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Structural and Electrical Properties of Cd Implanted GaTe Single Crystals Grown by Bridgman Technique

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ABSTRACT

p-GaTe:Cd crystal was grown in our crystal growth laboratory by using a modified Bridgman method. Structural properties of crystals (GaTe:Cd) has been studied by means of Scanning electron microscopy (SEM), energy dispersive X-rays (EDX) techniques. The effect of annealing temperatures at (100, 200, 300, 350, 400, 500, 600 and 700 ^{o}C) for 10, 20 and 30 minutes on structural properties has been investigated using X-ray diffraction (XRD). XRD measurements indicate that there is an increase in peak intensities at specific annealing temperatures (300 and 500 ^{o}C) and a decrease in higher annealing temperatures (700 ^{o}C). The lattice parameters of these crystals have found to be a = 17.45 Å, b = 10.47 Å, c = 4.09 Å which correspond to a monoclinic structure exhibiting B2/m (12) space-group symmetry. The crystallite size has been calculated to be 490- 980 Å for GaTe from the SEM result. It has been observed from EDX result that GaTe contains Ga=36.49 %, Te =58.14 %, Cd= 0.97 % and O = 0.05. Then, Zn/p-GaTe Schottky diode has been fabricated. The temperature dependence of current–voltage (I–V) characteristics of Zn/p-GaTe Schottky diode has been investigated in the temperature range of 40–360 K with a temperature step of 10 K under dark conditions. The forward I–V characteristics have been analyzed on the basis of standard thermionic emission theory. It has been shown that the ideality factor increases while the barrier height decreases with decreasing temperature.

Keywords: Structural, Electrical Properties, GaTe:Cd Single Crystals

1 INTRODUCTION

Binary semiconductor compounds have attracted the technological interest owing to their promises for practical application in the areas of visible and infrared light emitting diodes, infrared detectors, optical parametric oscillators, nonlinear optics, solar cells, optical frequency conversion, second harmonic

generation devices and many other electro-optical devices. The characteristics of these crystals which are important fort the Nano and optoelectronics technology will be explored in detail by analyzing the all obtained results. GaTe binary semiconductor compound was grown in our crystal growth laboratory by the Bridgman-Stockbarger method. GaTe is a layered semiconductor belonging to the III–VI metal– chalcogen family and it is a native p-type semiconductor. It has direct band-gap. So, it can be also used in various optical applications such as LEDs, solar cells and photovoltaic devices. However, the crystal structure of GaTe is considerably more complex than others. This relatively unstudied semiconductor has high atomic number (Ga - 31 and Te - 52) and wide bandgap energy (1.7 eV at 300K), which is important for the use of GaTe as a window material for solar cells and radiation detectors [1-2]. The physical and chemical properties of this material are amenable to conventional material processing procedures and crystal growth at moderate temperature. For these reasons, GaTe has recently received special attraction for potential use in the fields of optoelectronic devices [3-5], terahertz sources [6-7], radiation detectors [8-10] and solar cells [11].

Metal semiconductor (MS) contact is one of the most widely used rectifying contacts in electronics industry [2-4]. The interface states and interfacial-oxide layer at the MS-rectifying contact play an important role in the determination of the SBH and other characteristic parameters of the devices and affect the device performance. The surface states can be viewed as electronic states generated by unsaturated dangling bonds of the surface atoms [5]. These states will create a charge distribution at the interface, which will affect value of the capture cross-sections of the traps [6]. Growth of GaTe single crystals entails serious difficulties because of significant anisotropy of chemical bonds, structure and properties of layered semiconductors. Conventionally bulk layered semiconductors, such as pure and doped GaSe, GaTe are grown by the Bridgman technique [12–15]. Growth rates are quite low, about 2–6 mm/day [10, 13]. Four crystallographic phases of GaTe are represented in international X-ray diffraction data- bases: 3 monoclinic phases and 1 hexagonal phase. In this study, we present the results of the systematic studies on the structural analysis of the GaTe:Cd grown by using the Bridgman/Stockbarger method. The experimental investigations were carried out on GaTe single crystals, grown by the Bridgman method, which were Cd doped. For the characterization, both surface sensitive methods (energy dispersive X-rays (EDX) and electron microscopy (SEM) and bulk characterization method (X-ray diffraction (XRD)) were used. The temperature dependence of current–voltage (I–V) characteristics of Zn/p-GaTe Schottky diode has been investigated in the temperature range of 40–360 K with a temperature step of 10 K under dark conditions.

2 BASIC EQUATIONS

The average grain size of GaTe was determined using Debye - Sherrer's equation [16],

$$D = \frac{K\lambda}{(\beta Cos\ \theta)} \tag{1}$$

where θ is the Bragg angle, λ is the wavelength of the X-ray and β is the total broadening measured at the peak's full width at half maximum (FWHM) in radians and K is the Scherer constant (=0,91). The average crystallite size and micro strain σ_p were also obtained from the Rietveld analysis through the relationship

$$\left(\frac{\beta\cos\theta}{k\lambda}\right) = \frac{1}{d^2} + \sigma_p^2\left(\frac{\sin\theta}{k\lambda}\right)^2 \tag{2}$$

One can see that considerable crystallite growth and micro strain reduction occurred due to ageing. The lattice parameters were calculated using the following relation

$$\frac{1}{d^2} = \frac{1}{\sin\beta^2}\left(\frac{h^2}{a^2} + \frac{k^2\sin\beta^2}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right) \tag{3}$$

Where a,b and c are the lattice parameters and "d" is the lattice spacing. The dislocation density δ, defined as the length of dislocation lines per unit volume of the crystal has been evaluated using the formula [17] the dislocation density decreases with increase of grain size.

$$\delta=1/D^2 \quad (4)$$

The full-width at half-maximum β can be expressed as a linear combination of the contributions from the particle size, D and strain, ε through the relation [18]

$$\beta\cos\theta/\lambda = 1/D + \varepsilon \sin\theta/\lambda \quad (5)$$

The strain (ε) value evaluated using the relation

$$\varepsilon = \frac{(\beta Cos\ \theta)}{4} \quad (6)$$

The dislocation density (δ) may be calculated by using the formula [15].

$$\delta = \frac{15\,\varepsilon}{(axD)} \quad (7)$$

The number of crystallites per unit area (N) of the crystal was determined using the relation [15]:

$$N = \frac{t}{D^3} \quad (8)$$

3 RESULTS AND DISCUSSION

The effective barrier height $\emptyset_b$ and ideality factor n, were determined by using the thermionic emission current voltage expression:

$$I = I_0\left[\exp\left(\frac{qV}{nkT}\right) - 1\right] \quad (9)$$

where I_0 is the saturation current derived from the straight line intercept of lnI at V = 0 and is given by

$$I_0 = AA^*T^2\exp\left(\frac{-q\emptyset_b}{kT}\right) \quad (10)$$

Where V is the applied voltage, q is the electronic charge, k is the Boltzmann constant, T is the absolute temperature, A is the diode contact area (A = 7.85 × 10^{-3} cm^2), A^* is the effective Richardson constant, $\emptyset_b$ is the effective Schottky barrier height (SBH) at zero bias and n is the ideality factor. A theoretical A^*value of 56.4 A cm^{-2} K^{-2} was used for GaTe. The ideality factor is derived from;

$$n = \frac{q}{kT}\left(\frac{dv}{d\ln(I)}\right) \quad (11)$$

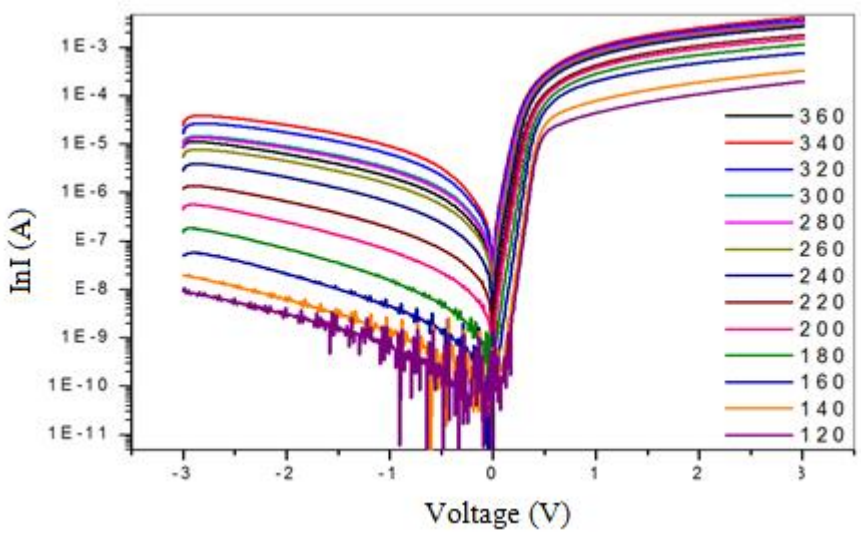
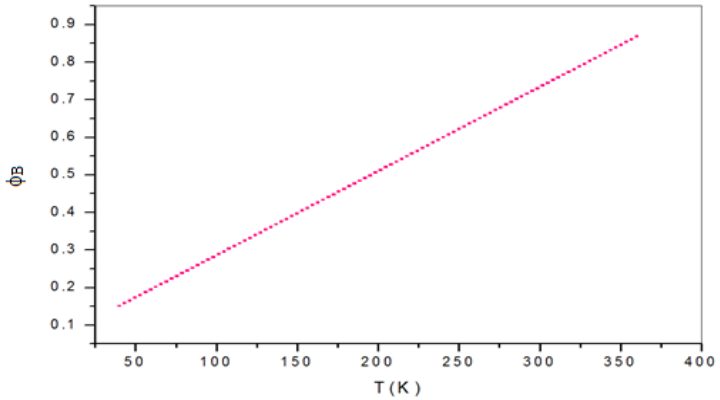


Figure 1: Current–voltage characteristics of the Zn/p-GaTe:Cd Schottky barrier diode at various temperatures(120-360K).

The current–voltage (I–V) characteristics of Zn/p-GaTe Schottky barrier diode (SBD) were measured in the temperature range 40–360K. The reverse and forward-bias I–V plots of Zn/p-GaTe:Cd SBD in the temperature range of 120–360 K are given in Fig.1. As can be seen, a change of both forward and reverse characteristics has occurred with temperature. The reverse-bias current of the Zn/p-GaTe:Cd SBD has increased with increasing temperature. The value of the ideality factor of the Zn/GaTe:Cd SBD was calculated from the slopes of the linear regions of the semi-log forward-biased I–V curves**(**Fig. 1**)** at each temperature. I_0wasobtainedbyextrapolatingthelinearregion of the semi-log forward I–V curves and $\emptyset_b$was determined by using equation (10). The determined values of n and $\emptyset_b$are presented in Fig. 2 as a function of temperature. As can be seen from Figure (2), the ideality factor (n) and $\emptyset_b$values obtained by analysing the forward-biased I–V characteristic based on the TE mechanism indicated that, although the ideality factor values have slightly increased, the $\emptyset_b$values have decreased with decreasing temperature.



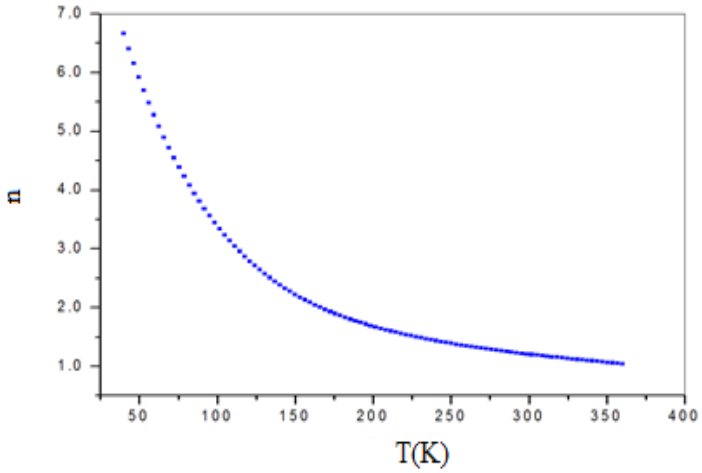


Figure 2: Temperature dependence of ideality factor and of the barrier height for the Zn/p-GaTe:Cd Schottky barrier diode.

The structural and lattice parameters of the Cd doped GaTe semiconductor was analyzed using a X-ray diffractometer (XRD) using Cu-Kα radiation with a wavelength of λ=1.54050 Å (Bruker). The values of 2θ were altered between 10 deg and 90 deg with the step of 0.1 deg/sec. Fig.3 shows the XRD pattern of the Cd doped GaTe semiconductor. It is found that the GaTe crystal has monoclinic structure, quite close 2θ peak values and dominant diffraction peak around 2θ= 24,57° degrees for the was the (410) plane. In this work, the XRD technique is used to determine the structure, the phases present and the orientation of the deposited GaTe crystals. XRD patterns of Cd doped GaTe crystals for as-grown and the samples annealed at 100, 300 and 500 ^{0}C, respectively (for 10, 20 and 30 min) are illustrated in Figs.3-6.

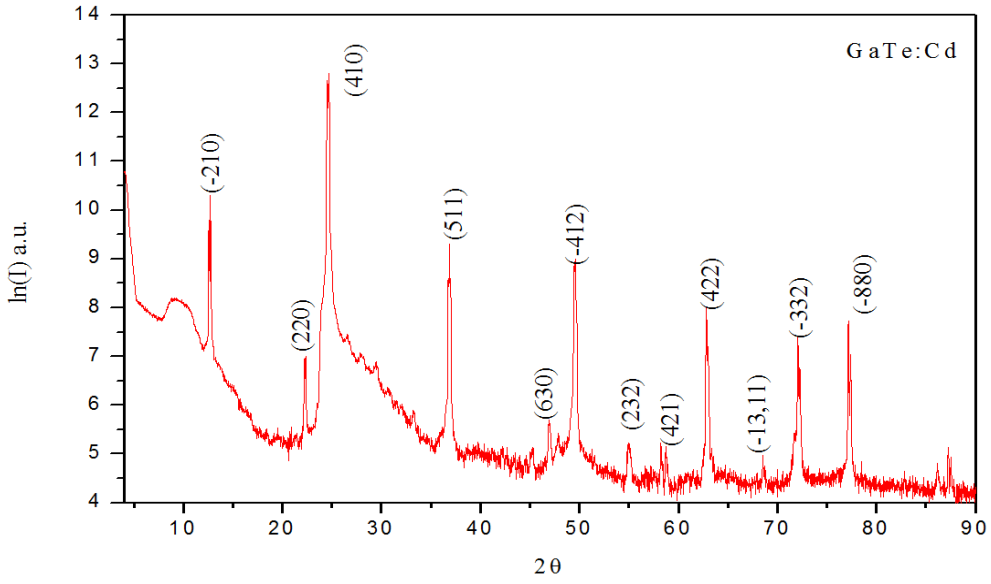


Figure 3**:** X-ray diffraction (XRD) spectra of GaTe:Cd (at room temperature).

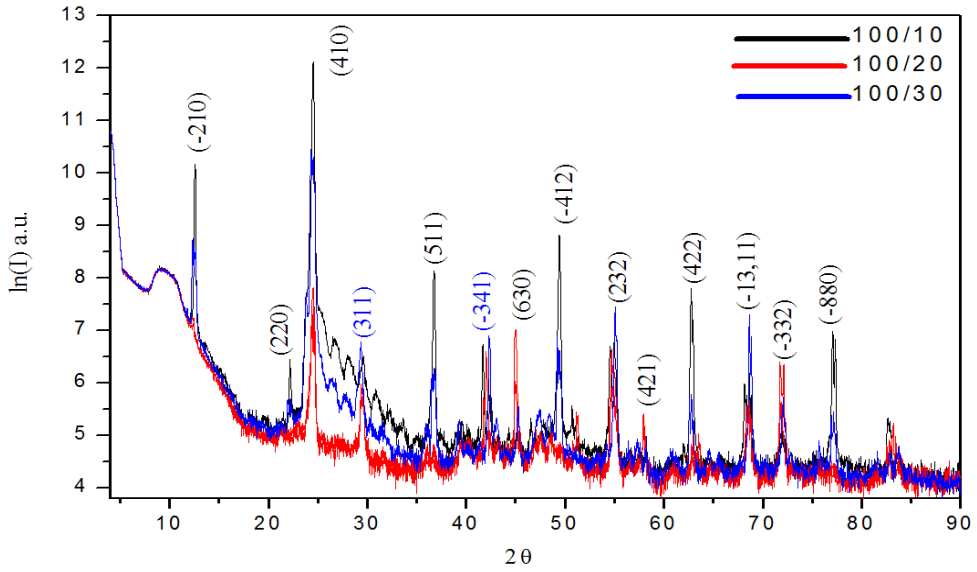


Figure 4: X-ray diffraction patterns of GaTe:Cd annealed at 100 ^{0}C for 10,20 and 30 min.

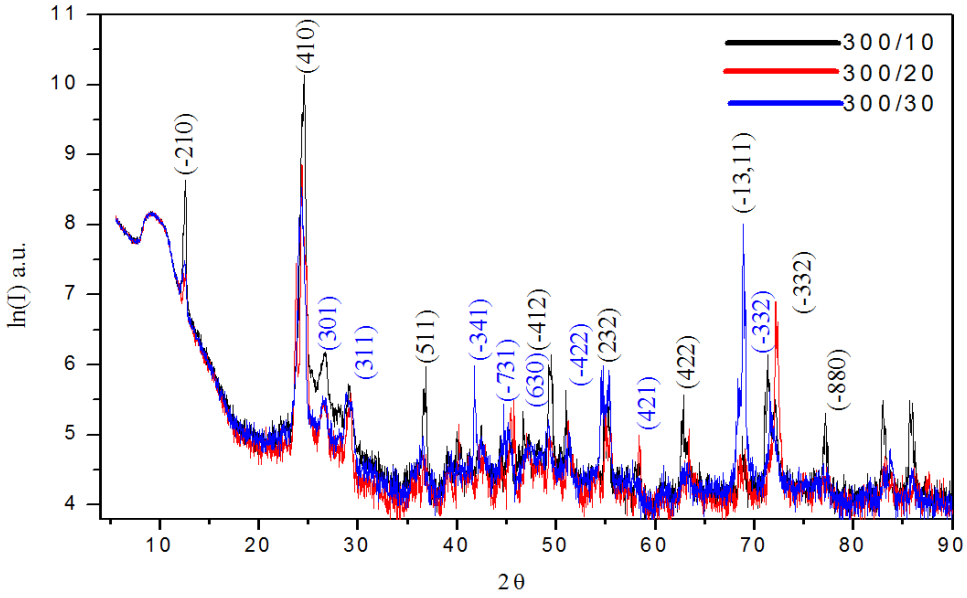


Figure 5: X-ray diffraction patterns of GaTe:Cd annealed at 300 ^{0}C for 10,20 and 30 min.

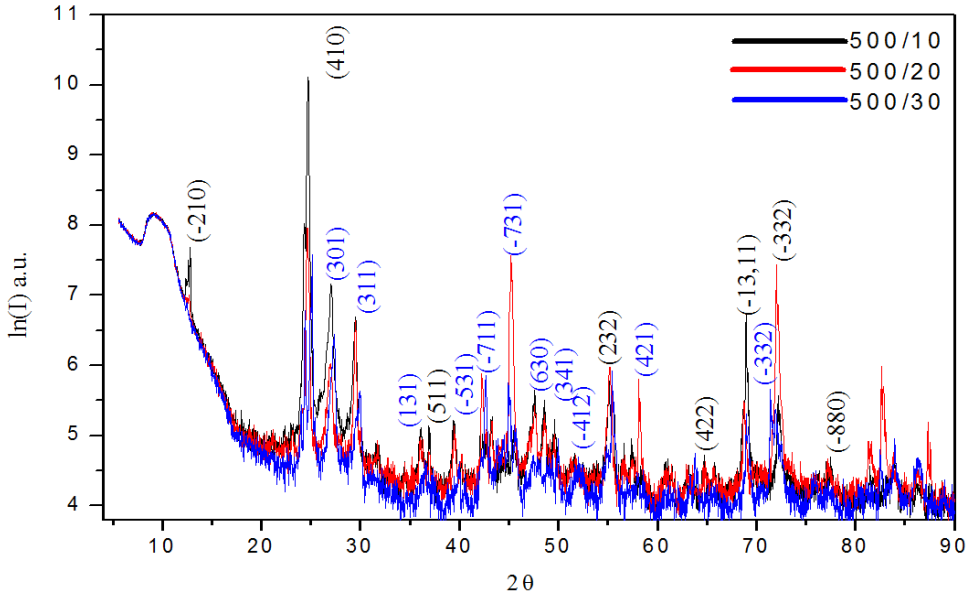


Figure 6: X-ray diffraction patterns of GaTe:Cd annealed at 500 ^{0}C for 10,20 and 30 min.

The values of standard inter planer distance ($d_{theoretical}$) and observed inter planer distance ($d_{experiment}$) calculated by using the Bragg's relation ($d_{hkl} = n\lambda / 2 \sin \theta$) along with the respective plane for GaTe:Cd semiconductor for as-grown and annealed at 300 ^{0}C has been given in Table 1. The experimental inter planar distance values have reported that GaTe crystals grown by Bridgman method had generally **monoclinic** structure [19].

Table 1 The standard and calculated XRD results for GaTe and GaTe:Cd crystals annealed at 300 ^{0}C for 10,20 and 30 min.

Sample name	Intensity (a.u.)	2θ (degree)	$d_{experiment}$ (Å)	$d_{theoretical}$ (Å)	Structure
GaTe:Cd-10	25309	24.570	3.620	3.623	Monoclinic
GaTe:Cd-20	7059	24.362	3.650	3.654	Monoclinic
GaTe:Cd-30	5089	24.307	3.659	3.662	Monoclinic

The crystallite size (D), dislocation density (ε), residual strain (δ) and number of crystallites per unit area (N) for GaTe:Cd crystals have been calculated using the Eqs. (4), Eq (5) and Eq (6), respectively. The analysis for as-grown and 300 ^{0}C has been presented in Table 2.

Table 2 the crystallite size (D), dislocation density (ε) and residual strain (δ) for Cd doped GaTe annealed at 300 ^{0}Cfor 10, 20 and 30 min.

Sample Name	2θ (degree)	FWHM (degree)	$d_{theoretical}$ (Å)	$d_{experiment}$ (Å)	ε ($lin^{-2}m^4$) x10^{-4}	δ (lin/m^2) x10^{14}	N (m^{-2}) x10^{18}	σ(%)
GaTe:Cd-10	24.570	0.261	325.6	345.5	11.127	8.377	12.123	0.699
GaTe:Cd-20	24.362	0.167	508.7	541.9	7.123	3.405	3.142	0.465
GaTe:Cd-30	24.307	0.144	589.9	626.4	6.142	2.549	2.034	0.393

The surface morphology images of the crystal were obtained by scanning electron microscope (SEM) technique at 30 kV with a 1.000 magnification (Figure 7). The surface of the GaTe:Cd was coated with Au for SEM image enhancement. SEM studies on GaTe:Cd slices showed smooth surface morphology without visible defects or micro cracks. The crystallite size has been calculated to be 490- 980 Å for GaTe:Cd.

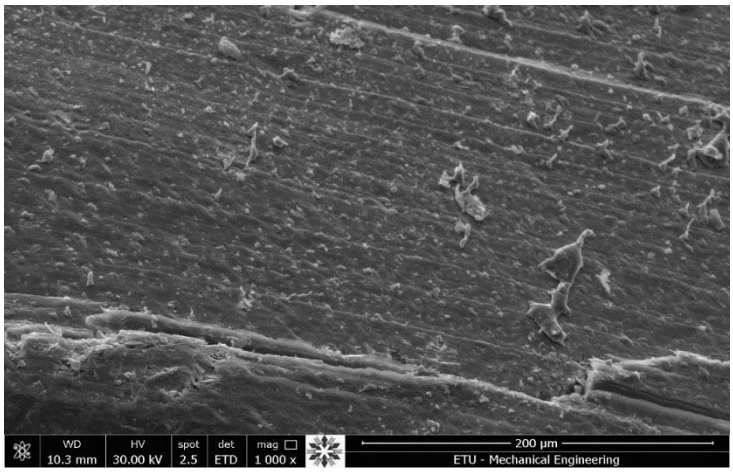


Figure 7: SEM images taken at 30 kV with a 1.000 magnification for GaTe:Cd crystal

A typical EDAX spectrum is shown in Figure 8, which confirmed Ga and Te to be the only components in the GaTe crystals grown by the vertical Bridgman technique. According to the EDX results, GaTe:Cd contains Ga=36.49 %, Te =58.14 %, Cd= 0.97 % and O = 0.05 % respectively. These values are quite close to the expected ones and a little amount of in has been got bonding with O.

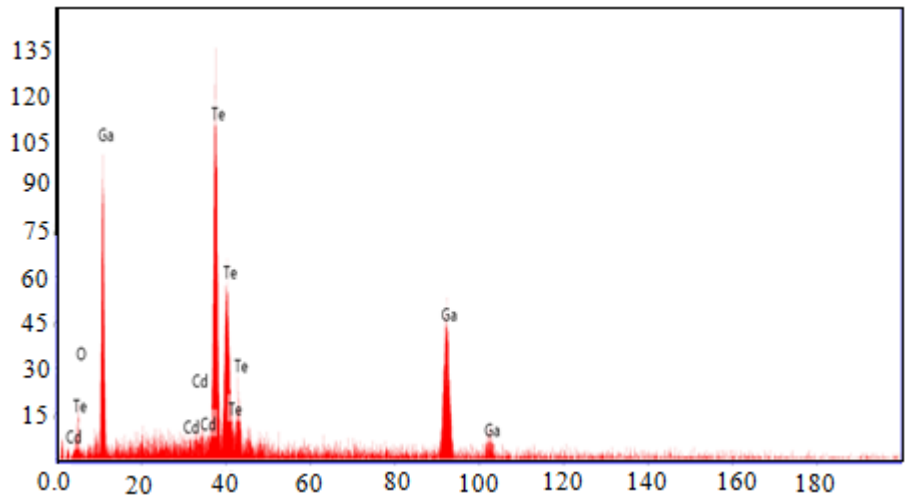


Figure 8: EDX spectra for Cd doped GaTe crystal.

4 CONCLUSION

We have reported the characterization of the GaTe:Cd compound semiconductor by the SEM, XRD and EDX. It is found that the Cd doped GaTe crystal has monoclinic structure; quite close 2θ peak values. XRD measurements indicate that there is an increase in peak intensities at specific annealing temperatures (300 and 500 $^{\circ}$C) and a decrease in higher annealing temperatures (700 $^{\circ}$C). The calculated lattice constants were found to be a= 17.404 Å; b= 10.456 Å; c=4.077 Å for GaTe which correspond to a monoclinic structure exhibiting B2/m (12) space-group symmetry. The crystallite size (589.9 Å), dislocation density (6.142 $lin^{-2}m^{4}$)) and residual strain (2.549 lin/m^{2}) (for the Cd doped GaTe crystal annealed at 300 ^{0}C for 30 min) values have been calculated using XRD results (410), respectively. The crystallite size has been calculated to be 490- 980 Å **for** GaTe:Cd from the SEM result**.** These results are in a good agreement with the ones obtained from EDX analysis**.** It has been observed that GaTe contains Ga=36.49 %, Te =58.14 %, Cd= 0.97 % and O = 0.05 % from EDX results, respectively.

5 ACKNOWLEDGEMENTS

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