Journal of Ovonic Research Vol. 6, No. 3, June 2010, p. 125 – 133

STRUCTURAL STUDY OF Se-Te-Zn SYSTEM USING XRD SPECTRA

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X-ray diffraction (XRD) analysis has been carried out on $Se_{19}Te_{81-x}Zn_x$ (x = 0, 3, 6, 9) samples and their diffractograms are analyzed to obtain information about various crystallographic aspects. XRD traces of all samples are taken at room temperature which shows almost similar trends. These traces confirm the formation of alloys of $Se_{19}Te_{81-x}Zn_x$. The presence of sharp structural peaks in these XRD patterns confirmed the polycrystalline nature of the material. In all the samples the average particle size of the alloy is found to be 4.4778 μm and mean density is found to be 120.73 g/cc.

(Received May 7, 2010; accepted June 5, 2010)

Keywords: XRD, density, Average particle size.

1. Introduction

From the past few decades chalcogenide semiconductors have attracted the attention of various research workers due to their potential ability in wide spectrum of the optoelectronics devices. These materials like Se-Te alloys are of great interest because of their higher photosensitivity, greater hardness, and higher crystallization temperature [1-4]. Moreover there is a great scope of doping these materials with a third element like Zn, Bi, Pb etc to enhance their properties and make them more suitable for various applications. A lot of work has therefore been done on ternary alloys containing Se-Te. Zinc based compound semiconductors such as zinc selenide and zinc telluride are applied to high energy conversion opto-electronic materials due to their wide band gap energy [5-8]. Among them zinc telluride (ZnTe) based diode is applicable to the green light emission device and photovoltaic solar cell because their large band gap energy (2.26 eV). ZnTe based semiconductors are one of the most widely used alloy semiconductors for a variety of applications in optics, electronics and optoelectronics, such as ultra fast optical sensors, holography, infrared lenses, ionic sensors etc. Wide band gap II–VI semiconductors present a large interest for visible light emitters in the blue/green spectrum [9-12]. These polycrystalline semiconducting materials are under increased scrutiny because of their wide use in the cost reduction of devices for photovoltaic applications.

Se Te Zn system is one of the II-VI ternary semiconductor materials whose band gap can be tailored to any value between 1.48 eV - 2.26 eV[2]. It is promising material for high-efficiency solar cells, switching and other optoelectronic devices.

In the present paper the structural studies of $Se_{19}Te_{81-x}Zn_x$ (x = 0, 3, 6, 9) system is analyzed by using XRD method. Various properties like density, particle size, volume etc. are studied. It is also observed that with the increasing proportion of Zn, the system moves to more crystalline state.

2. Experimental

$Se_{19}Te_{81-x}Zn_x$ (x = 0, 3, 6, 9) polycrystalline material were prepared by well known melt quenching technique. The exact proportions of high purity (99.999%) Se, Te and Zn elements, in

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accordance with their atomic percentages, were weighed using an electronic balance (LIBROR, AEG-120) with the least count of 10^{-4} G The material was then sealed in evacuated (~10^{-5} Torr) quartz ampoule (length ~ 10 cm and internal diameter ~ 8 mm). The ampoule containing material was heated to 800° C and was held at that temperature for 12 h. The temperature of the furnace was raised slowly at a rate of 3-4° C / minute. During heating, the ampoule was constantly rocked, by rotating a ceramic rod to which the ampoule was tucked away in the furnace. This was done to obtain homogeneous alloy. After rocking for about 12 hours, the obtained melt was quenched in air. The quenched sample was then taken out by breaking the quartz ampoule. The nature of the alloy was ascertained by X-ray diffraction. For this, X-ray diffraction (XRD) patterns of sample were taken at room temperature by using an X-ray diffractometer (Philips, PW 3064). The copper target was used as a source of X-rays with $\lambda = 1.54$ Å (Cu Kα_1).

3. Results and discussion

In the present work the X-ray diffraction patterns for the $Se_{19}Te_{81-x}Zn_x$ (x = 0, 3, 6, 9) system are studied by using the X-ray diffractometer XPERT-PRO (Philips, PW3064) with Cu Kα radiation $\lambda = 1.5405$ Å. The graphical study of the XRD pattern of the system is showing polycrystalline nature. The package program POWDER is used in the specification of the crystal systems through the lattice constants and Miller Indices for each phase [17-25].

Results

XRD graphs and related parameters of $Se_{19}Te_{81-x}Zn_x$ (x = 0, 3, 6, 9) system are studied.

$Se_{19}Te_{81}$ system

The XRD of $Se_{19}Te_{81}$ sample is shown in figure 1. In this figure peaks are appearing at the regular intervals. This system is showing the behavior of cubic as well as of the hexagonal system. Miller indices at the points (110), (111), (220) are showing the cubic part of the system under consideration and the Miller indices at the points (222), (211), (102), (210) are the hexagonal one. The cubic phase together with the hexagonal one was due to the polycrystalline behavior of the compound tending to present a multiphase structure [26-35]. Various (h, k, l) values corresponding to the peaks obtained in the figure 1 are shown in Table 1.1. From these values we have calculated the lattice parameters for cubic systems [15,27]

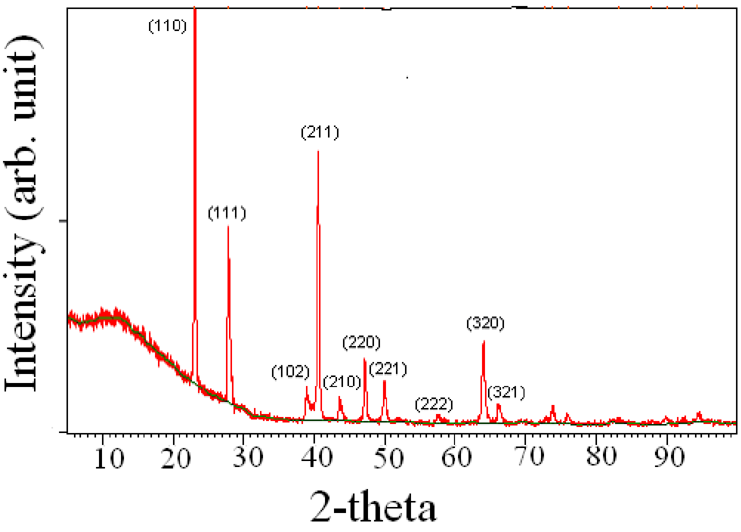

Fig. 1. Shows the XRD graph of $Se_{19}Te_{81}$ system.

Table 1.1 h,k,l values of the peaks of $Se_{19}Te_{81}$ *system*

2θ	**hkl**	**Crystal system**
23.12	110	Cubic
27.80	111	Cubic
38.95	210,102	Cubic/ Hexagonal
40.60	211,112	Cubic/ Hexagonal
43.56	210	Hexagonal
47.18	220	Cubic
49.88	221,300	Cubic/ Hexagonal
57.62	222	Cubic/ Hexagonal
63.86	320	Cubic/ Hexagonal
66.15	321	Cubic

For the cubic system

$$a = (\lambda/2)(N/Sin^2\theta)^{1/2}$$

Also

$$a = d(h^2 + k^2 + l^2)^{1/2}$$

which give us a=5.41 Å. Then volume

$$V = a^3 = 158.34\ Å^3$$

The density of the material in this case is found to be 124.09 g/cm^3.

The particle size is found by [27]

$$t = \frac{0.9\lambda}{B\cos\theta}$$

where B = broadening of the diffraction line measured at half its maximum intensity (radians) and t = diameter of the crystal particle and the density by using the relation $\rho = \frac{1.66020\sum A}{V}$

where $\sum A$ is the sum of the atomic weights of the atoms in the unit cell,ρ is the density in (gm/cm^3) and V is the volume of the unit cell ($\overset{o}{A}{}^3$).Here the substance is a compound whose composition can be represented by the simple chemical formula, then

$$\sum A = n_1 M$$

where n_l is the number of the molecules per unit cell and M is the molecular weight, here in our case n_l =1. The particle size and the Lorentz factor's variation calculated using XRD data `are shown in Table 1.2. From the calculated values the mean value of the particle size is found to be 0.0437 μm.

Table 1.2 Calculated values of the particle size and the lorentz's factor of $Se_{19}Te_{81}$ *system*

θ(in degree)	**cosθ**	**B(in radian)**	**t (Particle size in A^o)**	**Lorentz's factor**
11.56	0.9797	0.00209	673.67	47.43
13.90	0.9707	0.00209	679.92	31.82
19.48	0.9427	0.00408	360.35	15.27
20.30	0.9378	0.00467	316.47	13.97
21.78	0.9286	0.00175	852.90	11.91
23.58	0.9165	0.00467	323.82	9.95
24.93	0.9068	0.00356	429.34	8.81
28.81	0.8762	0.007	225.97	6.33
31.93	0.8486	0.00525	311.06	5.04
33.07	0.8380	0.00817	202.44	4.66

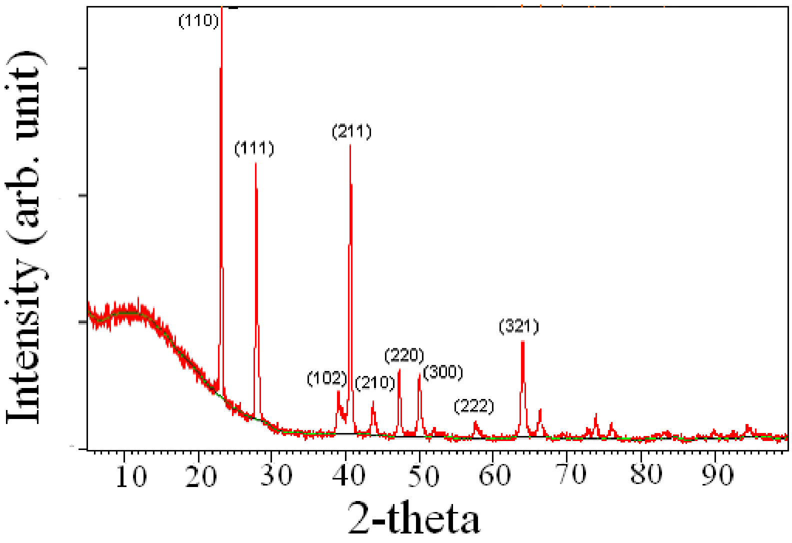

Fig. 2 Shows the XRD graph of $Se_{19}Te_{78}Zn_3$ system.

$Se_{19}Te_{78}Zn_3$ system

The XRD of $Se_{19}Te_{78}Zn_3$ sample is shown in figure 2. In the same way in this diffractogram too the peaks are appearing at the regular intervals Table 2.1 from which the value of a=5.4 Å. Then volume $V=a^3=158.34$ Å^3 the density of the material in this case is found to be 122.07g/cc. The particle size and the Lorentz factor's variation calculated using XRD data are shown in Table 2.2. The particle size is found to be 0.0405 µm.

Table 2.1 h,k,l values of the peaks of $Se_{19}Te_{78}Zn_3$ system

2θ	hkl	Crystal System
23.17	110	Cubic
27.88	111	Cubic
38.94	210, 102	Cubic/ Hexagonal
40.63	211, 112	Cubic/ Hexagonal
43.69	210	Hexagonal
47.12	220	Cubic
49.88	300,221	Cubic/ Hexagonal
57.52	222	Cubic/ Hexagonal
63.95	321	Cubic

Se_{19} Te_{75} Zn_6

In this sample Se_{19} Te_{75} Zn_6 XRD is shown in figure 3 .Table 3.1 Shows various h, k, l values of the peaks of the sample from which a=5.41 Å. Then volume $V=a^3=158.34$ Å ^{3}. The density of the material in this case is found to be 120.05gg/cc. The particle size and the Lorentz factor's variation calculated using XRD data are shown in Table 3.2. The average value of the particle size for this sample is 0.0437 µm.

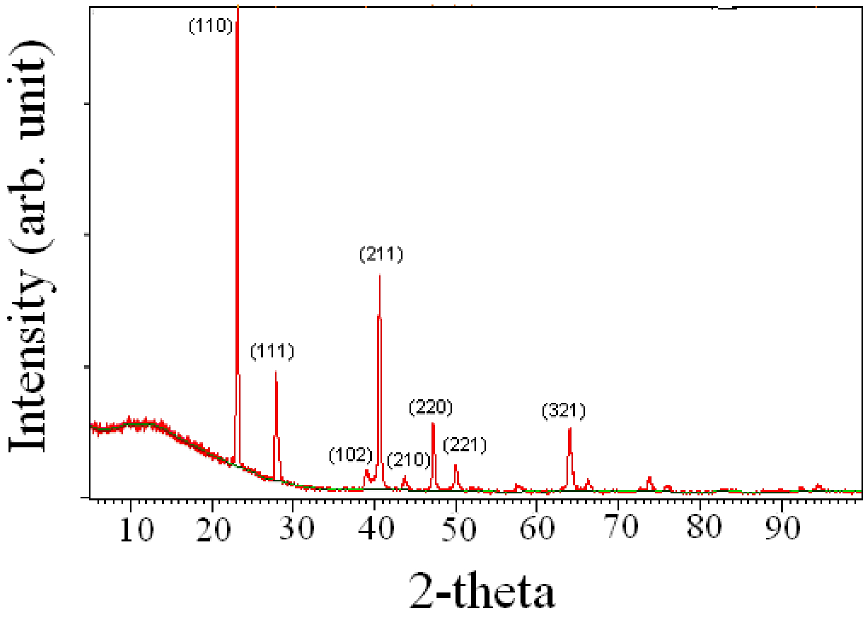

Fig. 3 shows the XRD graph of Se_{19} Te_{75} Zn_6 *system.*

Table 2.2 Calculated values of the particle size and the lorentz's factor of $Se_{19}Te_{78}Zn_3$ *system*

θ(in Degree)	cosθ	B(in radian)	Particle size t(Å)	Lorentz's factor
11.58	0.9797	0.00279	505.25	47.43
13.94	0.9706	0.00209	679.99	31.82
19.47	0.9428	0.00523	282.70	15.27
20.32	0.9378	0.00467	321.28	13.97
21.85	0.9281	0.007	213.33	11.91
23.61	0.9162	0.0035	432.17	9.95
24.94	0.9067	0.00204	749.32	8.81
28.76	0.8766	0.00817	193.52	6.33
31.98	0.8482	0.00642	272.34	5.04

$Se_{19}Te_{72}Zn_9$

The XRD of this sample $Se_{19}Te_{72}Zn_9$ is shown in figure 4. The various h, k, l values corresponding to the peak positions are given in Table 4.1. In this case parameters for cubic systems are a=5.43 Å. and volume $V = a^3 = 160.10$ Å ^{3}. The density of the material in this case is found to be 116.74g/cc. The particle size and the Lorentz factor's variation calculated using XRD data are shown in Table 3.2. The average value of the particle size for this sample is found to be 0.0496 µm. Then the averages of the values calculated are shown in Table-5.

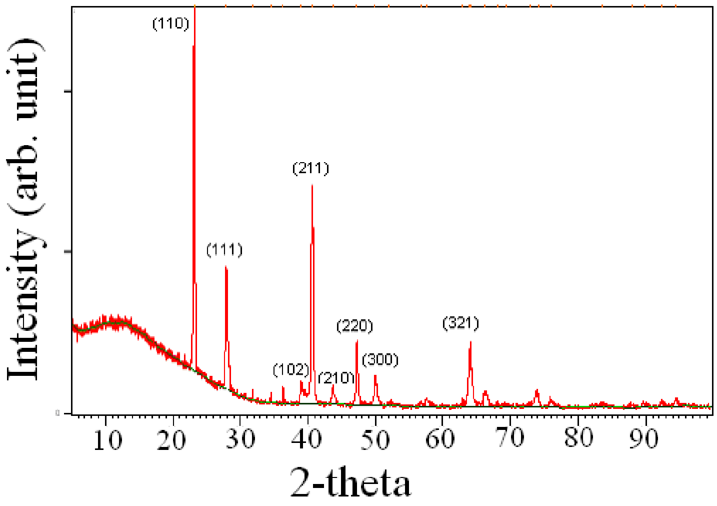

Fig. 4 Shows the XRD graph of $Se_{19}Te_{72}Zn_9$ system.

Table 3.1 h,k,l values of the peaks of Se_{19} Te_{75} Zn_6 system

2θ	**hkl**	**Crystal System**
23.15	110	Cubic
27.83	111	Cubic
38.91	210, 102	Cubic/ Hexagonal
40.54	211, 112	Cubic/ Hexagonal
43.66	210	Hexagonal
47.21	220	Cubic
49.89	300,221	Cubic/ Hexagonal
63.93	321	Cubic

Table 3.2 Calculated values of the particle size and the lorentz's factor of Se_{19} Te_{75} Zn_6 system

θ(in Degree)	**cosθ**	**B(in radian)**	**Particle size t(Å)**	**Lorentz's factor**
11.57	0.9796	0.00262	540.02	47.43
13.92	0.9706	0.00174	820.67	31.82
19.46	0.9428	0.00471	312.12	15.27
20.27	0.9380	0.00262	563.97	13.97
21.83	0.9282	0.00576	259.24	11.91
23.60	0.9163	0.00279	542.15	9.95
24.95	0.9066	0.00523	292.31	8.81
31.96	0.8484	0.00576	283.62	5.04

Table 4.1 h,k,l values of the peaks of the $Se_{19}Te_{72}Zn_9$ system

2θ	**hkl**	**Crystal System**
23.16	110	Cubic
27.89	111	Cubic
39.02	210, 102	Cubic/ Hexagonal
40.61	211, 112	Cubic/ Hexagonal
43.73	210	Hexagonal
47.21	220	Cubic
49.89	300,221	Cubic/ Hexagonal
64.13	321	Cubic

Table 4.2 Calculated values of the particle size and the lorentz's factor of $Se_{19}Te_{72}Zn_9$ system

θ(in Degree)	cosθ	B(in radian)	Particle size t(Å)	Lorentz's factor
11.58	0.9797	0.00279	505.25	47.43
13.94	0.9706	0.00209	679.99	31.82
19.51	0.9428	0.00523	282.70	15.27
20.31	0.9378	0.00467	321.28	13.97
21.87	0.9281	0.007	213.33	11.91
23.61	0.9162	0.0035	432.17	9.95
24.95	0.9067	0.00204	749.32	8.81
32.06	0.8482	0.00642	272.34	5.04

Table 5 Average particle size and the density of the materials.

Sample	Particle Size	Density
1. $Se_{19}Te_{81}$	0.437×10^{-5}cm.	124.09gm/cm^3
2. $Se_{19}Te_{78}Zn_3$	0.405×10^{-5}cm	122.07gm/cm^3
3. Se_{19} Te_{75} Zn_6	0.437×10^{-5}cm	120.05gm/cm^3
4. $Se_{19}Te_{72}Zn_9$	0.496×10^{-5}cm	116.74gm/cm^3

The average of all the particle sizes of all the samples is 0.0447 μm and the density is the 120.73g/cc. The variations of the Bragg's angle θ with the Lorentz factor for all the samples are shown here [36-40].

Discussions

In the present work the structure of the aggregate is studied, using the term in the wide sense to mean the relative size, perfection and orientations of the particles or grains making up the aggregate. Whether these particles are large or small, strained or unstrained, oriented at random or in some preferred directions, frequently has very important effects on the properties of the materials. If the material contains more than one phase, its property naturally depend upon the properties of each phase considered separately and on the way these phase occur in the aggregate. Such materials offers wide structural possibilities since the size, perfection and orientations of the particles or the grains of one phase may differ from those of the other phases. Here the polycrystalline material is prepared by the annealing process, so here in this case the materials are under the many kinds of the crystal imperfection such as non uniform strain because it is so characteristics of the cold worked states of metals and alloys, that is why in this case distorted hexagonal structure are obtained. The change in the shape of any particle is not only determined by the force applied to the piece as a whole but also by the fact that each particle retains contact on its boundary surface with all its neighbors. As a result of these restraints by its neighbors plastically deformed particle in the solid aggregate usually has regions of its lattice left in an elastically bent or twisted condition or more rarely in a state of uniform tension or compression. So we can say that a cold worked metal or the alloy have the deformed texture, twinned annealed crystals or become polygonal in shape. II-VI wide band gap semiconductors are of great interest as blue and green light emitters. For these, as well as for many other devices, good bipolar conductivity is required. The II-VI group ternary materials provide a possibility of tailoring their properties as per requirements and hence project themselves, as important semiconducting material, for future advancements in the field of device fabrication.The $Se_{19}Te_{81-x}Zn_x$ (x=0, 3, 6, 9) system taken is showing both the cubic and hexagonal system behaviour. The cubic phase together with the hexagonal one was due to the polycrystalline behavior of the compound tending to present a multiphase structure. In the intensity calculations Lorentz factor is combined with the polarization factor and further the variation of the Lorentz's factor with the Bragg angle (θ) is shown [47-52].

The overall effect of Lorentz factor is to decrease the intensity of the reflections at intermediate angles compared to those in the forward or backward directions.

4. Conclusions

Polycrystalline $Se_{19}Te_{81-x}Zn_x$ alloys are obtained by the annealing of the Se-Te-Zn material; under the controlled conditions. The material strongly possesses the polycrystalline behaviors showing the peaks almost at the same positions in all the samples. The cubic phase together with the hexagonal phase represents the polycrystalline behaviors. The effect of the Zn doping is very small, systems showing the cubic as well as the hexagonal phase but with some distortion due to the strain and deformation effects of the cold work or the annealing. The density of the material is found to be 120.73gm/cm^3 and the particle size is found to be 0.447×10^{-5}cm. It is promising material for high- efficiency solar cells, switching, and other optoelectronic devices.

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