - e.m.f. at low temperatures agrees qualitatively with author. (T) calculated under supposing constancy of concentration and efficient mass of a charge carriers, as well a factor of dispersion "r" equal to zero. Above temperature ~523K for both compositions an apparent decrease in the coefficient of thermal - e.m.f. is observed. In is probably connected, on one hand, with coming own field of conductivity, and on the other hand, with increase in a degree of degeneration of the charge. In whole studied temperature range the coefficient of thermal - e.m.f. possesses the negative sign of conductivity.

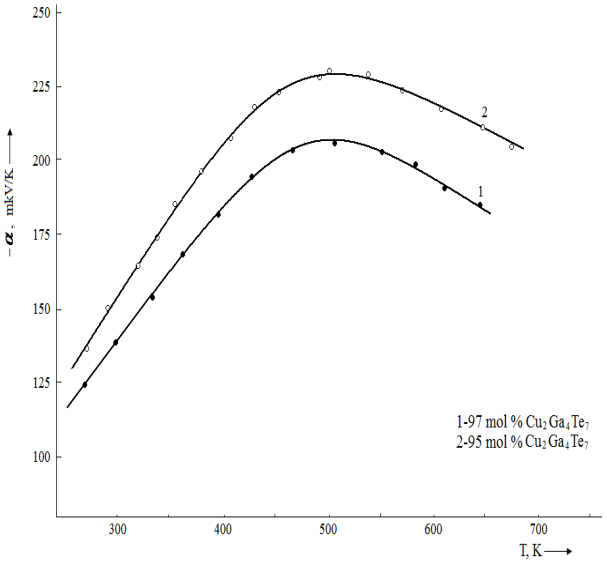

Fig.4. Temperature dependence of coefficient of thermal - e.m.f. of the alloys of solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$

Temperature dependence of Halls mobility of charge carriers of both composition of solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$ is offered in Fig.5 It has been established that till temperature ~ (403-423)K Halls mobility of current carriers changes by law~$T^{1.5}$. this testifies to dispersion of charge carriers flow ionized mixture atoms. Passing through gently sloping maximum dependence curves lgU_H ~lgT then display a tendency to noticeable decrease at high temperatures, where the law $T^{1.7}$ becomes varying one in dispersion of charge carriers. It corresponds to dispersion from heat fluctuations of crystalline lattice. However, sloping maximum on temperature dependences proves an existence of one more chanism of dispersion of electrons – dispersion from polarized optical vibrations.

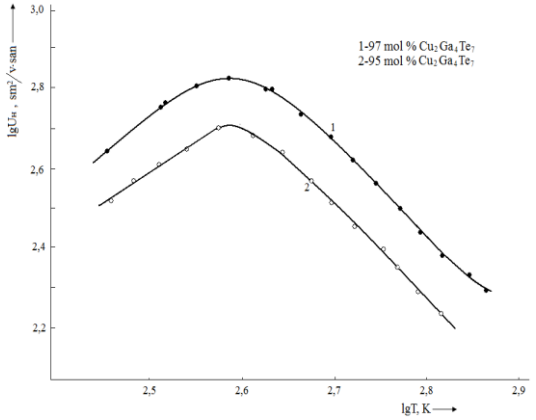

Fig.5. Temperature dependence of Halls mobility of current carriers in solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$

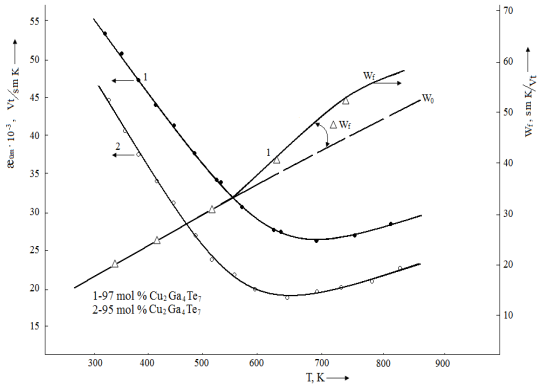

Fig.6. Temperature dependence of general heat conductivity ($æ_{gen}$) the allows of solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$ and heat resistance (W_f) of the alloy composition $(Cu_2Ga_4Te_7)_{0.97}(In_2Te_3)_{0.03}$.

In Fig.6 temperature dependence of general heat conductivity of the alloys of solid solutions $(Cu_2Ga_4Te_7)_{1-x}(In_2Te_3)_x$ is presented. As is seen at high temperatures general heat conductivity of both compositions changes by the negative degree law, what testifies to normal phonon processes of heat transfer. However, beginning since 600K general heat conductivity displays a tendency to increase that may be a consequence of bipolar constituent of heat conductivity [11]. The calculations showed that a general heat conductivity at law temperatures changes by $T^{0.1}$ law, and at higher ones by $T^{-0.12}$. Therefore, heat transfer in the examined compositions takes place according to one phone processes. The third curve in Fig.6 reflects dependence of phonon heat resistance (W_{II}) of the alloy of composition $(Cu_2Ga_4Te_7)_{0.97}(In_2Te_3)_{0.03}$. As is seen, at relatively law temperatures the change of phonon heat resistance agrees qualitatively with a change of theoretically calculated value of the same parameter (W_0) by temperature. However, beginning with ~550K the outlined composition displays an additional heat resistance (W_r). It testifies to the existence of one more source of dispersion of phonons-dispersion from defects of a crystalline lattice. An additional phonon heat resistance may be valued qualitatively as, $\Delta W_f = W_f - W$ one phon.

Further, the values of thermoelectric durability of the composition $(Cu_2Ga_4Te_7)_{0.95}(In_2Te_3)_{0.05}$ have been calculated by formula $Z=a^2\sigma/\varkappa_{gen}$. It has been exposed that at 700K thermoelectric efficiency of this composition has a value $Z=0.5\times10^{-3}K^{-1}$,what is admissible for technics of thermoelectricity. Thus, investigation of physical-chemical and thermoelectric properties of the alloys of the system $Cu_2Ga_4Te_7$- In_2Te_3 revealed some perspective compositions and a new complex compound $CuGa_2InTe_5$, which may be suitable for solid leady electronic structures.

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