

Research Article

Infrared Absorption Study of Bonding and Lattice Vibrations in the Cu_2NiTe_2 Chalcogenide Semiconductor

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Abstract

Cu_2NiTe_2 was synthesized, and its crystal lattice and vibrational behavior were investigated in this study. As a consequence, the structural analysis demonstrated a hexagonal arrangement assigned to the space group $P6_3/mmc$, consistent with hexagonal symmetry. Atomic motions were examined using infrared spectroscopy and interpreted spectroscopically. Six dominant absorption maxima appeared distinctly within the $400\text{--}4000\text{ cm}^{-1}$ region. These features are primarily linked to the vibrations of metal chalcogen bonds, as described chemically.

Keywords: vibrational properties, infrared spectroscopy, Cu_2NiTe_2 , chalcogenide, crystal structure

1. Introduction

Chalcogenide semiconductors are widely used in various electronic technologies. Their usefulness comes from their ability to conduct electricity well and their strong interactions with light, both in terms of electricity and optics [1]. These components are used in many different types of sensors and transducers [2]. Therefore, they remain a popular and active area of research in materials science [3]. With improvements in experimental techniques and modeling, we can now more reliably determine necessary parameters [4]. Therefore, a thorough study of their structural, electrical, and optical properties using modern analytical methods is crucial [5].

Among these materials, the Cu_2NiX_2 (where X is S, Se, or Te) compounds are particularly remarkable. These crystals always exhibit copper in a monovalent state, while nickel is always in a divalent state. The lattice structure is characterized by a highly symmetric hexagonal arrangement, which reflects hexagonal symmetry. This symmetry contributes to a relatively stable structure, both physically and chemically. Differential scanning calorimetry and thermogravimetric results indicate no phase transitions at elevated temperatures, thermally. The release of gas molecules from the sample explains the observed thermoelectric effects [6], [7], [8]. It has been established that these chalcogenides can also serve as model objects for studying thermodynamic functions.

There are many methods for studying crystal lattice vibrations. These methods allow one to study lattice vibrations both theoretically and experimentally. Among the research methods, Raman spectroscopy and infrared (IR) spectroscopy occupy a special place. The applicability of these methods changes depending on the chemical composition and shape of the sample. Since Raman spectroscopy is quite sensitive, it is also used to determine phase transitions [9], [10], [11], [12]. Infrared spectroscopy is one of the most widely used analytical methods for studying solids. It has been established that this method is one of the unique methods for studying the vibration modes of interatomic bonds, determining the properties of the atoms that make up the sample, and the nature of the bonds.

Therefore, various studies are being conducted in the direction of studying functional materials using infrared spectroscopy [13], [14], [15]. Although many physicochemical properties of chalcogenide semiconductors, Cu_2NiX_2 studied using infrared spectroscopy.

In this work, Cu_2NiTe_2 has been studied, their atomic dynamics have not been crystal was synthesized, and its crystal structure and atomic dynamics at room temperature were studied. The research utilized X-ray diffraction (XRD) and infrared spectroscopy (FTIR), which are considered modern analytical methods. The results were analyzed using state-of-the-art software.

2. Materials and Methods

2.1. Synthesis of Samples

The Cu_2NiTe_2 compound was synthesized using a standard method typical for chalcogenide semiconductors. To prevent oxidation during the reaction, the synthesis process was carried out under closed conditions (high vacuum). In a single-zone furnace, the chemical elements of copper, nickel, and tellurium, deposited according to the stoichiometric composition, were collected in a quartz ampoule. The ampoule was reduced to approximately 10^{-4} mmHg, and it was subsequently closed. Following this, the ampoule's temperature was maintained at 300°C , and it was introduced into the furnace. After a one-hour hold, the furnace temperature was gradually increased. The program included 30-minute holds at 800 , 900 , and 1000°C , in sequence, within the range of 700 - 1050°C . To achieve uniformity, the closed ampoule was periodically stirred together in the furnace. Afterward, the temperature was adjusted to 50°C and maintained for 1.5 hours steadily. In the next step, the temperature was gradually reduced to $T = 600^\circ\text{C}$. After holding at the homogenization temperature for 3 days, the process was stopped. After the synthesis process was complete, samples were prepared for structural and atomic dynamics studies.

2.2. Study of Crystal Structure

The crystal structure of the Cu_2NiTe_2 compound was studied using X-ray diffraction. The studies were conducted on a D8 ADVANCE diffractometer (Bruker, Germany). The diffractometer parameters are 40 kV, 40 mA, $\text{Cu K}\alpha$ radiation, and λ is 1.5406 \AA . A polycrystalline Cu_2 sample was first crushed and ground into powder. An X-ray spectrum of the powder sample was then obtained. The X-ray diffraction spectrum, obtained at room temperature, was analyzed using the Rietveld method in Mag2Pol software. It was established that the sample was obtained in a single-phase state with a highly symmetric hexagonal crystal structure.

2.3. Study of Vibrational Properties

The atomic dynamics (vibrational properties) of the Cu_2NiTe_2 compound were studied at room temperature using infrared spectroscopy. The samples for Fourier-transform infrared experiments were prepared in a cylindrical form with a diameter of 7 mm and a length of 1 mm at a pressure of P is 0.5 kN/cm^2 Cu_2NiTe_2 by using a press machine. The infrared spectra of the samples were analyzed within the wave number range of 400 - 4000 cm^{-1} by using the Varian 640 FTIR device. The obtained spectrum was analyzed, the modes corresponding to the lattice vibrations were determined, and the atomic dynamics of the Cu_2NiTe_2 were studied using the wave numbers of these modes.

3. Results and Discussion

3.1. Structural Properties

The crystal structure of the Cu_2NiTe_2 compound, synthesized in polycrystalline form, was studied using X-ray diffraction. The spectrum, obtained at room temperature and under normal conditions, was analyzed using the Rietveld method in the Mag2Pol program. During the spectrum analysis, it was determined that the crystal structure of the Cu_2NiTe_2 compound corresponds to hexagonal symmetry with the space group $\text{P6}_3/\text{mmc}$. The lattice parameters were determined to be $a = b = 3.944 \text{ \AA}$, $c = 17.138 \text{ \AA}$. As can be seen, when monovalent copper



and divalent nickel atoms combine with tellurium chalcogenide atoms with the formation of covalent bonds, a single-phase, highly symmetric system is formed. Such systems are stable under external influences (temperature, pressure, radiation, etc.). However, under external influences, internal fluctuations may occur. Therefore, when studying the structural aspects of such systems, lattice vibrations, atomic dynamics, and bond characteristics should be studied.

3.2. Vibrational Properties

Based on the above, the atomic dynamics of the Cu_2NiTe_2 semiconductor compound were studied using infrared spectroscopy. The infrared spectrum, obtained under normal conditions at room temperature, in the wavelength range of $400\text{--}4000\text{ cm}^{-1}$, is shown in Figure 1.

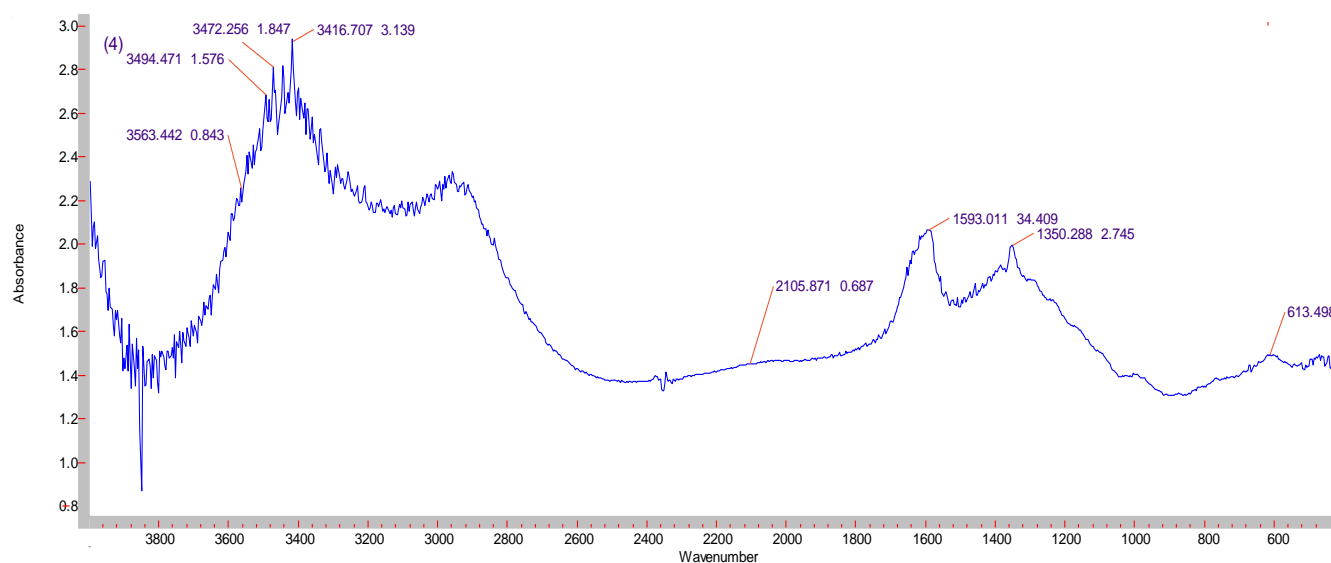


Figure 1. Infrared spectrum of Cu_2NiTe_2 crystal.

The spectrum shown in Figure 1 shows the infrared spectrum of the Cu_2NiTe_2 crystal in the wavenumber range. These peaks correspond to wavenumbers of approximately $500, 600, 1300, 1600, 3000,$ and 3400 cm^{-1} . These values correspond to vibrations of the bonds formed by metal atoms with chalcogen atoms. When the crystal lattice consists of atoms of heavy elements, the lattice vibration frequencies are low. Examples of such atoms include atoms of metals such as Tl and Pb. The frequencies of the bonds they form are low. However, when light elements such as H, Li, and O enter the crystal, the bond frequencies become higher. Since the atoms that form the Cu_2NiTe_2 crystal are not heavy elements, the frequencies of the vibrational modes observed in the infrared spectrum are quite high. As can be seen from the wavenumbers observed in the spectrum, the intensity of the observed peaks increases with increasing wavenumbers.

The infrared spectrum of Cu_2NiTe_2 indicates a vibrationally active lattice dynamically. When these spectral features are compared with crystallographic results, the Cu–Ni–Te framework is confirmed as highly symmetric and robust, structurally. This high symmetry supports stability against external perturbations, mechanically. As a result, no high-temperature phase transitions are expected for this system, consistently [7].

4. Conclusion

The structure and lattice motions of Cu_2NiTe_2 were examined using modern analytical approaches, systematically. The results show that the Cu–Ni–Te framework behaves as a highly symmetric, vibrationally active system, dynamically. Infrared measurements identified six dominant bands across the $400\text{--}4000\text{ cm}^{-1}$ region, clearly. These bands are attributed mainly to vibrations associated with metal-chalcogen bonding, chemically.

Comparison with related chalcogenide semiconductors indicates Cu₂NiTe₂ remains resilient to external disturbances because of its robust symmetry and lattice dynamics.

Author Contributions

All authors reviewed, edited, and approved the manuscript.

Conflict of Interest

The authors declare no conflicts of interest.

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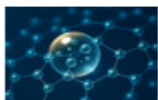
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Abbreviations

Nickel Telluride Copper (Cu₂NiTe₂), Sulphur (S), Selenium (Se), Tellurium (Te), Infrared (IR), X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Thallium (Tl), Plumbum (Pb), Copper-Nickel-Titanium (Cu–Ni–Te).

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