

Structural and electrical measurements of CdZnSe composite

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Abstract. The I - V characterization and the electrical resistivity of selenium rich $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ ($x = 0, 3, 7, 11$ and 15) system at room temperature have been studied. Samples were obtained using melt cooling technique. So prepared samples were then characterized in terms of their crystal structure and lattice parameter using X-ray diffraction method. The materials were found to be polycrystalline in nature, having zinc blend structure over the whole range of zinc concentration. The measurements of I - V characteristics have been carried out at different temperatures from room to 140°C . The electrical resistivity of the samples with composition at room temperature has been found to vary between maximum $2.7 \times 10^8 \Omega \text{ m}$ and minimum $7.3 \times 10^5 \Omega \text{ m}$ and shows a maximum at 3 at. wt.% of Zn. The carrier activation energy of the samples with composition has also been determined and found to vary from 0.026 eV to 0.111 eV.

Keywords. Resistivity; activation energy; polycrystalline; X-ray diffraction.

1. Introduction

Elements of II–VI group are attracting a great deal of attention because of their potential abilities in the wide spectrum optoelectronic devices (Sharma *et al* 1979; Burger and Roth 1984; Bassam *et al* 1988; Nasibov *et al* 1989; Gupta *et al* 1995a; Deshmukh *et al* 1998). High absorption coefficient, high efficiency of radiative recombination and nearly matching band gaps with the visible region of the solar spectrum are the root causes of the popularity of II–VI group semiconductors. Ternary materials provide a possibility of tailoring their properties as per requirements and hence project themselves as important semiconducting materials for further advancements in the field of device fabrication. CdZnSe is a n -type wide band gap material and plays a dominant role in modern technology (Ray 1969; Bassam 1990). The growth of ternary CdZnSe opens up the possibility of their application for novel optoelectronic devices such as light emitting diodes, photoelectrodes, blue green laser etc (Samarth *et al* 1990) in the visible region of electromagnetic radiation (Gupta *et al* 1995b). Further, research of optical and electrical properties of CdZnSe system, forms a basis of active region of laser and LED. An electrical characteristic on bulk crystal growth from the vapour phase was reported by Reimers (1969) and more recently by Burger and Roth (1984). Most of the work has been done on $\text{SeCd}_{1-x}\text{Zn}_x$ system. So far no work has been reported on selenium rich $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ polycrystalline material. Thus, the present study is aimed at investigating the electrical properties of $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ system in bulk form.

The I - V characteristic is an important tool for analysing the different conduction processes. Several workers (Gogoi and Barua 1982; Gould and Ismail 1992) studied the I - V curves in the II–VI semiconductor films with a variety of methods and thereby determined the various physical processes viz. Schottky, Poole–Frankel and space charge limited conduction depending upon the film growth and experimental ambient conditions. Efforts have also been made to study the temperature dependence of conductivity of thin films. But it is observed that most of the thin films suffered the problem of degradation as compared to their bulk. So in the above context, investigation has been made to study the I - V characteristics of $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ polycrystalline material. Besides that an effort has also been made to study the temperature dependence of resistivity under ambient conditions in their bulk form.

2. Experimental

$\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ (where $x = 0, 3, 7, 11$ and 15) system was prepared using slow cooling of the melt. High purity (99.999%) Se, Cd and Zn (in elemental form) were weighed according to their atomic percentages and sealed off in a vacuum of 10^{-5} torr in quartz ampoules. The sealed ampoules were then placed in a muffle furnace where the temperature was raised at the rate of 4 K/min up to 900°C and kept at that temperature for 8 h, with frequent rocking to ensure homogenization of the melt. Subsequently slow cooling process was carried out. The ingots of the sample were then taken out by breaking the ampoules. These ingots were then ground into fine powder. X-ray traces of all samples were taken at room temperature in order to study structure of the material. The materials

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were found to be polycrystalline in nature as shown in figure 1.

For resistivity measurement, bulk samples in the form of pellets (dia. 12 mm and thickness ≈ 1 mm) were prepared by compressing the fine powder of polycrystalline material under a load of 5 ton. The bulk materials were mounted between two copper electrodes in a sample holder for I - V measurement. For that purpose voltage was applied across the pellet and the resulting current was measured by Keithley electrometer/high resistance meter-6517A. The temperature range of the study was from room temperature to 140°C . The circuit diagram used for this study is given in figure 2. This electrometer has an in-built capability of output independent voltage source of ± 1000 V. So the same equipment was used to apply the voltage across the sample and to measure the current through the sample. To ensure proper connection of the sample, an indigenously designed sample holder was used with copper electrodes.

3. Results and discussion

X-ray diffraction studies were carried out on these samples using Philips mode PV1840 diffractometer with an iron K_α radiation source ($\lambda = 1.937355 \text{ \AA}$) and the diffractograms were analysed to obtain information about various crystallographic aspects. XRD patterns of all the samples were taken at room temperature. These patterns confirmed the formation of alloy CdZnSe system. The presence of sharp peaks in these XRD patterns confirmed the polycrystalline nature of the so prepared material.

The experimental d -values for the different compositions of $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ ($x = 0, 3, 7, 11$ and 15) system have been calculated from the peaks of XRD pattern (Cullity 1959) using the Bragg's diffraction law. These calculated d -values are compared with the d^* values obtained from Vegard's law for $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ system. The experimental d -values and d^* as obtained from Vegard's law values are shown in table 1 and were found to be in good agreement.

Typical I - V characteristics of the samples under test recorded at different temperatures, from room to 140°C , have been found to be linear as shown in figure 3. It shows the ohmic behaviour of the samples. From the I - V characteristics of the samples the electrical resistivity has been determined. A plot of resistivity vs composition has been drawn.

The electrical resistivity (r) of the samples has been determined using the relation,

$$r = (R \times A)/L, \quad (1)$$

where R is the resistance, L the thickness, and A the cross-section area of the sample. A typical graph between electrical resistivity and the composition at room temperature is shown in figure 4. This figure shows that the resistivity is maximum for $x = 3$ in the series $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ ($x = 0, 3, 7, 11$ and 15) system at room temperature. It is clear from figure 4 that the material $\text{Se}_{85}\text{Cd}_{15}$ shows the lowest resistivity. As we introduce Zn in this material the resistivity increases and reaches a maximum for 3 at. wt.% of Zn in CdSe system. This is due to the fact that as we add zinc into the CdSe lattice, initially it does not react with the CdSe and do not form alloy of CdZnSe.

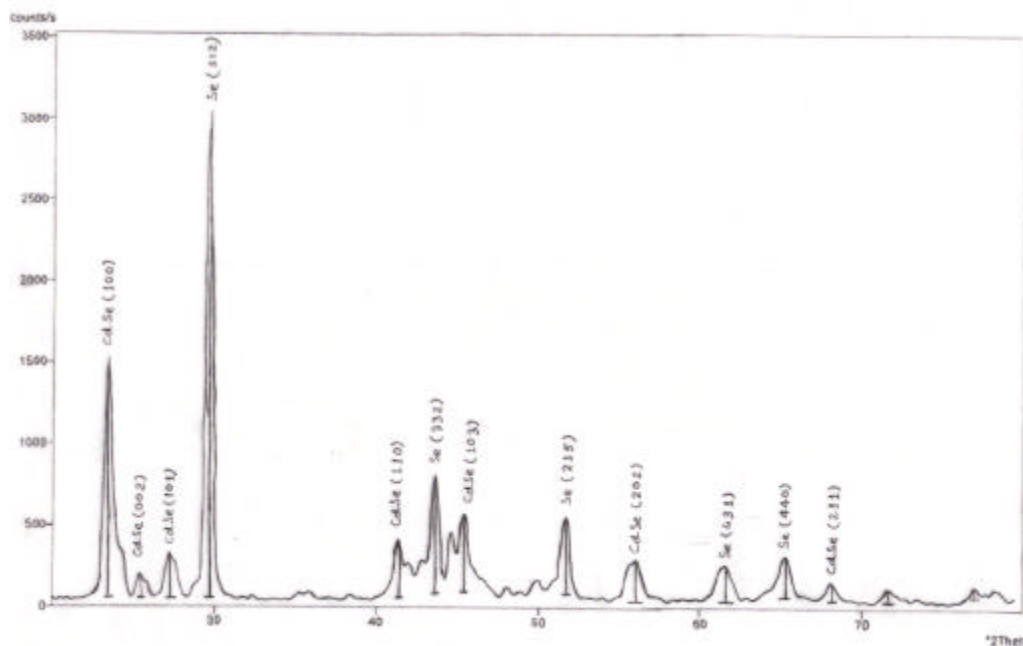


Figure 1. XRD pattern of $\text{Se}_{85}\text{Cd}_{12}\text{Zn}_3$ system.

Since the volume of Cd atom is greater than that of Zn atom and therefore, Zn settles down at the interstitial sites of CdSe lattice. This in turn increases the number of scattering centres in the material, hence the resistivity. This fact is also supported by the XRD pattern of $\text{Se}_{85}\text{Cd}_{12}\text{Zn}_3$ system, where no peaks of ZnSe and CdZnSe have been found. With further increment in at. wt.% of zinc in Se–Cd, some Zn atoms settle down at the interstitial sites of

the Se–Cd lattice whereas other atoms form the ZnSe as well as CdZnSe. As a result, CdZnSe (like $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Se}$, $\text{Cd}_{0.6}\text{Zn}_{0.4}\text{Se}$) dominates in the material and hence the numbers of scattering centres decrease, resulting in a decrease in resistivity. The XRD pattern which shows the peaks of ZnSe and CdZnSe in figure 1 also supports the above explanation. The same explanation can be given for the material containing 11 at. wt.% of zinc. At 15 at.

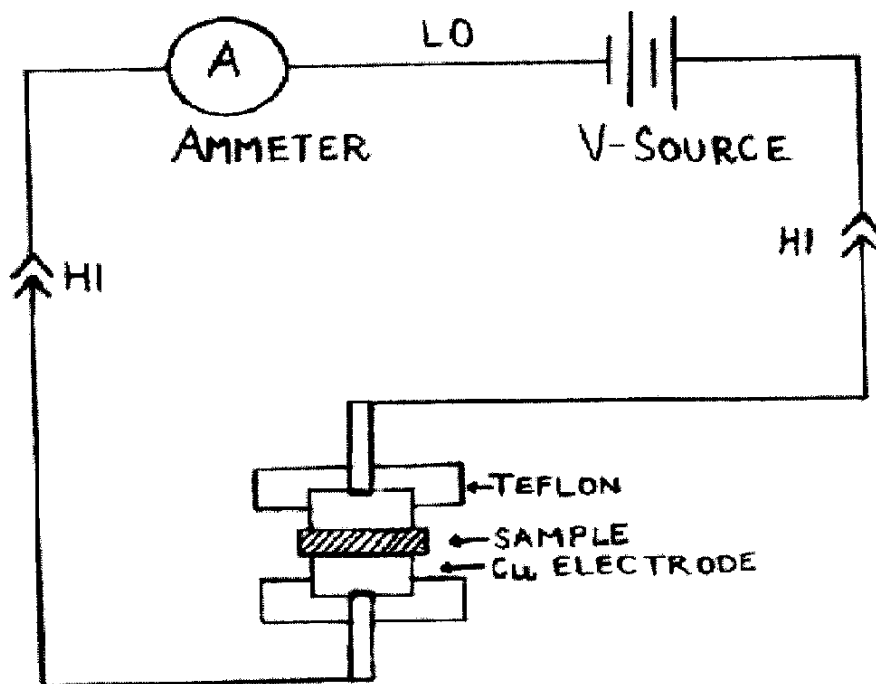


Figure 2. The circuit diagram used for I - V characteristic measurements.

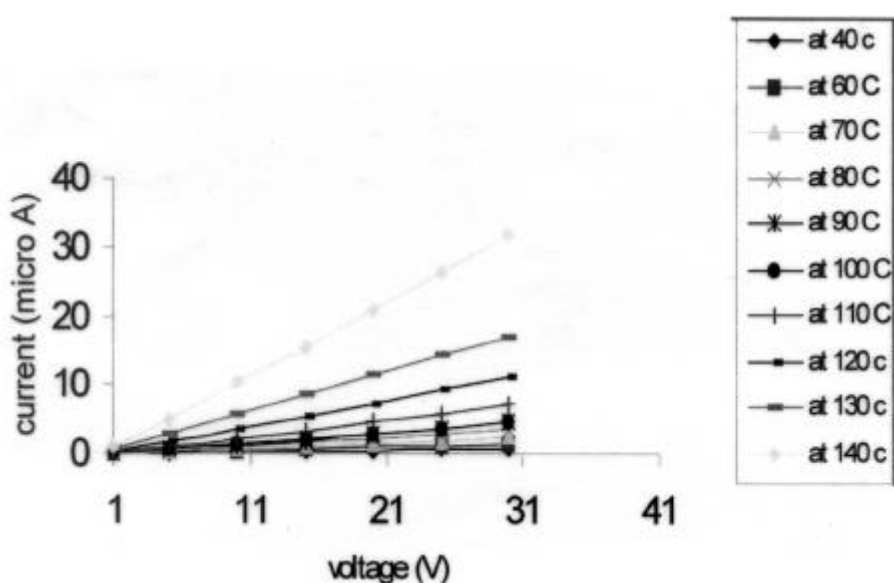


Figure 3. Temperature dependence of I - V characteristics of $\text{Se}_{85}\text{Cd}_{12}\text{Zn}_3$ system.

Table 1. XRD data of $\text{Se}_{85}\text{Cd}_{15}$, $\text{Se}_{85}\text{Cd}_{12}\text{Zn}_3$, $\text{Se}_{85}\text{Cd}_8\text{Zn}_7$, $\text{Se}_{85}\text{Cd}_4\text{Zn}_{11}$ and $\text{Se}_{85}\text{Zn}_{15}$.

Sl. no.	Exp. d (Å)	ASTM d^* (Å)	$h k l$	Chemical composition
$\text{Se}_{85}\text{Cd}_{15}$				
1.	3.77	3.77	1 1 0	Se
2.	3.52	3.51	0 0 2	CdSe
3.	3.02	3.00	$\bar{3}$ 1 2	Se
4.	2.54	2.55	1 0 2	CdSe
5.	2.14	2.15	1 1 0	CdSe
6.	2.08	2.08	3 2 3	Se
7.	1.98	1.98	1 0 3	Se
8.	1.86	1.86	2 0 0	Se
$\text{Se}_{85}\text{Cd}_{12}\text{Zn}_3$				
1.	3.78	3.72	1 0 0	CdSe
2.	3.49	3.51	0 0 2	CdSe
3.	3.27	3.29	1 0 1	CdSe
4.	3.00	3.00	$\bar{3}$ 1 2	Se
5.	2.18	2.15	1 1 0	CdSe
6.	2.07	2.07	$\bar{3}$ 3 2	Se
7.	1.99	1.98	1 0 3	CdSe
8.	1.76	1.76	$\bar{2}$ 1 5	Se
9.	1.64	1.65	2 0 2	CdSe
$\text{Se}_{85}\text{Cd}_8\text{Zn}_7$				
1.	3.86	3.86	2 0 2	Se
2.	3.37	3.38	0 0 2	$\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Se}$
3.	3.04	3.00	$\bar{3}$ 1 2	Se
4.	2.44	2.44	1 0 2	$\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Se}$
5.	2.19	2.18	1 4 0	Se
6.	2.16	2.15	1 1 0	CdSe
7.	2.08	2.09	1 1 0	$\text{Cd}_{0.6}\text{Zn}_{0.4}\text{Se}$
8.	2.01	1.99	1 1 0	ZnSe
9.	1.90	1.92	1 0 3	$\text{Cd}_{0.6}\text{Zn}_{0.4}\text{Se}$
10.	1.77	1.80	2 0 2	CdSe
$\text{Se}_{85}\text{Cd}_4\text{Zn}_{11}$				
1.	3.86	3.86	$\bar{2}$ 0 2	Se
2.	3.35	3.30	0 0 2	$\text{Cd}_{0.2}\text{Zn}_{0.8}\text{Se}$
3.	3.00	3.00	$\bar{3}$ 1 2	Se
4.	2.30	2.30	$\bar{1}$ 3 3	Se
5.	2.09	2.09	0 3 4	Se
6.	2.01	2.02	1 1 0	$\text{Cd}_{0.2}\text{Zn}_{0.8}\text{Se}$
7.	1.78	1.76	1 1 2	$\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Se}$
$\text{Se}_{85}\text{Zn}_{15}$				
1.	3.78	3.77	1 0 0	Se
2.	3.28	3.25	0 0 2	ZnSe
3.	3.00	3.00	$\bar{3}$ 1 2	Se
4.	2.18	2.18	1 1 4	Se
5.	2.07	2.07	$\bar{3}$ 3 2	Se
6.	2.00	1.99	1 1 0	ZnSe
7.	1.88	1.84	1 0 3	ZnSe
8.	1.76	1.76	$\bar{6}$ 1 3	Se
9.	1.70	1.70	1 1 2	ZnSe

wt.% of zinc, the formation of ZnSe takes place, which is confirmed from XRD. Since the density as well as the number of scattering centres of ZnSe increase, hence there is an increment in resistivity as compared to previous one.

The resistivity of a semiconductor at temperature, T , is given by

$$r = r_0 \exp(\Delta E/kT), \quad (2)$$

where r_0 is pre-exponential factor, ΔE the carrier activation energy for the generation process and k the Boltzmann constant (Hussain *et al* 2003).

A variation between $\ln(r)$ vs $1000/T$ is a straight line having a slope equal to $\Delta E/1000k$ and intercept $\ln(r_0)$. This slope gives information about the activation energy (ΔE). A plot of activation energy vs composition has been shown in figure 5. An effort has also been made to determine electrical resistivity of the samples in the range

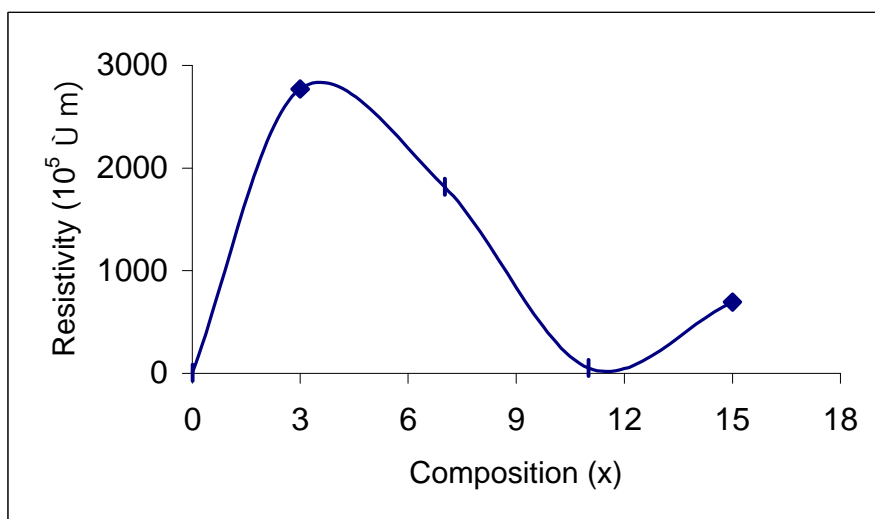


Figure 4. Composition dependence of resistivity of $Se_{85}Cd_{15-x}Zn_x$ ($x = 0, 3, 7, 11$ and 15) system.

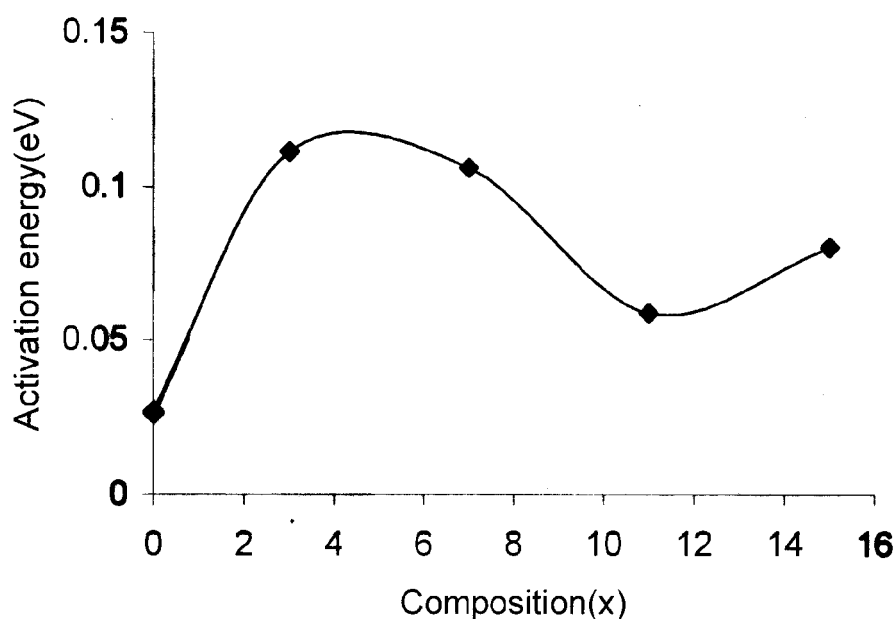


Figure 5. Composition dependence of activation energy of $Se_{85}Cd_{15-x}Zn_x$ ($x = 0, 3, 7, 11$ and 15) system.

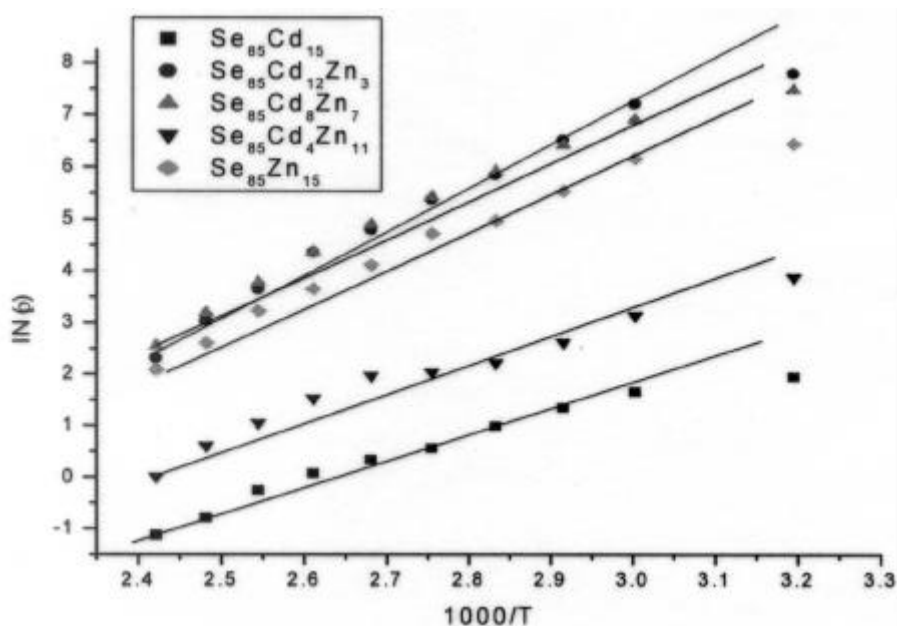


Figure 6. Linear relationship between $\ln(\rho)$ vs $1000/T$.

of temperature from 313 K to 413 K. The temperature dependence of resistivity is shown in figure 6. The resistivity of all the samples decreases with increase in temperature. The plots of $\ln(\rho)$ vs $1000/T$ are straight lines for all the samples indicating that conduction in these samples is through thermally activated process.

4. Conclusions

The electrical resistivity of $\text{Se}_{85}\text{Cd}_{15-x}\text{Zn}_x$ ($x = 0, 3, 7, 11$ and 15) system has been investigated. The resistivity is maximum at 3 at. wt.% of zinc because Zn does not occupy the lattice position in Cd–Zn–Se system while in other at. wt.%, Zn acquires the lattice position, resulting in decrement in scattering centres and hence in electrical resistivity. At 15 at. wt.% of Zn, most of zinc atoms reach at the lattice sites and decrease the volume of ZnSe, resulting into the increment in scattering centres as well as in resistivity.

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