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PREPARATION AND X-RAY DIFFRACTION INVESTIGATION OF $Cu_{1.80-x}ZnTe$ (x= 0.025, 0.050, 0.07 5, 0.10 at%) SINGLE CRYSTALS

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Absrtact: In the presented study, it was reviewed preparing of the $Cu_{1.80-x}ZnTe$ monocrystal systems (x = 0.025, 0.050, 0.075, 0.10 at.%), affection to crystal cage parameters and phase transition temperature of concentration increase of substituting isovalent metal atoms (Zn^{2+}) in crystalline form $Cu_{1.80}Te$ (so, the increase in the value of x).

Key words: elemental crystal cage, cage parameters, centered cube, solid solution, diffraction lines, isomorphism.

1. Introduction

The Cu_2Te combination at room temperature has a hexagonal structure with parameter a = 4.246 Å, c = 7.289Å, F.qr.D_{6h}^1-P6b/mm, Z = 2 [1]. The Cu_2Te combination in the 293-793 K temperature range is unstable and exposed to phase transition [2]. ZnTe combination is present in metastable form at room temperature and a = 4.31Å, c = 7.090Å, F.qr.$C6_v^4$-$P6_3mc$; crystallizes in hexagonal structure with Z = 2 parameter [3-7]. Cu_2Te and ZnTe compounds have a high temperature centralized high temperature cube (HMC) phase. The following crystal cage parameters have been defined for the cube phases of these compounds: a=6.104Å -For Cu2Te; a = 6.103Å - for ZnTe [3]. Based on the differential-thermal and microstructure analysis, the solubility of Cu2Te in the ZnTe combination was 51 mol%, the solution of the ZnTe compound in Cu_2Te combination is properly 3 mol% [5]. The room temperature of Cu_2Te and ZnTe compounds and crystal cage parameters of WPA phases, being close of ion radius of metal atoms Cu^{2+} and Zn^{2+}, as well as a wide range of solutions for the Cu_2Te combination Zn_2Te combination, in the crystal structure of $Cu_{2-x}Te$ compounds Cu^{2+} provides favorable conditions for the replacement of metal ions with isovalent Zn^{2+} metal ions.

2. Experimental

For the purpose of preparing and x-ray scanning of $Cu_{1.80-x}ZnTe$ monocrystals (x = 0.025, 0.050, 0.075, 0.10 at.%), highly clean Cu, Zn, Te chemical elements are extracted in the appropriate proportions, filled with quartz ampoules and synthesized directly by melting 10^{-2} Pa vacuum. During the synthesis, the ampoule was maintained at 750 K temperature (at elevated temperature of the tellurium) for 1 hour, the temperature was increased up to 1400 K (higher than the melting temperature of the Cu_2Te compound) and the temperature of the ampoule was reduced to 373 K after maintaining this temperature for 2 hours and maintained at this temperature for 24 hours for homogenization purposes. Examples of Cu1.80-xZnTe-synthesized by this method were thinned and filled with conical quartz ampoule and creating 10-2 Pa vacuum, their monocrystals have been obtained by the Bridgeman method. In order to determine the uniformity of the obtained monocrystalline $Cu_{1.80-x}ZnTe$ samples, their Laue grams were removed, and then putting into powder X-ray analysis was performed on DSC-910 ADVNCE-8D diffractometer. The results of the X-rays analysis are shown in table 1. As a result of the X-

ray analysis, the monocrystals of the acquired $Cu_{1.80-x}ZnTe$ system are monocrystalline and crystallized in hexagonal structure. As can be seen from table 1, all the diffraction lines are indexed on the basis of a = 8.37Å, c = 21.60Å defined for the hexagonal phase.

Report of the diffractogram of powder Cu1.80-xZnTe crystals.
CuKα -radiation, 40kv, 40ma, λ = 1.5418 Å, x = (0.025.0.050.0.075.0.10 at.%).

Table-1

№	$Cu_{1.80-x}ZnTe$							
	0.00	0.025	0.05	0.075	0.10	Hexagonal phase		T,K
	d.,ex.Å	d.,ex.Å	d.,ex.Å	d.,ex.Å	d.,ex.Å	d.,te.Å	hkl	
1	3.614	3.6187	3.6235	3.6285	3.6332	3.6182	1123	293
2	3.224	3.2280	3.2319	3.2357	3.2395	3.2243	1016	
3	3.015	3.0178	3.0212	3.0246	3.0279	3.0093	2024	
4	2.837	3.8400	2.8430	2.8459	2.8489	2.8392	1017	
5	2.777	2.7799	2.7826	2.7855	2.7883	2.7766	2025	
6	2.554	2.5565	2.5589	2.5613	2.5636	2.5541	2026	
7	2.350	2.3520	2.3540	2.3559	2.3579	2.3495	2027	
8	2.269	2.2703	2.2721	2.2740	2.2758	2.2688	1128	
9	2.160	2.1626	2.1659	2.1692	2.1726	2.160	2028000.10	
10	2.071	2.0743	2.0773	2.0804	2.0834	2.070	101.10	
11	2.005	2.0074	2.0102	2.0131	2.0159	2.0062	3036	
12	1.999	2.0018	2.0046	2.0074	2.0102	2.0010	2029	
13	1.807	1.8095	1.8117	1.8139	1.8162	1.8058	4041	
14	1.783	1.7852	1.7874	1.7896	1.7918	1.7872	4042	
15	1.750	1.7523	1.7544	1.7565	1.7586	1.7553	3146	
16	1.613	1.6148	1.6165	1.6182	1.6199	1.6125	3148	
17	1.512	1.5137	1.5152	1.5767	1.5182	1.5097	3256	
18	1.445	1.4474	1.4487	1.4507	1.4527	1.4462	4049	
19	1.356	1.3576	1.3593	1.3606	1.3622	1.3590	4262	
20	1.343	1.3451	1.3474	1.3496	1.3519	1.3448	5056	
21	1.274	1.2755	1.2775	1.2795	1.2815	1.2762	415.10	
22	1.211	1.2128	1.2145	1.2163	1.2180	1.2081	6060	
23	1.206	1.2077	1.2094	1.2111	1.2128	1.2061	6061	
24	1.138	1.1403	1.1425	1.1447	1.1469	1.1348	5274	
25	1.087	1.0885	1.090	1.0924	1.0950	1.0864	5277	
26	1.045	1.0463	1.0476	1.0490	1.0503	1.0450	4481	
27	0.998	0.9901	1.000	1.0012	1.0024	0.9956	62	
28	0.965	0.9712	0.0722	0.0733	0.9743	0.9669	70	
29	0.925	0.9261	0.9272	0.9282	0.9293	0.9247	50	
30	0.903	0.9042	0.9052	0.9061	0.9072	0.9029	80	

3. Experimental results and discussion

The calculated elemental crystal cage parameters for $Cu_{1.80-x}ZnTe$ system crystals are given in table 2.

As can be seen from table 2, with the increase in the concentration of isovalent metal ions of substituted Zn^{2+} - 0.83Å and being replaced Cu^{2+} - 0.80Å in crystalline form $Cu_{1.80}Te$ that is, the value of x, increases with crystal cage settings. This increase in crystal cage settings in crystalline form $Cu_{1.80}Te$ is connected with the radius difference of substituted and substituted isovalent metal ions.

Calculated elementary crystal cage parameters for samples containing $Cu_{1-80-x}ZnTe$ (x=0.025, 0.050, 0.075, 0.10 at %).

Table-2

a,c,Å	$Cu_{1.80-x}ZnTe$							
	0.000	0.025	0.050	0.075	0.10	Hexagonal phase		T,K
a_{or}	8.37	8.3772	8.3844	8.392	8.399	-	-	293
c_{or}	21.60	21.626	21.659	21.692	21.726	-	-	

Since the Zn^{2+} and replaced Cu^{2+} metal ions which are substituted in $Cu_{1.80}Te$ crystal structure are isovalent, one of the main conditions of isomorphism is the electron-beam of the crystal cage. In this case, the difference between substituting and substituted isovalent metal ions is 3.75%. Apparently, this difference is a 15% limit for V.M.Goldshmitt. Note that $Cu_{1.80}Te$ is an isovalent substituent in the crystalline structure differential lines in x-ray diffractograms obtained from $Cu_{1.80-x}ZnTe$ crystals and the number of molecules in the crystal cage does not change, however some of their intensity, crystal cage settings change. This indicates the formation of a solid solution based on $Cu_{1.80}Te$ crystal structure. The phase transition temperature occurring in monocrystals of $Cu_{1.80-x}ZnTe$, and to learn the effect of Zn^{2+} metal atom on the transition temperature to this phase X-ray diffractometric study was performed at temperature range 293-793K. As a result, the hexagonal phase of $Cu_{1.80}Te$ at 773 ± 1K is exactly turns into a centralized high temperature cube (UMC) phase. During this conversion, all 12 diffraction lines from the $Cu_{1.80}Te$ monocrystalline at room temperature were all lost and occurs three new diffraction lines (111), (220), (311) belonging to the FPC phase.

Different types of monocrystals Cu1-80-xZnTe.
CuKα irradiation, 40kv, 40mA, λ = 1.5418Å, (x = 0.025.0.050.0.075.0.10 at%).

Table 3.

№	$Cu_{1-80-x}ZnTe$									T,K
	0.00	0.025	0.050	0.075	0.10	Hexagonal phase		ÜMK-phase		
	$d._{təc}$Å	$d._{təc}$Å	$d._{təc}$Å	$d._{təc}$Å	$d._{təc}$Å	$d_{nəz.}$Å	Hkl	$d_{nəz.}$Å	hkl	
1	3.614	3.6187	3.6235	3.6285	3.6332	3.6182	1123			293
2	3.224	3.2280	3.2319	3.2357	3.2395	3.2243	1016			
3	3.015	3.0178	3.0212	3.0246	3.0279	3.0093	2024			
4	2.777	2.7797	2.7826	2.7855	2.7883	2.7766	2025			
5	2.554	2.5565	2.5589	2.5613	2.5636	2.5541	2026			
6	2.4338	2.4359	2.4380	2.4402	2.4423	2.4332	3031			
7	2.350	2.3520	2.3540	2.3559	2.3579	2.3495	2027			
8	2.160	2.1626	2.1659	2.1692	2.1726	2.1600	2028			
9	2.005	2.0074	2.0102	2.0131	2.0159	2.0062	3036			
10	1.807	1.8095	1.8117	1.8139	1.8162	1.8058	4041			
11	1.750	1.7523	1.7544	1.7565	1.7586	1.7553	3146			
12	1.445	1.4474	1.4487	1.4507	1.4527	1.4462	4049			

1	3.5136	3.5203	3.5248	3.5293	3.5340	-	-	3.5121	111	793
2	2.1528	2.1561	2.1593	2.1626	2.1659	-	-	2.1509	220	
3	2.4338	1.8380	1.8402	1.8425	1.8448	-	-	1.8341	311	
a_{or} Å	6.0888	6.0972	6.1053	6.1135	6.1220	-	-	-	-	

As the concentration of the Zn^{2+} metal atom replaced by the crystalline structure of $Cu_{1.80}Te$ increases, i.e. the x-in price increases, the phase transition temperature shifts to the higher temperature. Crystal cage parameters set for the $Cu_{1.80-x}ZnTe$ crystals for the high temperature cube phase are given in table 3. As seen from the table, by increasing the x, at 793 K crystal cage settings also increase. The observed dependency graph is shown in figure 2. As can be seen from the picture, dependence crystal cage parameters on x are linear character. The $Cu_{1.80-x}ZnTe$ crystals are associated with the concentration of Cu^{2+} and Zn^{2+} metal ions that are soluble in the cube phase when the phase of the crystal cage phase depends on the x-phase phase.

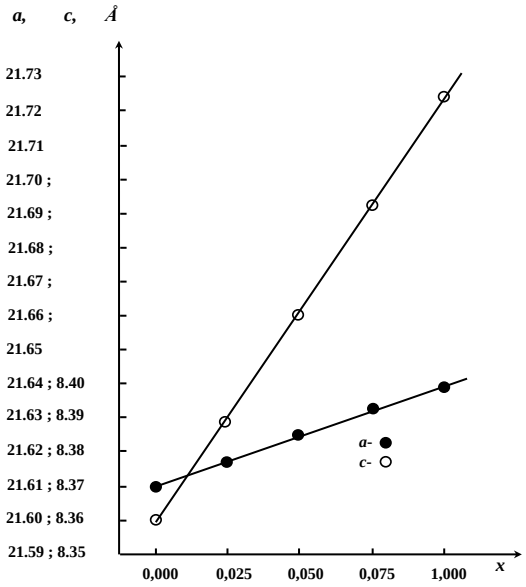

Fig. 1. Dependence of crystal lattice parameters of $Cu_{1.80-x}ZnTe$ monocrystals on the x.

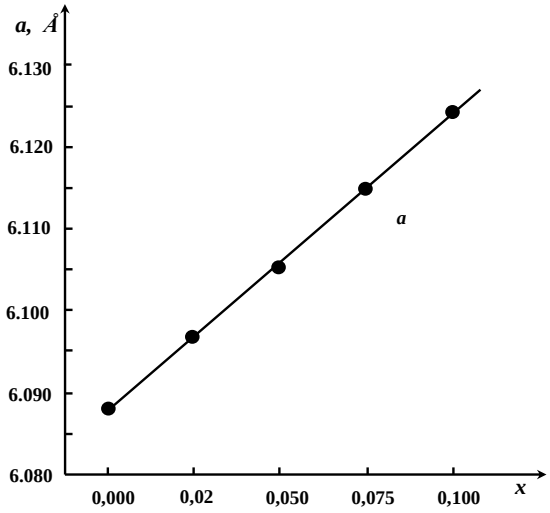

Fig. 2. Dependence of high temperature cubic phase of $Cu_{1.80-x}ZnTe$ systems crystals on the x. T=793K.

Note that, during $Cu_{1.80-x}ZnTe$ monocrystals phase transition monocrystalline is not violated and phase transition is monocrystalline type.

4. Conclusions

The results of the X-ray study based on $Cu_{1.80-x}ZnTe$ system monocrystals can be summarized as follows:

- $Cu_{1.80-x}ZnTe$ system samples (x = 0.025, 0.050, 0.075, 0.10 at.%) were synthesized and their monocrystals were prepared by Bridgman method. The prepared monocrystalline samples are uniform and crystallize in hexagonal structure at room temperature.
- In $Cu_{1.80}Te$ crystal structure with increased concentration of substituted Zn^{2+} and replaced Cu^{2+} isovalent metal atoms, i.e. with the increase in the value of x , increase of crystal cage parameters replaced and being replaced metal atoms differs in radius and this growth is a linear characteristic.
- with the rising price of x there is no change in the number of crystals of the $Cu_{1.80-x}ZnTe$ system crystal and the number of molecules in the crystal cage, but the intensity of some of the

diffraction lines increases or decreases, which indicates the formation of a solid solution based on $Cu_{1.80}Te$ crystal structure.
- with the increase in the x-price of mono crystals of the Cu1.80-xZnTe system temperature from 770 K to the phase that occurs at high temperatures and the crystal cage settings of the centralized high temperature cube phase are increasing.

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$Cu_{1.80-X}ZnTe$ MONOKRİSTALLARININ ALINMASI VƏ RENTGENEQRAFİK TƏDQİQİ (x= 0.025, 0.050, 0.075, 0.10 at.%).

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Xülasə: Təqdim olunan işdə $Cu_{1.80-x}ZnTe$ sisteminin (x=0.025, 0.050, 0.075, 0.10 at.%) monokristallarının alınmasına, $Cu_{1.80}Te$ kristal quruluşda əvəzedən izovalent metal atomlarının (Zn^{2+}) konsentrasiyasının artımının (yəni, x-in qiymətinin artımının) kristal qəfəs parametrlərinə və faza keçid temperaturuna təsirinə baxılmışdır.

Açar sözlər: elementar kristal qəfəs, qəfəs parametrləri, üzdən mərkəzləşmiş kub, bərk məhlul, difraksiya xətləri, izomorfizm.

ПОЛУЧЕНИЕ И РЕНТГЕНОГРАФИЧЕСКОЕ ИССЛЕДОВАНИЕ МОНОКРИСТАЛЛОВ $Cu_{1.80-X}ZnTe$ (x= 0.025, 0.050, 0.075, 0.10 at.%)

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Резюме: В представленной статье было рассмотрено получение монокристаллов системы $Cu_{1.80-x}ZnTe$ (x=0.025, 0.050, 0.075, 0.10 at.%), а также влияние увеличения концентрации (т.е. с повышением значения x) изовалентных атомов (Zn^{2+}) в кристаллической структуре $Cu_{1.80}Te$ на температуру фазовых переходов и параметров кристаллической решетки.

Ключевые слова: элементарная кристаллическая решетка, параметры кристаллической решетки, гранецентрированный куб, твердых раствор, линии дифракции, изоморфизм