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STUDY OF THERMOPHYSICAL PROPERTIES OF Cu_2NiTe_2 COMPOUND AT HIGH TEMPERATURES BY DSC SPECTROSCOPY

Y.I. Aliyev[1,2]*, Kh.M. Guliyeva[3], N.N. Mursakulov[3], Kh.N. Ahmadova[3,4,5], A.I. Bayramova[2], L.N. Ibrahimova[6]
[1]*Azerbaijan State Pedagogical University, Baku, AZ-1000, Azerbaijan*
[2]*Azerbaijan University of Architecture and Construction, Baku, AZ-1073, Azerbaijan*
[3]*Institute of Physics, Ministry of Science and Education, Republic of Azerbaijan, Baku, AZ-1143, Azerbaijan*
[4]*Azerbaijan State Oil and Industry University, Baku, AZ-1010, Azerbaijan*
[5]*Khazar University, Baku, AZ-1096, Azerbaijan*
[6]*Nakhchivan State University, Nakhchivan, AZ-7012, Azerbaijan*
Corresponding Author email: yusifafshar@gmail.com
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The crystal structure and thermophysical properties of the chalcogenide semiconductor Cu_2NiTe_2 were comprehensively investigated using X-ray diffraction and differential scanning calorimetry. Structural characterization at room temperature revealed that the synthesized compound crystallizes in the hexagonal crystal system with the space group $P6_3/mmc$, indicating the formation of a highly ordered polycrystalline phase. The diffraction peaks were sharp and well-defined, confirming the material's good crystallinity and structural homogeneity. The absence of additional impurity peaks in the diffraction pattern also suggests that the synthesized compound possesses a predominantly single-phase structure.
Key words: *Cu_2NiTe_2; Chalcogenide; Semiconductor; DSC; X-ray diffraction; Crystal structure; Thermal properties*
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1. INTRODUCTION

Studying the thermal properties of semiconductor compounds provides information on both their structure and various physical properties. Thermal energy significantly influences the formation of these properties. Changing the temperature of a system alters the thermodynamic parameters, which in turn influence its physical properties. Therefore, extensive research has recently been conducted on the thermal properties of condensed systems and the influence of temperature on their physical properties [1-5].

The development of analytical methods allows for both increasing the accuracy of the results obtained and conducting comparative analysis. These methods enable the study of structural changes and thermal effects in various systems [6-8]. One of them is Differential Scanning Calorimetry (DSC). It has been established that, in studies conducted using the DSC method, it is possible to investigate structural transformations, thermal effects, melting, and other processes occurring in semiconductors, and to determine the mechanism of changes in thermodynamic parameters during these processes [9-11]. The thermodynamic functions of many semiconductor crystals have been studied by the DSC method. The thermal properties of the $Cu_2NiSeTe$ compound at high temperatures have been studied [12]. It has been established that 4 thermal transitions occur within the specified temperature range. The transition at T = 144°C is attributed to the escape of water molecules from the sample. It has been shown that thermal transitions at T = 587 and 647°C increase system stability by rupturing weak bonds in polycrystals, whereas the transition at T = 714°C corresponds to a structural phase transition.

There are certain difficulties in studying the thermal properties of chalcogenide semiconductors. Since these compounds are non-oxide materials, an oxide layer forms on their surfaces as the temperature increases. To avoid this, the thermophysical properties of chalcogenide semiconductors are studied in vacuum conditions [13]. When conducting studies in vacuum conditions, the mass of the samples does not change. Therefore, studies by Thermogravimetric Analysis (TGA) cannot be performed. However, by analyzing the DSC spectra, it is possible to study the processes of evaporation, decomposition, phase transitions, and melting occurring in the system.

Copper chalcogenides are compounds with interesting physical properties. Since Cu atoms have variable valence, various structures and physical properties are observed in the compounds they form [14-16]. One of such compounds is Cu_2NiTe_2. Although many properties of this compound have been studied, its thermal properties at high temperatures remain underexplored. In this work, a Cu_2NiTe_2 crystal was synthesized, its crystal structure at room temperature and thermophysical properties at elevated temperatures were studied.

2. EXPERIMENTAL PART

Sample synthesis. The Cu_2NiTe_2 compound was synthesized using a standard method typical for chalcogenide semiconductors. To prevent oxidation, the synthesis was carried out under vacuum. In a single-zone furnace, the elements

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(copper, nickel, and tellurium), deposited in stoichiometric proportions, were collected in a quartz ampoule. Air was evacuated from the ampoule to a vacuum of 10^{-4} Hg, and the ampoule's neck was closed. The ampoule's temperature was stabilized at T = 300°C inserted into the furnace. After holding the process for 1 hour, the furnace temperature was gradually increased. The temperature was stopped at 800°C, 900°C, and 1000°C for 30 minutes in the range of T = 700-1050°C. To ensure homogeneity, the synthesis ampoule was shaken while the furnace was running. After this, the temperature was also increased by T = 1050°C and maintained for 1.5 hours. In the next step, the temperature was gradually reduced to T = 600°C. After holding at the homogenization temperature for 3 days, the process was stopped. To study the structure of the resulting sample, X-ray diffraction analysis was performed. Based on the data obtained, the Cu_2NiTe_2 crystal was synthesized as a single-phase polycrystalline material.

Study of crystal structure. There are various methods for studying the crystal structure of solids. The research method is selected depending on the shape and chemical composition of the samples being studied. One such method is X-ray diffraction (XRD). It was used to study the crystal structure of the Cu_2NiTe_2 compound. Modern X-ray diffractometers make it possible to study the structure of crystalline solids and determine crystallographic parameters. The studies were conducted on a D8 ADVANCE diffractometer (Bruker, Germany). Its parameters were: 40 kV, 40 mA, CuK_α radiation, λ = 1.54184 Å. After the synthesis, samples for study were prepared from a polycrystal of Cu_2NiTe_2. For X-ray diffraction studies, the sample was crushed and ground into powder. The X-ray diffraction spectrum obtained at room temperature was analyzed using the Rietveld method in Mag2Pol. Miller indices were determined from the diffraction maxima. The symmetry, syngony, space group, and lattice parameters of the crystal were determined.

Study of thermophysical properties. Various approaches are used to investigate the thermophysical properties of condensed matter systems. Each experimental technique has its own advantages and limitations, depending on the nature of the material under investigation and the measurement conditions. Among the existing experimental techniques employed for thermophysical characterization, Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA) hold particular importance due to their high sensitivity and broad applicability [17-19]. The DSC method is based on the passage of heat flux through the sample, and the temperature dependence of the heat flux function is given in the DSC spectrum. The TGA method is based on the temperature dependence of a substance's mass. In studies conducted under vacuum conditions, it is not possible to control the change in mass. Because the mass of the ampoule generally remains unchanged. However, it is possible to obtain a DSC spectrum. Therefore, the thermophysical properties of the Cu_2NiTe_2 compound were studied at high temperatures using the DSC method. Those measurements were carried out using the DSC3 STAR Systems manufactured by METTLER TOLEDO, and temperature-corrected MULTISTAR sensors. The standard adiabatic calorimetry was performed in the temperature range from 20 °C up to 1000 °C at a heating rate of 5 °/min in argon atmosphere at a flow rate of 20 mL·min^{-1} (which is previously calibrated with indium). The cooling process was achieved with the help of the NITROGEN UN 1977 REFRIGERATED LIQUID analyzer cooling system and "digital temperature controller". The error of weight determination did not exceed **0.02**% at 20 °C and 1% at 1000 °C.

3. RESULTS AND DISCUSSION

The crystal structure of the Cu_2NiTe_2 compound was studied by X-ray diffraction at room temperature and normal conditions. The spectrum, obtained in the diffraction angle range of 25° ≤ 2θ ≤ 70°, is shown in Figure 1.

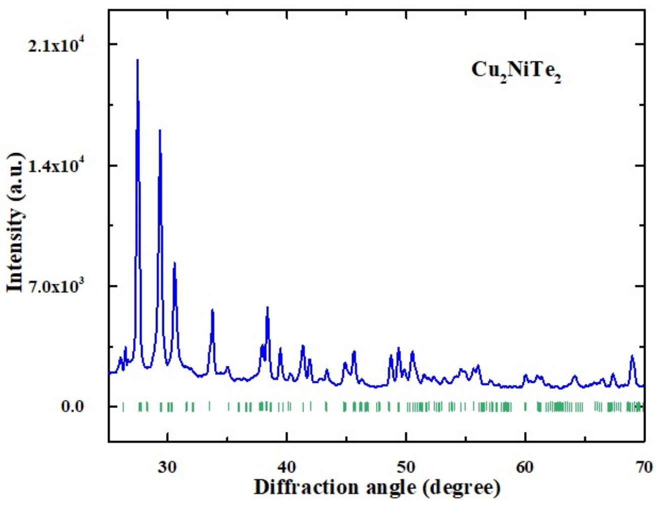

Figure 1. X-ray diffraction spectrum of the compound Cu_2NiTe_2. The experimentally obtained spectrum is shown by the blue line, and the diffraction planes are shown by the green lines

An analysis of the X-ray spectrum using the Rietveld method in the Mag2Pol program revealed that the crystal structure of the Cu_2NiTe_2 compound has high symmetry. The values of the crystallographic parameters were determined for this compound. It was found that the crystal structure of the Cu_2NiTe_2 compound has hexagonal symmetry and space group P6$_3$/mmc. The values of the lattice parameters were determined: $a = b = 3.9447(5)$ Å, $c = 17.1382(6)$ Å. The results are consistent with those from studies of the structure of copper- and nickel-containing chalcogenide dielectrics. Previous studies have established that the crystal structure of the $Cu_2NiSeTe$ compound is also hexagonal [12]. Certain variations were observed in the lattice parameters of these compounds. Such changes are mainly associated with the nature and atomic characteristics of the elements forming the crystal structure. In the $Cu_2NiSeTe$ compound, a portion of the Te atoms is substituted by Se atoms, resulting in modifications of the lattice parameters. This behavior can be explained by the mismatch between the ionic radii of selenium and tellurium atoms, which influences the interatomic distances and consequently affects the crystal lattice dimensions. It has been established that in the divalent state, the ionic radius of the selenium atoms is $R_{Se2-} = 0.69$ Å, and the ionic radius of the tellurium atoms is $R_{Te2-} = 0.85$ Å [20]. Between the ionic radii of these atoms, there is a distance of $\Delta R = 0.16$ Å. When a covalent chemical bond is formed between the metal and chalcogen atoms, the distance ΔR has a significant effect. Therefore, differences in the lattice parameters of the $Cu_2NiSeTe$ and Cu_2NiTe_2 compounds arise.

The results from structural studies indicate that the Cu_2NiTe_2 compound has a single-phase, highly symmetric hexagonal structure. Covalent bonds formed by Cu and Ni metals with Te chalcogen atoms are capable of forming a dense, highly symmetric system in a small volume. Such systems are resistant to external influences.

Semiconductor materials are known as functional materials with potential applications across various fields. Cu_2NiTe_2, in particular, has a wide range of applications. Therefore, it is important to study the processes occurring under external influences. When considering external influences, temperature is primarily considered, since heating occurs in electronic devices. As the temperature increases, the functionality of semiconductor converters changes. Therefore, when studying each research object, it is necessary to examine the fundamental physical properties that arise with temperature. With this in mind, the thermophysical properties of Cu_2NiTe_2 at high temperatures were studied.

Thermal properties were studied at high temperatures using DSC. The heat flow spectrum in the temperature range $20°C \leq T \leq 1000°C$ is shown in Figure 2.

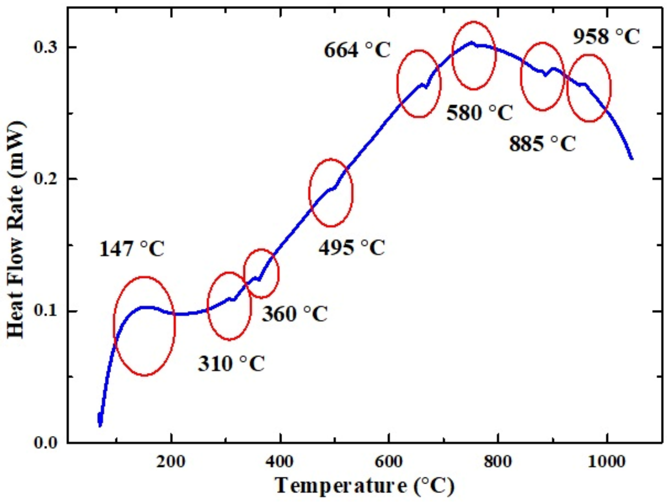

Figure 2. Heat flow rate function of Cu_2NiTe_2 sample at the 20 °C $\leq T \leq 1000$ °C temperature ranges

As can be seen from Figure 2, the temperature dependence of the heat flux spectrum can be divided into four distinct regions, each corresponding to specific thermophysical processes occurring within the investigated material. In the first region, the heat flux value increases abruptly to $\Phi = 0.1$ mW. In the second region, it remains practically at the level of $\Phi \sim 0.1$ mW. In the third region, a abrupt increase in the heat flux value to $\Phi = 0.3$ mW is observed. In the last region, a decrease in the value of the heat flux function is observed. The abrupt increase in the heat flux in a small temperature range is associated with the quantum region of heat capacity in high-entropy compounds. At this time, the frequencies of harmonic oscillations of the atoms forming the structure begin to increase. When analyzing the DSC spectrum of the Cu_2NiTe_2 compound, it was determined that the thermal properties of this compound are quite complex. Each of the 4 different regions observed at high temperatures has its own thermal properties. In some regions, the lattice vibration frequencies increase due to thermal energy, in some regions they remain stable, and in some regions a decrease is observed. The observation of these effects is associated with thermal transitions occurring in the system. From the spectrum presented in Figure 2, it is evident that 8 different thermal effects were observed at high temperatures. These effects occurred at temperatures of $T = 147$ °C, 310 °C, 360 °C, 495 °C, 664 °C, 580 °C, 885 °C, and 958 °C. As can be seen from the spectrum, the effect centered at $T = 147$ °C differs from the others. This effect is caused by a small number of water molecules leaving the sample. Beginning at approximately $T = 100$ °C, water molecules undergo evaporation and gradually leave the sample in the gaseous phase. Although water molecules are free, in some cases they combine with metal atoms in the material, forming hydroxide groups. In this case, as the temperature increases, the hydroxide groups first break down and water molecules form. Then, the water molecules begin to leave the substance. Thermal effects in this case occur at higher temperatures.

The spectrum in Figure 2 shows that the remaining thermal effects are endoeffects, which are virtually identical to each other. The energy required to generate the effects is of the same order. These effects, which arise with low energy absorption, are primarily associated with the release of air gases from the substance. For example, gas atoms adsorbed from the air, primarily carbon dioxide, exist in a space between grains. These molecules exist both freely and form specific chemical bonds with the metal atoms within the sample. As the temperature increases, the vibrational amplitudes of the bonds between the atoms increase, breaking weak chemical bonds. When bonds are broken, the gas molecules escape the sample. This effect is observed by energy absorption in the DSC spectrum. The thermal effects observed for the Cu_2NiTe_2 compound at high temperatures are virtually identical. No phase transition is observed in the system.

4. CONCLUSIONS

The crystal structure and thermophysical properties of the Cu_2NiTe_2 compound were comparatively studied. Structural studies revealed that this compound has a highly symmetrical hexagonal crystal structure. The thermal properties of Cu_2NiTe_2 were studied in the temperature range of T = 20-1000°C. Eight thermal effects were observed in this temperature range. The transition at T = 147°C is attributed to the release of water molecules from the sample. Other effects, occurring at higher temperatures, are explained by the rupture of bonds between gas atoms within the sample and the release of gases from it. It was determined that the hexagonal system is sufficiently stable at this temperature, and no phase transition occurs in this temperature range.

ORCID

Y.I. Aliyev, https://orcid.org/0000-0001-8896-2180; **Kh.M. Guliyeva,** https://orcid.org/0000-0001-8061-3189; **N.N. Mursakulov,** https://orcid.org/0000-0001-5121-9289; **Kh.N. Ahmadova,** https://orcid.org/0000-0001-5974-5400

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ДОСЛІДЖЕННЯ ТЕПЛОФІЗИЧНИХ ВЛАСТИВОСТЕЙ СПОЛУКИ Cu_2NiTe_2 ЗА ВИСОКИХ ТЕМПЕРАТУР МЕТОДОМ ДСК-СПЕКТРОСКОПІЇ

Ю.І. Алієв[1,2], Х.М. Гулієва[3], Н.Н. Мурсакулов[3], Х.Н. Ахмадова[3,4,5], А.І. Байрамова[2], Л.Н. Ібрагімова[6]
[1]*Азербайджанський державний педагогічний університет, Баку, AZ-1000, Азербайджан*
[2]*Азербайджанський університет архітектури та будівництва, Баку, AZ-1073, Азербайджан*
[3]*Інститут фізики, Міністерство науки та освіти, Азербайджанська Республіка, Баку, AZ-1143, Азербайджан*
[4]*Азербайджанський державний університет нафти та промисловості, Баку, AZ-1010, Азербайджан*
[5]*Хазарський університет, Баку, AZ-1096, Азербайджан*
[6]*Нахчиванський державний університет, Нахчивань, AZ-7012, Азербайджан*

Кристалічну структуру та теплофізичні властивості халькогенідного напівпровідника $Cu2NiTe_2$ було всебічно досліджено за допомогою рентгенівської дифракції та диференціальної скануючої калориметрії. Структурна характеристика за кімнатної температури показала, що синтезована сполука кристалізується в гексагональній кристалічній системі з просторовою групою $P6_3/mmc$, що вказує на утворення високовпорядкованої полікристалічної фази. Дифракційні піки були різкими та добре визначеними, що підтверджує добру кристалічність та структурну однорідність матеріалу. Відсутність додаткових домішкових піків на дифракційній картині також свідчить про те, що синтезована сполука має переважно однофазну структуру.

Ключові слова: *Cu_2NiTe_2; халькогенід; напівпровідник; ДСК; рентгенівська дифракція; кристалічна структура; теплові властивості*