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Structural, Morphology and Some Optical Properties of Chalcogenide $Ga_{80-x}Se_xTe_{20}$ (Where x = 10%, 15% and 20%) Glassy Material

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Abstract

$Ga_{80-x}Se_xTe_{20}$ amorphous system was prepared by conventional technique. Structural, morphology and optical properties have been investigated. X-ray diffraction (XRD) patterns reveal the non-crystalline nature of the prepared sample. Differential thermal analysis (DTA) traces indicate the presence glass transition temperature T_g for all samples below 500˚C. Addition T_g values increases by increasing Se content. Energy dispersive X-ray spectroscopy (EDX) data shows good agreement with actual composition. Moreover, surface characterization was achieved by scanning electron microscope (SEM). The patterns confirmed the non-crystalline nature. In order to analyze the data, the cohesive energy C.E was calculated by all three composition optical properties that have been investigated in the wavelength range 500 - 2500 nm. Reflectivity R and transmitivity T spectrum were used to estimate the band gap energy using UV-Visible absorption spectrum. It is worthy mention that the optical band gap follows the T_g and cohesive energy behavior, where it increases by increasing Se content.

Keywords

Chalcogenide Glasses, Structure, Optical, Cohesive Energy

1. Introduction

Chalcogenide glasses find wide applications in various fields of up-to-date technology due to their peculiar properties [1], such as target materials of television

cameras, microwave devices, switching and diodes [2] [3]. This is most likely due to their high optical transparency in the IR region, strong optical nonlinearity, high photo sensitivity, ease of fabrication and processing, and good chemical durability. Chalcogenide glasses based on the chalcogen elements S, Se, Te are used widely in ultra-fast optical switches, frequency converters, optical amplifiers, optical recording devices, an optical integrated circuit for IR operations and infrared transmitting optical fibers [4]-[10]. Ga-X systems where elements X = S, Se or Te have revealed to be particular interest [10]. In the present article, the structural, morphological and some optical properties of $Ga_{80-x}Se_xTe_{20}$ (where X = 10%, 15% and 20%) have been studied with thickness ranging between 165 nm, 615 nm and 1027 nm.

2. Experimental Procedure

Bulk amorphous of $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) chalcogenide glass were prepared by conventional melt quenching technique [11]. High purity (99.9999% purity) materials of Ga, Se, and Te were weighed according to their atomic percentage and sealed in quartz ampoules with a vacuum of 10^{-5} Torr. The samples were then heated and melted in a rocking furnace, where temperature was raised at a rate of 4 K per minute for up to 1273 ˚K for 15 h. During heating process, the ampoules were frequently rocked by rotating a ceramic rod to which the amorphous were tucked away in the furnace is order to obtain a compositionally homogeneous melt. The molten samples were then rapidly quenched in ice cooled water. The quenched samples were taken out by breaking the ampoules. The glassy nature of the samples was established by the non-isothermal differential scanning (DTA-50) Measurements at a constant heating rate of 20 K/min. The DTA scan was obtained by heating 8 mg of powdered samples sealed in an aluminum pan.

The x-ray diffraction machine (XD-D ShimadZu) was used to study nature of the prepared sample). Moreover the scanning electron microscope (Joel-SEM-5400) which connected by energy dispersive spectroscopy (EDX) technique was used to study the morphology together with chemical compositions of samples, constitutes fully quantitative analyses results were obtained from the spectra by processing date through Zaf correction program. The transmittance and reflectance were measured using a double beam UV-VIS Spectrophotometer in the wavelength range 500 - 2500 nm.

3. Results and Discussion

3.1. Thermal Properties

Figure 1 represents the DTA thermogram of the investigated system. It was obtained for a bulk glass sample by heating 8mg using a heating rate of 20 k/min. By increasing Se content T_g shows tendency to increase Figure 1. The temperature was found to be 433 K, 445 K, and 447 K respectively.

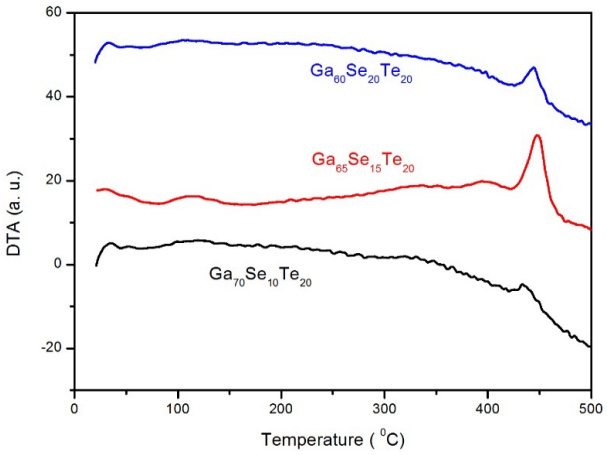

Figure 1. DTA thermograms of $Ga_{80-x}Se_xTe_{20}$ Glass composition.

3.2. Structural of Characterization

The X-ray diffraction pattern of the$Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) glass composition was presented in **Figure 2**. It is clear that the absence of sharp diffraction lines and the presence of hump only confirm the amorphous nature of the prepared samples.

3.3. Surface Morphology

Morphological inspections performed by SEM on as-grown films have shown a flat surface without the presence of cracks agglomerates and precipitated **Figure 3**. SEM image has confirmed the absence of spurious phase. The morphology of thin films of different compositions has been found to be of coniform contrast. The diffraction pattern for the as-prepared thin films of different compositions is similar, indicating the amorphous nature of as-prepared thin films of different compositions. The elemental compositions of $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) chalcogenide glasses were checked by energy dispersive X-ray analysis (EDX). It is noticed that **Figure 4** which clearly show that amount of selenium increase with the increase of X.

3.4. Cohesive Energy

The possible bonds formed in chalcogenids system $Ga_{80-x}Se_xTe_{20}$ are Se-Ga, Se-Se, Se-Te. According to chemical bond approach (CBA) [12] combination in different type in the atoms takes place more easily rather in the atoms of same type. These bonds are formed in the sequence of decreasing bond energy until the available valence of atoms is saturated. The Ga-Se glassy system is covalent chalcogenide system. The bond energy of homopolar bonds can be estimated by The Pauling method in terms of the bond energy of homopolar bonds and the electronegativity of the atoms involved.

The bond energy E(A-B) of hetero nuclear bond, can be calculated by Equation [13]

$$E_{A-B} = \left(E_{A-A} - E_{B-B}\right)^{1/2} + 30\left(x_A - x_B\right)^2 \quad (1)$$

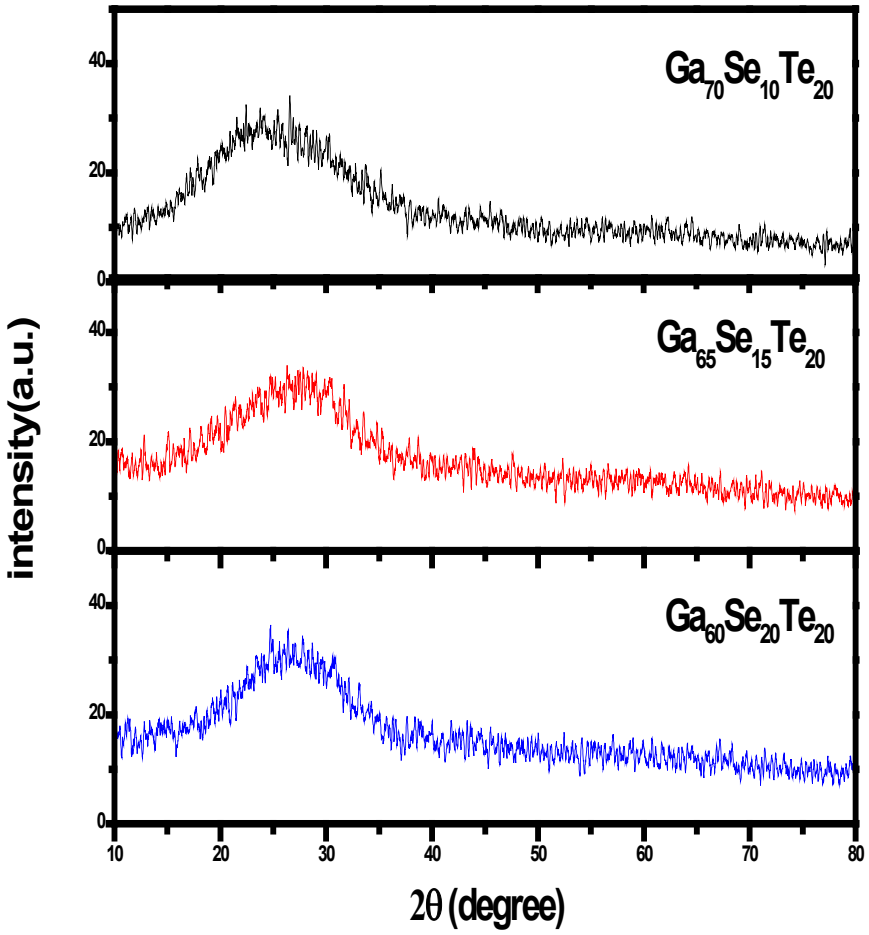

Figure 2. X-ray diffraction patterns of as-prepared $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) glass composition.

Figure 3. SEM images of $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) glass composition.

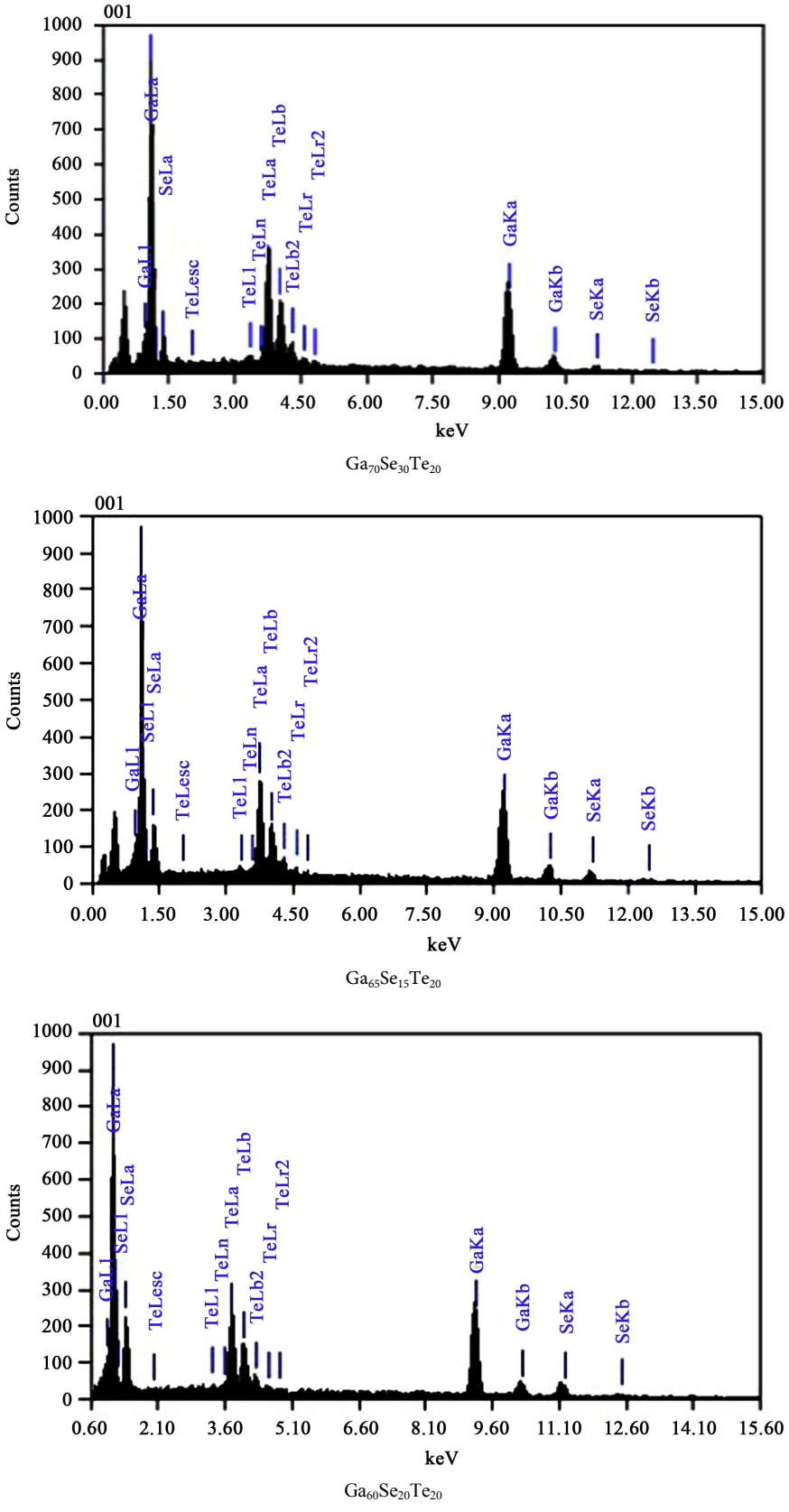

Figure 4. The energy dispersive X-ray spectroscopy (EDAX) of $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) glassy material.

E_{A-A} and E_{B-B} are the bonds energies of homo nuclear bonds, x_A and x_B are electronegativity values of A and B Elements.

The bond energy of the homo polar bonds E_{Ga-Ga} is 31.82, E_{Se-Se} is 44, and E_{Te-Te} is 33 Kal/mol [14] [15].

The electronegativity value are 1.81, 2.55, and 2.10 for Ga, Se and Te respectively [13].

By using Equation (1) values of E_{Ga-Se}, E_{Se-Te} and E_{Te-Se} are gives as 53.85, 44.93 and 44.18 respectively.

The bonds are formed in order of decreasing bond energy.

Ga-Se bonds having maximum energy are first followed by E_{Te-Se} then E_{Ga-Te} bonds.

As these bond energies are assumed to be addition, so cohesive energies calculated by summing the bond energies over all possible in a compound. Cohesive energies calculated as:

$$C_E = \sum C_i E_i \tag{2}$$

where C_i is the probability of formation of expected bonds, and E_i is the energy of the corresponding bond present in the system.

Table 1 listed the chemical distribution of bonds, electronegativity, and cohesive energy of the sample.

Table 1. Electronegativity, distribution of chemical bonds and cohesive energy for the composition $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %).

Composition	Electronegativity	Distribution of chemical bonds			Cohesive energy
		Ga-Se	Ga-Te	Ga-Ga	CE ev
$Ga_{70}Se_{10}Te_{20}$	1.81	0.09523810	0.1904762	0.7143857	1.496454
$Ga_{65}Se_{15}Te_{20}$	2.55	0.1538462	0.2051282	0.6410256	1.5544054
$Ga_{60}Se_{20}Te_{20}$	2.10	0.2222222	0.2222222	0.5555556	1.6220154

It is observed that by increasing Se content leads to increasing the cohesive energy in chalcogenide system $Ga_{80-x}Se_xTe_{20}$.

3.5. Optical Properties

Optical properties of $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) have been investigated in the wavelength (500 - 2500) nm. Figures 5(a)-(c) show reflectivity R and transmition T of investigated then films with wavelength.

The data of (Figure 5(a)) $Ga_{70}Se_{10}Te_{20}$ reveled reflectivity R decrees by increasing wavelength, while transimtion T is increase by increasing wavelength. It is worthy to mention that the observed edg in transmtion spectra extended over wide wavelength ranged, confirming a non-crystalline nature of the films.

Figure 5(b) and Figure 5(c) of composition $Ga_{65}Se_{15}Te_{20}$ and $Ga_{60}Se_{20}Te_{20}$ show that the dependence of R and T is non-linear, by increasing the selenium content, the transimtion increase up to 1750 nm with minimum reflection at the same wavelength. Such observed nonlinearity allows to conclude that we are dealing with more than one absorption mechanism.

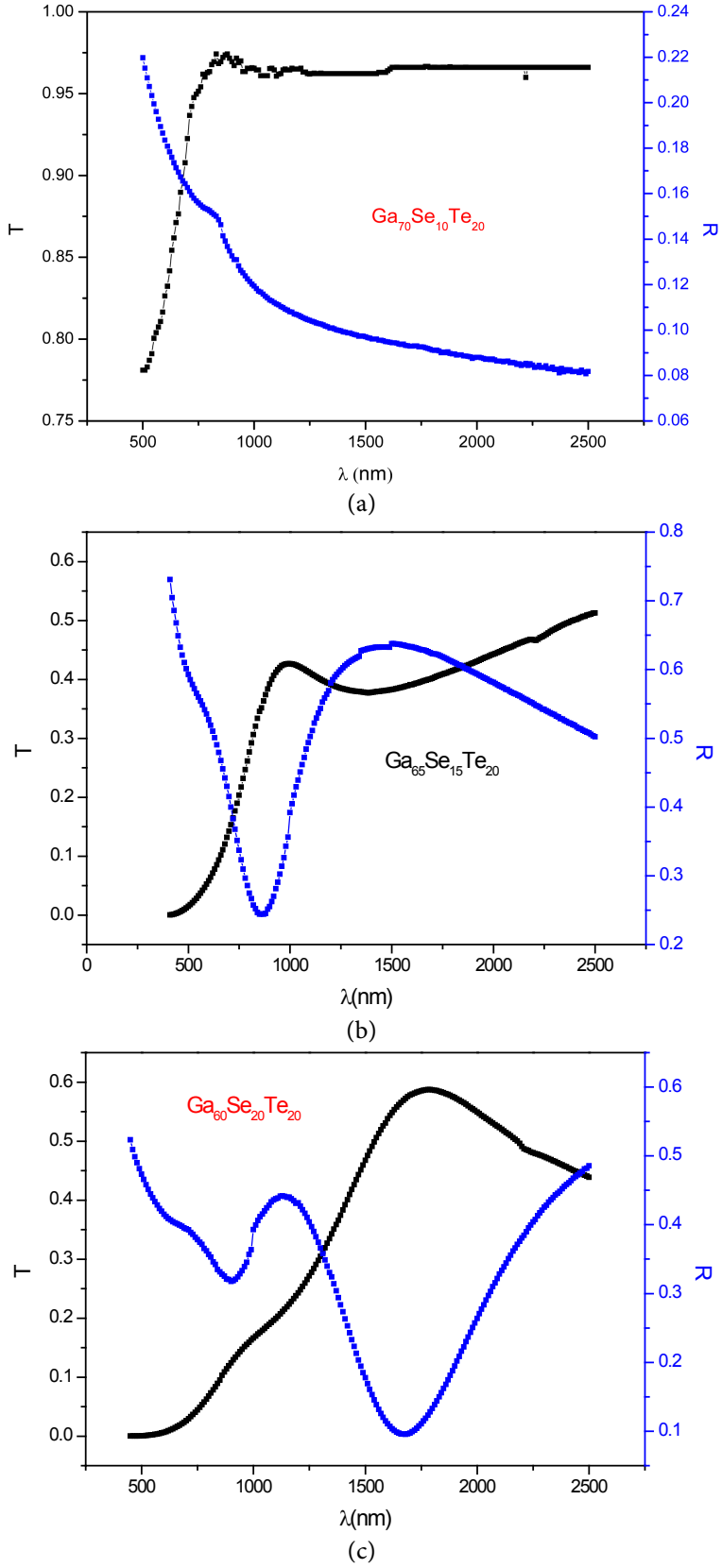

Figure 5. Transmission and reflection spectra for $Ga_{80-x}Se_xTe_{20}$ (where x = 10, 15 and 20 at %) glassy material.

The obtained spectra were used to estimate the optical band gap energies as 0.721 ev, 0.97 ev, and 1.007 ev for $Ga_{70}Se_{10}Te_{20}$, $Ga_{65}Se_{15}Te_{20}$ and $Ga_{60}Se_{20}Te_{20}$ respectively.

It is worthy to mention that the band gap increases by increase Se content, *i.e.* by increasing C.E the letter represent the average binding energy of the system.

4. Conclusions

Glassy system of $Ga_{80-x}Se_xTe_{20}$ (where x = 10%, 15% and 20%) Chalcogenide Semiconductors has been successfully prepared. The study includes DTA, XRD, SEM, EDX and UV-visible absorption spectrum. The analysis of DTA reveals the absence of any sharp exothermic peak indicating the absence of structural change, which is in a good agreement with X-ray diffraction, confirmed the amorphous state of the system. Also (SEM) and (EDX) are confirmed the absence of serious phase. Moreover, the cohesive energy of the investigated has been calculated by using chemical bond. It follows the T_g behavior, and by increasing Se content, cohesive energy increases.

Addition of selenium content in the $Ga_{80-x}Se_xTe_{20}$ system modifies the properties of the present sample especially the optical (T & R). Optical measurements indicate that the non-direct transition is dominant in mechanism responsible for the photon absorption inside the investigated samples. It is also observed that the increasing of Se content leads to increase of band gap. This is in fair agreement with T_g and cohesive energy data.

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