

Raman Studies On Cupric Telluride Thin Films: An Empirical Study On Cupric Telluride

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Cupric telluride thin films (CuTe) of 100 nm and 200 nm thickness were produced using a thermal evaporation process and deposited at a rate of 15.3 Å/s on a well-cleaned glass substrate held at 300 K under a vacuum of greater than 10^{-5} mbar. A bulk sample of (CuTe) was also collected for study. The deposited films were annealed for one hour at 375 K before being used for characterization. CuTe bulk material and thin (CuTe) films have had their Raman spectra recorded. The composition and polycrystalline character of CuTe films were confirmed by X-ray diffraction experiments. Raman bands at 231cm^{-1} , 240cm^{-1} , and 259cm^{-1} were found on (CuTe) thin films as well as bulk samples. The Raman peak position of CuTe films did not vary significantly, but the peak intensity increased. Atomic Force Microscopy (AFM) tests indicate that the grain size of CuTe thin films is roughly 40 nm. This work is motivated by the works of [1 - 10].

Keywords: Cupric telluride, thin film, thermal evaporation, AFM.

1 Introduction

AIBVI compounds, which include copper telluride, are being extensively researched in relation to their potential use in thermoelectric generators, rapid switches, and heterojunctions. Thin films of copper chalcogenides have attracted the interest of researchers for many years, owing to their diverse uses in solar cells, super-ionic conductors, photothermal converters, electroconductive electrodes, microwave shielding, solar control coating, and so on. The CuTe recording media can utilize run-length-limited codes successfully, allowing for very large data storage capacity and data transfer rates (see [11-20]). At ambient temperature, the binary semiconductor (CuTe) has an energy gap E_g of roughly 1.5 eV, which is quite near to the range for best solar energy conversion. As a result, this material is quite interesting for device applications. The mineral vulcanite (CuTe) has an orthorhombic crystalline structure ($a = 3.155\text{Å}$, $b = 4.086\text{Å}$, and $c = 6.946\text{Å}$). It belongs to the D_{2h}^{13} pmn space group and is strongly birefringent and pleiochroic. Bahl examined the K absorption edge on CuTe and concluded that the shift towards the high-energy side is caused by electron transfer from tellurium to copper. CuTe has been attempted to be used as a solar cell. Several workers have conducted detailed structural and optical studies on CuTe. According to Maheshwari and Sharma, the

vibrational frequency of CuTe is around 254cm^{-1} , and the force constant is approximately $1.612 \times 10^{-5}\text{dyn/cm}$. According to Lefebure and Bocquet, the vibrational frequency of the CuTe molecule is approximately 253cm^{-1} . Baranova et al. investigated electron di raction on CuTe alloys. CuTe possesses metallic properties in bulk and semiconducting qualities in thin lms.

Seong used Te-Te bonding to explain the metallic and semiconducting behavior of CuTe. Their research also revealed that there is no phase transition in CuTe and that the material is a p-type semiconductor with great electrical conductivity. However, Copper Telluride has received little attention.

Raman spectrometry has evolved as a helpful tool for studying lattice vibrations and their interactions with other excitations in recent years. Raman spectroscopy is a nondestructive, very sensitive spectrometer technique used to characterize semiconductor structure and molecular vibrations. We provide the preliminary results of a Raman spectroscopy analysis of the optical properties of thin lms in this paper because no attempt has previously been made to analyze the Raman spectrum of CuTe(see[21-51]).

2 Experimental

Cooper Telluride (CuTe) alloy with 99.99 purity acquired from M/S Aldrich (India) was utilized to prepare thin lms by thermal evaporation. On properly cleaned glass substrates of $0.01 \times 0.03\text{ m}^2$, a known amount of CuTe material was extracted and evaporated the entire charge from a molybdenum boat under a vacuum better than $2 \times 10^{-5}\text{mbar}$. Before placing the glass substrates in the vacuum chamber, they were cleaned with hot chromic acid and distilled water. Energy Dispersive Analysis of X-rays (EDAX) measurements were also used to gather compositional information. Figure 2 shows an AFM image of a CuTe thin lm with a thickness of 200 nm. The surface roughness and grain size of CuTe lms were estimated using AFM measurements. Raman characterisation was performed using a Reinshow in through Laser Raman microscope. A He-Ne laser source with a power of 18 mW was operating at a wavelength of 633 nm. At normal temperature, raman spectra with wave numbers ranging from 100 to 800 cm^{-1} were obtained.

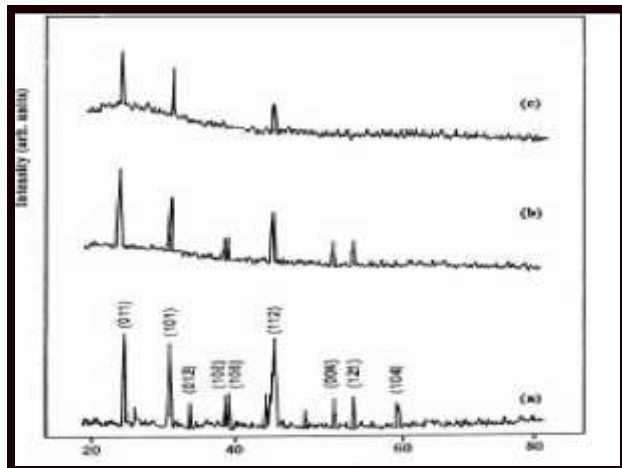


Figure 1: XRD pattern of CuTe (a) bulk, (b) 200 nm and (c) 100 nm

3 Results and discussion

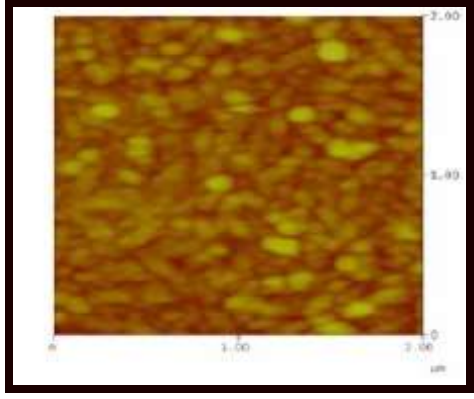


Fig. 3 depicts the Raman spectra of CuTe thin lms and bulk material. Diatomic molecules have only one vibration along their chemical link. We discovered the following symmetries of zone center optical phonon modes from a group theoretical investigation of CuTe lms:

$$2A_g + 2B_{2g} + 2B_{3g} + B_{1u} + B_{2u} + B_{3u}$$

where six modes of $2A_g + 2B_{2g} + 2B_{3g}$ are active in Raman spectra.

Factor group analysis of CuTe Figure 2: AFM picture of CuTe thin lms (Crystal Space group: D_{2h}^{13} ; $Z = 2$; $Z^b = 2$)

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	Modes and degrees of freedom for each species	site symmetry species C_{2v}	Factor group Species D_{2h}
Cu atoms	Vibrational	A_1	$A_g + B_{1u}$
		B_1	$A_{2g} + B_{3u}$
		B_2	$A_{3g} + B_{2u}$
Te atoms	Vibrational	A_1	$A_g + B_{1u}$
		B_1	$A_{2g} + B_{3u}$
		B_2	$A_{3g} + B_{2u}$

$$\Gamma_{\text{vibCuTe}} = 2 A_g + 2 B_{2g} + 2 B_{3g} + B_{1u} + B_{2u} + B_{3u}$$

We found a strong sharp band at 259 cm^{-1} and a shoulder peak at 231 cm^{-1} and 240 cm^{-1} in a CuTe bulk sample. The Raman spectra of CuTe thin lms are extremely similar to the corresponding Raman spectra of bulk sample. Figure shows that a conspicuous peak is located about 259 cm^{-1} and that other peaks are present in all other lms. This corresponds to the reported values. The A_1 mode is clearly responsible for the most strong Raman line, which emerges at 259 cm^{-1} . This mode is caused by the interaction of Te and Cu atoms. The Raman spectrum's sharp Raman Intensity (arb. units) peak suggests that the polycrystalline phase is prevalent in CuTe thin sheets. There is no substantial change in peak location, however there is some change in intensity.

The intensity of Raman bands was thought to increase with the number of scattering molecules or the intensity of input light. The extent of the increase in Raman scattering cross section relies on the chemical composition of the adsorbed molecule, the roughness of the surface, and the adsorbent's optical properties. In our situation, the roughness of the CuTe lm surfaces increases the intensity of the Raman spectra.

AFM measurements reveal that the roughness RMS value is around 3.2 nm and the grain size is approximately 40 nm . Sherrer's formula, when applied

to XRD peaks, corroborated this. This lm's X-ray diffraction pattern demonstrates that these materials

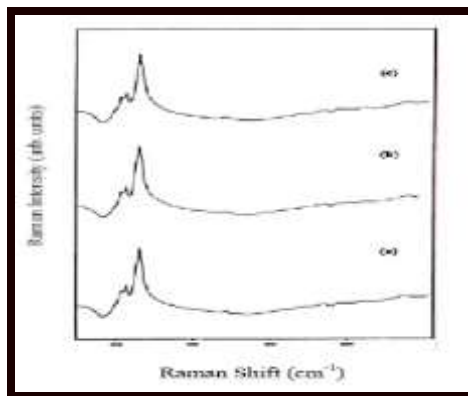


Figure 3: Raman Spectrum of CuTe (a) bulk, (b) 100 nm and (c) 200 nm

are polycrystalline and confirm the compound composition. The

emergence of a prominent peak may

indicate that the lm is well crystalline. The surface quality of vacuum evaporated CuTe thin lms was independently checked using atomic force microscopy (AFM). The 2D AFM pictures of the room temperature deposited lms are shown in Fig. 2. The RMS value of surface roughness determined by AFM measurements of vacuum evaporated CuTe thin lms at ambient temperature is around 3.2 nm . After annealing, the RMS roughness of the lms ranges from 2.7 to 2.9 nm . This could be attributed to the elimination of surface imperfections from the lms during heating.

4 Conclusion

Thermal evaporation was used to create thin lms of copper telluride (CuTe) under a vacuum of $2 \times 10^{-3}\text{ mbar}$. The Raman spectra of copper telluride thin lms and bulk materials were recorded. There are three Raman lines, with the strongest peak occurring at 259 cm^{-1} . This is because of the A_1 mode. It is formed by the motion of Te atoms in conjunction with Cu atoms. The X-ray diffraction technique detected the extent of crystallinity and polycrystalline nature, which is reflected in the Raman spectra of the thin lms. The surface of CuTe thin lms was found to be smooth in SEM and AFM tests, and the grain size was calculated to be around 40 nm .

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