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EFFECT OF γ -RADIATION DEFECTS ON THE ELECTROPHYSICAL PROPERTIES IN THE p-CuTIS MONOCRYSTAL

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Abstract: The surface morphology of p-type CuTIS single crystal with specific resistance $\rho = 40 \ \Omega \cdot cm$ in the initial state and after exposure to gamma radiation is studied by atomic force microscopy. It is shown that the surface relief undergoes modification in the absorbed dose region of $D_{\gamma} \leq 500$ krad. Experimental results show that the activation energy of the retention center during radiation depends on the radiation dose, and the gradient of the curve does not change at $\Phi < 500$ krad, increases at $\Phi > 500$ krad, and the resulting defects have a deeper energy level.

Keywords: Radiation, semiconductors, surface morphology, electrical conductivity, current, defects

1. Introduction

Triple compounds of the A^IB^{III}C^{VI} ₂ type with a chalcopyrite structure have long attracted the attention of researchers in connection with the prospects for their practical application as elements of solar energy converters, nonlinear optics, efficient emitting LEDs, and photodetectors [1,2]. In the study of phase transitions (PT), one of the important aspects is to identify the relationship between the structural and thermal characteristics of the material. To determine this relationship, it is necessary to investigate the physical properties of the material in the temperature range of the PT, which makes it possible to obtain information about the PT process itself. Another topical issue is the determination of the distribution of coexisting phases in the PT region. As is known, PTs occurring as a result of fluctuations in the physical state of matter are responsible for all changes in physical properties that occur in this area. The phenomenological theory of diffuse phase transitions [1] is based on the theory of heterophase fluctuations, the phase inclusion function L is introduced, which characterizes the distribution of coexisting phases in the phase transition region and its temperature derivative dL/dT (temperature velocity of the phase transition). In essence, the function L can determine the change in all thermodynamic parameters of the system occurring in the PT region. Various solid solutions with high values of thermal efficiency [3] were obtained by replacing copper atoms with atoms of various metals in chalcogenides of the Cu_2X type (where, X = S, Se, Te).

Stoichiometric and non-stoichiometric compounds formed in Cu-S (Se) systems have been one of the main objects of study for many years due to their application-oriented properties. This interest is related to their physical and chemical properties. It should be noted that these classes of compounds are also interesting objects in terms of crystal structure and structural phase transitions.

One of the important issues of modern materials science, as well as solid state physics is the acquisition of new materials with high thermal conductivity and the development of methods for the purposeful management of their properties. Based on the literature [4–9], we can say that copper thallium chalcogenides- Cu-Tl-X (x = S, Se) are an interesting research object for the creation of new thermo materials.

There is no more information about the electrical conductivity, thermoelectric and optical properties of this crystal in the scientific literature. Although there is some information about their electronic structure and anomalies of conductivity at low temperatures, but they do not allow to make model suggestions about the properties of conductivity. To complete the above theoretical and experimental results and obtain new data, the current transfer mechanism in the CuTIS single crystal was studied in the temperature range of 100–300K.

2. Experimental part

The studied p-CuTlS compound was grown at high temperature using the Bridgman– Stockbarger method. Using materials with a high degree of purity (Tl 99.99%; Cu 99.999%; S 99.99%) in the crucible is completely melted in the hot zone at 775K of the two-zone Bridgman furnace and is transferred to the cold zone (580K) at speed of 1.2mm/h. The obtained single crystal had a diameter of 1cm, a length of 8cm and a specific resistance of ~ 40 Ω · cm. Crystal structure and lattice parameters of the sample obtained by X-ray analysis method a = 4.08; c = 8.16Å; z = 2 were calculated, and it was determined that the compound crystallizes in tetragonal crystal system and the results were given in [17].

Silver paste was used for the conductive ohmic contact and the distance between the contacts was L = 6mm. The size of the studied sample is $2 \times 0.5 \times 6mm$. Measurements were made on a B7-30 universal ampere-voltmeter at a voltage of 0–20V (E ~ 10–105V/cm) and a temperature range of 100–300K.

The surface of the samples was examined with an AGM microscope in contact mode using a 50 nm nanoEducator probe scanning microscope.

Figure 1 shows three-dimensional surface images of the CuTIS compound before irradiation — initial (a), thermally evaporated (b), and after irradiation ((D = 500krad (c))). From the illustrations shown in Figure 1, it can be seen that the initial sample consists of a set of particles with a surface height of 202 nm and is unevenly distributed along the surface. At 100° C, the surface of the thermally evaporated sample is 130 nm high, and evenly distributed particles are formed on the surface. After irradiation with gamma quanta at a dose of 500 krad, large particles of height 500 nm and evenly distributed are observed (Figure 1 (c)).



Fig. 1. Study of microscopic surface of CuTlS compound, three-dimensional surface images(3D):a) initial; b) termal brewed; c) irradiated(D_{γ} =500krad)



Fig. 2. Study of microscopic surface of CuTlS compound, histograms: a) initial; b) termal brewed; c) irradiated $(D_{\gamma}=500krad)$

Confirmation of three-dimensional surface images can be clearly seen from histograms (distribution curves of surface elements according to dimensions). As shown in Figure 2, the initial (non-irradiated) CuTIS compound contains mainly one type of nanoparticles with a size of 200 nm (number 80). After thermal evaporation, the size of the nanoparticles in the sample increased to 350 nm (number 125) (Figure 2 (b)). After irradiation with gamma quanta at a dose of 500 krad, the size of the nanoparticles in the samples was 250 nm (number 70). (Figure 2 (c)).

2. Discussion of experimental section and conclusions

The dependence of ΔE_t (E) ~ f (E^{1/2}) is shown in Fig.3. As can be seen from the figure, ΔE decreases linearly with $E^{1/2}$ increase. From the extra polarization of the linear dependence $\Delta E \sim f$ (E^{1/2}) under the condition E = 0, the activation energy of the trap was determined and was 0.05eV for low temperature and 0.07eV for high temperature. The obtained experimental and theoretical analyzes [10, 11] show that the field dependence of the electrical conductivity at values of field intensity E > 40V/cm is obeyed by Frenkel's law.

Based on experimental results and literature data [10], the value of the β —Frenkel coefficient was calculated according to the following expression:

$$\beta = 1/\kappa T (e^3/\pi \epsilon \epsilon_0)^{1/2}$$

Taking into account the expression $\sigma 0$ in the Frenkel formula, the dependence $\Delta E \sim f(E^{1/2})$ can be written as follows [11]:

$$\Delta E_t(E) = E_t(0) - (e^3 E / \pi \epsilon \epsilon_0)^{1/2}$$

and its graphical description at different radiation doses is given in Fig. 3. It can be seen from the figure that after irradiation $\Delta E_t \sim E^{1/2}$ - dependence also retains its linear character, but its gradient changes concerning the original sample. It is known from the study that the ionization process in metallic materials with a high concentration of free charge carriers does not affect the process of defect formation and distribution of structural defects. As shown in [12] work, this can be related

to the change in the permittivity of the medium- ε_0 which is caused by the defects that were created during the emission. The activation energy of the trap from the extrapolarization of the linear dependence $\Delta E - f(E^{1/2})$ under the condition E = 0 was determined and was 0.05 eV for low 25 temperature and 0.08 eV for high temperature. Experimental results show that the activation energy of the retention center during radiation depends on the radiation dose, and the gradient of the curve does not change at $\Phi < 500$ krad, increases at $\Phi > 500$ krad, and the resulting defects have a deeper energy level.



Fig. 3. The dependence of the activation energy of the trap on $E^{1/2}$ at different temperatures and doses

[12-15] - studies show that the permittivity of the medium increases to a certain value of the dose due to the parabolic dependence on the radiation dose, which decreases with the subsequent dose increase. According to this result, it can be assumed that the dependence of the gradient of $\Delta Et \sim E^{1/2}$ and dependence of the β - coefficient on the radiation dose is due to changes in the permittivity of the medium[16].

Thus, the effect of γ -quantum on the current transfer mechanism in the p-CuTlS single crystal was studied in different ranges of electric field and temperature and compared with the corresponding theoretical and experimental results.

References

- 1. J.M. Stewart, W.S. Chen, W.E. Devany, R.A. Mickelsen. Ternary and Multinary Compounds, ed. by S.K. Deb, A. Zunger. (Pitsburgh, PA, Materials Research Society, 1987).
- 2. S. Shirakata, K. Murakami, S. Isomura. Jpn. J. Appl. Phys., 28, 1728 (1989).
- L. Cuangminq, T. Schulmeyer, J. Brotz, A. Klein, W. Jaedermann. Thin Sol. Films, 431, 472 (2003).
- Z.S. Aliev, Y.M. Koroteev, T. Breczewski, N.B. Babanly, I.R. Amiraslanov, A. Politano, G. Madariaga, M.B. Babanly, E.V. Chulkov, Insight on a novel layered semiconductors: CuTlS and CuTlSe. J. Solid State Chem. 242, 1–7 (2016).
- 5. E. Wimmer, H. Krakauer, M. Weinert, A.J., Freeman, Full-potential self-consistent linearized-augmented-plane-wave method for calculating the electronic structure of

molecules and surfaces:O2molecule. Phys. Rev. B 24(2), 864–875 (1981). https:// doi. org/ 10. 1103/ physr evb. 24. 864

- 6. H.T. Joshua, T. Zhongjia, L. Bing, S. Kalyan, L. Bernd, C.W. Paul, M.G. Arnold, Insight on a novel layered semiconductors: CuTlS and CuTlSe. Phys. Rev. B. 78, 060505 (2008)
- 7. K. Momma, F.J. Izumi, VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. J. Appl. Cryst. 44, 1926–1928 (2011)
- 8. V.T. Abishov, M.B. Babanly, A.A. Kuliev, Crystalline lattice of Cu(Ag)TlS(Se) compounds and phase-equilibria in the Cu(Ag)TlS-Cu(Ag) TlSe systems. Inorg. Mater. 15, 1514–1516 (1979)
- 9. M.B. Babanly, A.A. Kuliev, Phase equilbiria and thermodynamic properties of the Ag–Tl-Se system. Russian J. İnorganic Chem. 27, 1336–1340. İSSN 0036–0236 (1982)
- 10. Y.I. Frenkel, Application of the Fermi-Pauli theory to the question of the forces of clinging. Phys. Rev. 54, 109–121 (1928)
- 11. B.G. Tagiev, O.B. Tagiev, N.N. Musaev, Injection and field ioniza-tion of traps in MnGa2Se4 single crystals. Physc Techn. Semic. 29, 1403–1405 (1995)
- 12. O.B. Tagiev, T.Sh. Gashimova, I.M. Askerov, Study of the influence of a strong electric field on the electrical conductivity of a single crystal MnGaInS4: Eu Physc.Techn.Semic.; 32, 701703(1998)
- 13. R.M. Hill. Phil.Mag. Poole-Frenkel conduction in amorphous solids. A Journal of Theoretical Experimental and Applied Physics; 23, 59-61 (1971)
- 14. B.G. Tagiyev, O.V. Tagiev, G.A. Kasimova, Injection currents and thermionic effect of Frenkel-Pool in single crystals Phys.St.Sol.(a); 128, 167(1991)
- 15. N.G. Volkov, V.K. Lyapidevsky Weak Coupling Produced in Superconductors by Irradiation. Physcs. Techn. Semicon.; 14, 1337(1972)
- 16. R.S.Madatov, R.M.Mamishova, G.B.Baylarov, Characteristics of current injection in the narrow-band p-CuTlS single crystal, Applied Physics A (2021) 127:364 https://doi.org/10.1007/s00339-021-04515-8
- 17. R.S. Madatov, G.B. Baylarov, R.M. Mamishova, M.N. Mirzayev, Crystallin structure and differential thermal analysis of CuTlS compound, Journal of Radiation Researches, vol.6, №2, 2019, Baku, p. 50-54

ВЛИЯНИЕ γ-ИЗЛУЧЕНИЯ НА ЭЛЕКТРОФИЗИЧЕСКИЕ СВОЙСТВА В МОНОКРИСТАЛЛЕ p-CuTIS

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Резюме: Методом атомно-силовой микроскопии исследована морфология поверхности монокристалла CuTlS p-типа с удельным сопротивлением $\rho = 40 \ \Omega \cdot \text{см}$ в исходном состоянии и после воздействия гамма-излучения. Показано, что в области поглощенной дозы D $\gamma \leq 500$ крад происходит модификация рельефа поверхности. Результаты экспериментов показывают, что энергия активации удерживающего центра при облучении зависит от дозы облучения, и градиент кривой не изменяется при $\Phi < 500$ крад, увеличивается при $\Phi > 500$ крад, а образующиеся дефекты имеют более глубокий энергетический уровень.

Ключевые слова: Излучение, полупроводники, морфология поверхности, электропроводность, ток, дефекты

p-CuTIS MONOKRİSTALINDA γ-ŞÜALANMANIN ELEKTROFİZİKİ XASSƏLƏRİNƏ TƏSİRİ

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Xülasə: İşdə ilkin və qamma şüalarına məruz qalmış xüsusi müqaviməti $\rho = 40 \ \Omega \cdot \text{sm}$ olan p tipli CuTIS monokristalının səth morfologiyası atom qüvvə mikroskopu(AQM) ilə öyrənilmişdir. Göstərilmişdir ki, şüalanma dozasının $D_{\gamma} \leq 500$ krad qiymətində səth relyefinin modifikasiyası baş verir. Alınmış təcrübi nəticələr göstərir ki, şüalanma zamanı yaranan tutma mərkəzinin aktivləşmə enerjisi şüalanma dozasından asılıdır və dozanın $\Phi < 500$ krad qiymətlərində əyrinin meyli dəyişmir, $\Phi > 500$ krad qiymətlərində isə artır və yaranan defektlər daha dərin energetik səviyyəli olur.

Açar sözlər: Radiasiya, yarımkeçirici, səth morfologiyası, elektrik keçiriciliyi, cərəyan, defektlər