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# Characteristics of synthesized CdSeTe powder

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CdSeTe semiconducting material was synthesized for the first time by a chemical method using selenium and tellurium with cadmium oxide in the presence of reducing atmosphere. Hexagonal mono phase CdSeTe powder of different compositions were prepared and characterized by X-ray diffraction and optical absorption studies. © *1999 Kluwer Academic Publishers*

## 1. Introduction

Semiconducting compounds CdSe, CdTe and CdSeTe are suitable for the conversion of solar energy into useful electric energy by Photo-Voltaic or Photo electrochemical devices. CdSeTe is a promising semiconductor which is used for various applications. In the case of mixed compounds such as $CdSe_xTe_{(1-x)}$, the optimal direct bandgap 1 to 1.7 eV can be achieved by changing the value of $x$ which in turn changes the opto electronic properties [1, 2]. Preparation of $CdSe_xTe_{(1-x)}$ by sintering the mixtures of CdSe and CdTe were reported earlier [3, 4]. The films prepared by using the material obtained by sintering method show a mixture of cubic and hexagonal phases, moreover the desired uniformity in distribution of CdSe and CdTe was not achieved throughout the samples. In order to avoid these difficulties, a novel method was adopted for the first time by an easy and convenient low temperature wet chemical method in which selenium and tellurium were reacted with CdO. Samples with different $x$ values varying from $x = 0$ to 1 have been synthesized and results on structural and optical properties are reported.

## 2. Experiment

Semiconducting compound CdSeTe was synthesized at 80° to 90° by the reaction of cadmium oxide with elemental selenium and tellurium in the presence of oxalic acid. This technique consists of the reduction of cadmium oxide and the reaction of Cd with Se and Te.

3 to 4 g of CdO powder was taken in an aqueous oxalic acid solution and 1.5 to 2 g of Se and 0.5 to 2.5 g Te was added to the solutions. By changing the selenium to tellurium ratio the different ratios of $CdSe_xTe_{(1-x)}$ were obtained. In each step after 1 to 10 hours of refluxing at 80° to 90° powders of requried Se to Te ratios have been formed. The resulting powder was dried in an electric oven at 60 °C. The materials were then treated with hot KOH solution to remove any unreacted Se and Te. Finally the powders were treated with acetic acid to remove traces of unreacted CdO. The dried powders were ground into fine powder using an agate mortar. 70% yield was obtained by this process.

The powders were characterised by X-ray diffraction technique using JEOL X-ray diffraction unit with Cu$K_\alpha$ radiation. Diffuse reflectivity measurement was conducted using Hitachi U-3400 UV-Vis-NIR spectrophotometer and density measurement was carried out by gravimetric method.

## 3. Results and discussion

Cadmium seleno telluride powder with different composition of CdSe and CdTe were arrived as per the following schematic chemical reaction.

$$CdO + xSe + (1-x)Te \rightarrow CdSe_xTe_{(1-x)} + 1/2O_2$$

X-ray diffraction studies on prepared powders of all compositions indicated the polycrystalline nature of the powder with hexagonal phase only. X-ray diffractogram of the representative samples $CdSe_{.55}Te_{.45}$ is shown in Fig. 1. The composition of powder has been calculated using Vegard's law expressed as follows:

$$x(a_{CdSe}) + (1-x)(a_{CdTe}) = a_{CdSe_xTe_{(1-x)}} \quad \text{obtained} \tag{1}$$

$$x(c_{CdSe}) + (1-x)(c_{CdTe}) = c_{CdSe_xTe_{(1-x)}} \quad \text{obtained} \tag{2}$$

where $a$ and $c$ are the lattice constants attained from

$$1/d^2 = 4(h^2 + hk + k^2)/3a^2 + l^2/c^2 \tag{3}$$

where $d$ is the distance between lattice planes and $h$, $k$, $l$ the miller indices.

The end composition of CdSe and CdTe were also prepared by this method. X-ray studies on the $CdSe_xTe_{(1-x)}$ powders indicated that the $d$ value changes as composition was varied from 0 to 1. Lattice parameters versus composition listed in Table I.

Generally the alloy structures depends on the composition and mode of preparation. Conventional method of preparation resulted in CdSeTe with mixed of cubic and hexagonal phases. Conversion of cubic to hexagonal phases required an additional heat treatment step

TABLE I Lattice parameters for different composition of $CdSe_xTe_{1-x}$

| S. No. | $x$ | $1-x$ | Hexa % | Cubic % | $a$ (Å) | $c$ (Å) |
|---|---|---|---|---|---|---|
| 1 | 0.93 | 0.07 | 100 | 0 | 4.31 | 7.03 |
| 2 | 0.86 | 0.14 | 100 | 0 | 4.33 | 7.07 |
| 3 | 0.82 | 0.18 | 100 | 0 | 4.34 | 7.08 |
| 4 | 0.65 | 0.35 | 100 | 0 | 4.40 | 7.18 |
| 5 | 0.55 | 0.45 | 100 | 0 | 4.42 | 7.27 |
| 6 | 0.48 | 0.52 | 100 | 0 | 4.44 | 7.25 |
| 7 | 0.41 | 0.59 | 100 | 0 | 4.46 | 7.28 |

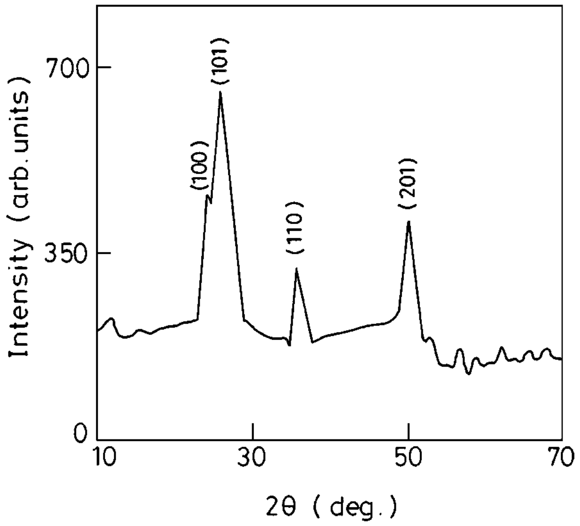

*Figure 1* X-ray diffractogram for $CdSe_{.55}Te_{.45}$ Powder.

[3, 5–7]. By this synthesis method only hexagonal phase is obtained for all compositions.

Diffuse reflectance measurements indicated that the band gap values varied from 1.49 to 1.65 eV as the composition was varied from CdTe to CdSe. The energy gap as a function of composition for the wurtzite phases of the $(CdTe)_{1-x}(CdSe)_x$ system is given in Fig. 2. This variation of band gap with composition is in good agreement with variation of $d$ with composition. This is illustrated in the Table II. Experimentally estimated density values of the synthesised powder with varying composition were in close agreement with theoretically calculated values of the same. This is shown in Table III.

TABLE II Comparison of crystallographic data and band gap

| S. No. | Composition | Structure | Interplanar distance $d$ (Å) | Band gap (eV) |
|---|---|---|---|---|
| 1 | $CdSe_{.93}Te_{.07}$ | Hexagonal | 3.736 | 1.65 |
| 2 | $CdSe_{.86}Te_{.14}$ | Hexagonal | 3.750 | 1.62 |
| 3 | $CdSe_{.82}Te_{.18}$ | Hexagonal | 3.767 | 1.61 |
| 4 | $CdSe_{.65}Te_{.35}$ | Hexagonal | 3.815 | 1.565 |
| 5 | $CdSe_{.55}Te_{.45}$ | Hexagonal | 3.831 | 1.535 |
| 6 | $CdSe_{.48}Te_{.52}$ | Hexagonal | 3.847 | 1.52 |
| 7 | $CdSe_{.41}Te_{.59}$ | Hexagonal | 3.864 | 1.51 |
| 8 | $CdSe_{.34}Te_{.66}$ | Hexagonal | 3.880 | 1.50 |

TABLE III Density vs. composition

| | | Density values | |
|---|---|---|---|
| S.No. | Composition | Theoretical | Experimental |
| 1 | $CdSe_{.97}Te_{.03}$ | 5.7436 | 5.680 |
| 2 | $CdSe_{.93}Te_{.07}$ | 5.7840 | 5.685 |
| 3 | $CdSe_{.86}Te_{.14}$ | 5.7568 | 5.662 |
| 4 | $CdSe_{.82}Te_{.18}$ | 5.7616 | 5.720 |
| 5 | $CdSe_{.65}Te_{.35}$ | 5.7820 | 5.730 |
| 6 | $CdSe_{.48}Te_{.52}$ | 5.8024 | 5.760 |
| 7 | $CdSe_{.34}Te_{.66}$ | 5.8192 | 5.756 |

The variation of the direct energy gap with composition in semiconductor alloys is expressed conventionally as a quadratic form [3, 8, 9].

$$E_x = E_{\mathrm{A}} + (E_{\mathrm{B}} - E_{\mathrm{A}} - C)x + Cx^2$$

where $E_{\mathrm{A}}$ and $E_{\mathrm{B}}$ are the energy gap of the pure compounds A and B, $E_x$ is the energy gap of the alloy $A_{1-x}$,

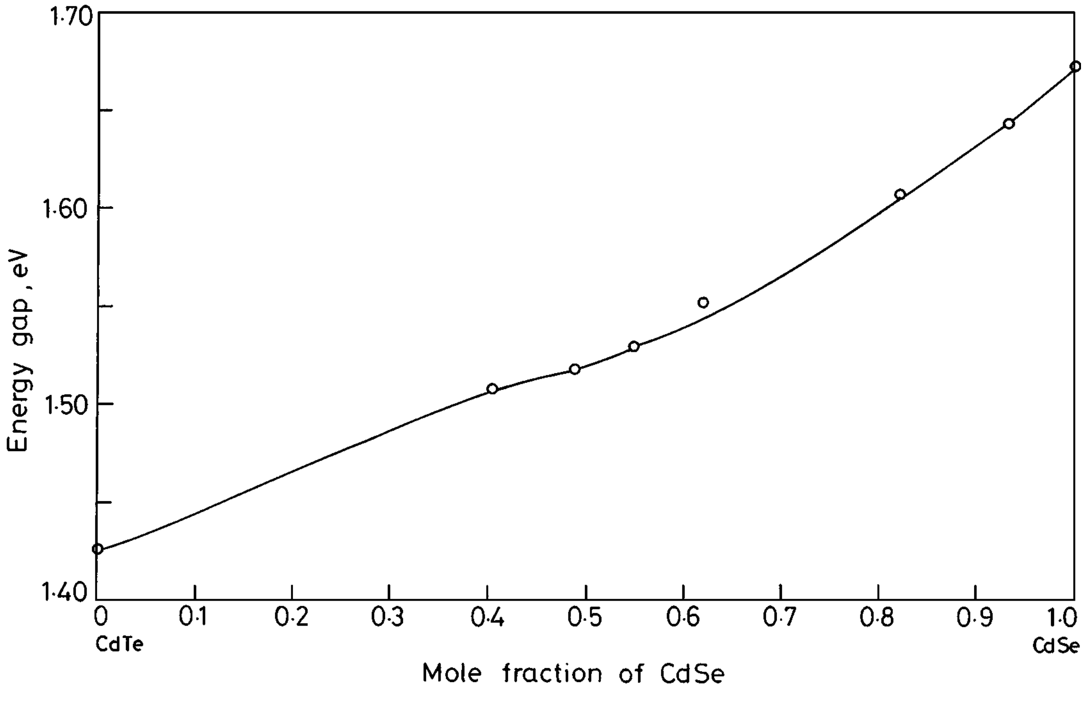

*Figure 2* Variation of band gap with mole fraction of CdSe.

TABLE IV Bowing parameter values for different composition $CdSe_xTe_{1-x}$

| S. No. | Composition | Energy gap of the end component $E_A$ (eV) | $E_B$ (eV) | Bowing parameter ($C$) |
|---|---|---|---|---|
| 1 | $CdSe_{.93}Te_{.07}$ | 1.47 | 1.70 | 0.46 |
| 2 | $CdSe_{.86}Te_{.14}$ | 1.47 | 1.70 | 0.39 |
| 3 | $CdSe_{.82}Te_{.18}$ | 1.47 | 1.70 | 0.32 |
| 4 | $CdSe_{.65}Te_{.35}$ | 1.47 | 1.70 | 0.24 |
| 5 | $CdSe_{.55}Te_{.45}$ | 1.47 | 1.70 | 0.24 |
| 6 | $CdSe_{.48}Te_{.52}$ | 1.47 | 1.70 | 0.24 |
| 7 | $CdSe_{.41}Te_{.59}$ | 1.47 | 1.70 | 0.22 |
| 8 | $CdSe_{.34}Te_{.66}$ | 1.47 | 1.70 | 0.21 |

$B_x$ and $C$ is the bowing parameter. The bowing parameter fitted to the experimental results shown in Fig. 2 and listed in the Table IV.

## 4. Conclusion

A novel method has been attempted for the synthesis of CdSeTe. This method of preparation has the following advantages:

1. 70% yield is obtained.
2. All the compositions exhibit hexagonal structure.
3. It is a low temperature synthesis technique.
4. Does not involve costly imported material and costly imported equipment.
5. Experimentally estimated density values for all compositions are reported for the first time.

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