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## RESEARCH ARTICLE

### EFFECT OF ANNEALING OF ELECTRON BEAM EVAPORATED CdSe FILMS

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#### ABSTRACT

Cadmium selenide (cdse) thin films on glass substrates were prepared by electron beam evaporation technique at various substrate temperatures and annealed at room temperature (RT), 100, 200 and 300 ° C respectively. XRD spectra indicates that films are polycrystalline with the hexagonal structure. When the heat treatment temperature is increased to 100° C, the films became highly oriented along (002) plane. The microstructure parameters like particle size, stress, strain, and dislocation density were calculated. The grain size is within the range of 24 to 44 nm.

#### INTRODUCTION

Nanocrystalline semiconductors have been used in electronic, optoelectronic and solar energy conversion devices. CdSe (Cadmium selenide) is a direct band gap material belonging to II-VI group, possessing excellent optoelectronic properties. It is used as an n-type window layer material in thin film solar cells and it is the suitable material for photovoltaic applications (Chate *et al.*, 2010; Nair *et al.*, 1993; Hankare *et al.*, 2010). Among all methods, EBE is one of the most promising methods for making high quality thin films for photovoltaic applications because it is an efficient and reasonably cost effective method (Pathinettam Padiyan *et al.*, 2002; Hernandez-Perez *et al.*, 2008; Murali *et al.*, 1991; Yamamoto *et al.*, 1998; Mane and Lokhande 1997; Kale and Lokhande 2000). CdSe films have been prepared by EB (Electron Beam) evaporation technique (Hus and Parlak 2008; Patel *et al.*, 2008) at room temperature and annealed at different temperatures were characterized by XRD (X ray Diffraction) (Arif *et al.*, 2008; Patidar *et al.*, 2008) and the results are presented. Grain size, dislocation density, strain and lattice constant variations of CdSe films have been calculated and discussed here.

#### MATERIALS AND METHODS

CdSe films were deposited using Hind Hivac electron beam evaporation (EBE) unit on glass substrates at different substrate temperatures in the range RT – 300 °C. Substrate temperature was fixed on the basis of the TGA data of the CdSe powder. The films were deposited with 5 kV and 10 mA under a vacuum of 10<sup>-6</sup> Torr. Film thickness was measured by the

stylus Profilometer (Mitutoyo). The films were characterized by X-ray diffraction (XRD) studies using CuK $\alpha$  radiation from an X'pert Pro PAN analytical XRD unit.

#### RESULTS AND DISCUSSION

XRD confirms the polycrystalline nature of the annealed films. The peaks correspond to the hexagonal structure for all the CdSe films. This is clearly supported by the published results that the bulk CdSe material acquires a highly stable hexagonal structure at temperatures varying from room temperature to the melting point of about 1240 ° C (Hus and Parlak 2008). At relatively low temperatures, CdSe exists with cubic structure, which is also a metastable phase. Hence, all the CdSe films deposited at various substrate temperatures and also annealed at RT, 100, 200 and 300 ° C showed only hexagonal structure in the present films deposited by the EB evaporation technique. All the films have thickness values of about 250 – 270 nm. A sharp peak at  $2\theta = 25.35^\circ$  appears in the XRD spectra of all the CdSe films, corresponding to the (002) reflection of the CdSe crystalline lattice. This observation suggests that the CdSe films grow according to the preferential orientation correspond to the hexagonal structure. Another peak that is commonly observed at about  $2\theta = 45.87^\circ$  with a broad and low intensity represents the (103) plane of the hexagonal structure for the CdSe film. Grain size, dislocation density, strain and lattice constant variations of CdSe films have been calculated and presented here.

Figure 1 shows the XRD patterns of CdSe thin films deposited at different temperatures. The spectra recorded for the CdSe film deposited at room temperature (RT) showed (002) peak along with the formation of other peaks like (101), (110) and (103) which are identified with the hexagonal structure.

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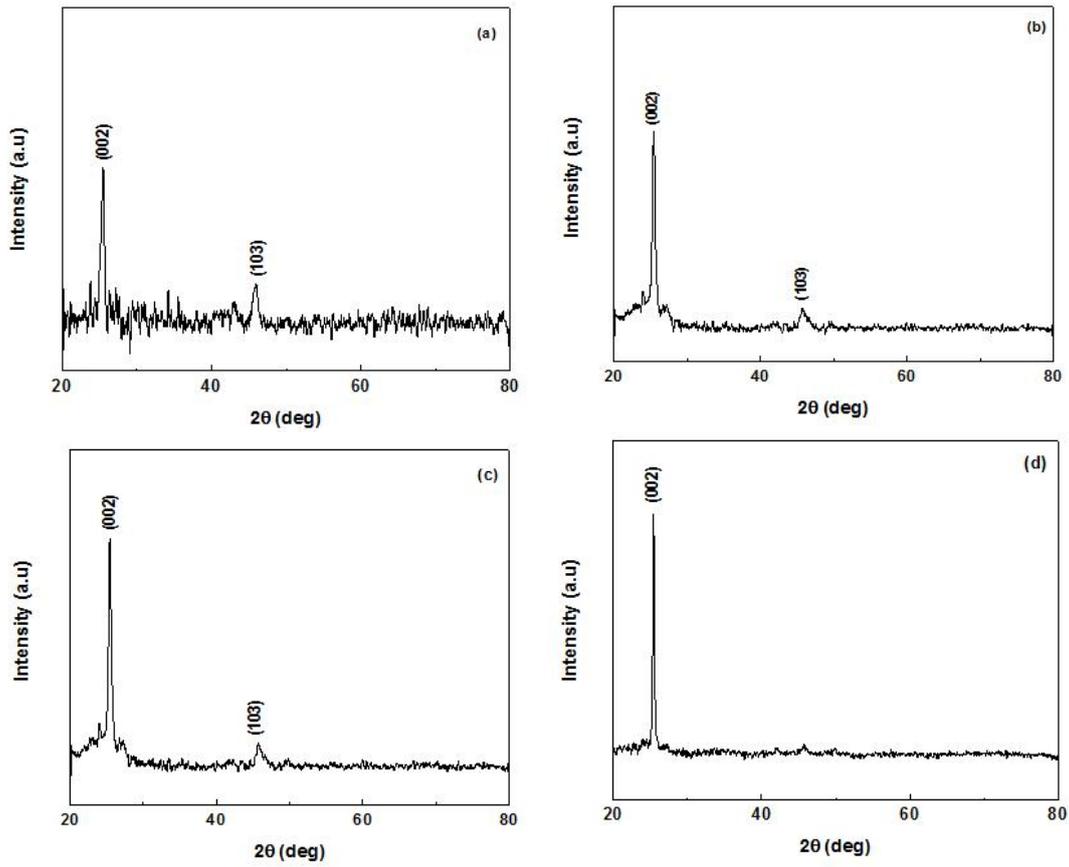


Fig. 1. XRD patterns of CdSe films deposited at (a) RT and annealed at (b) 100, (c) 200 and (d) 300 °C

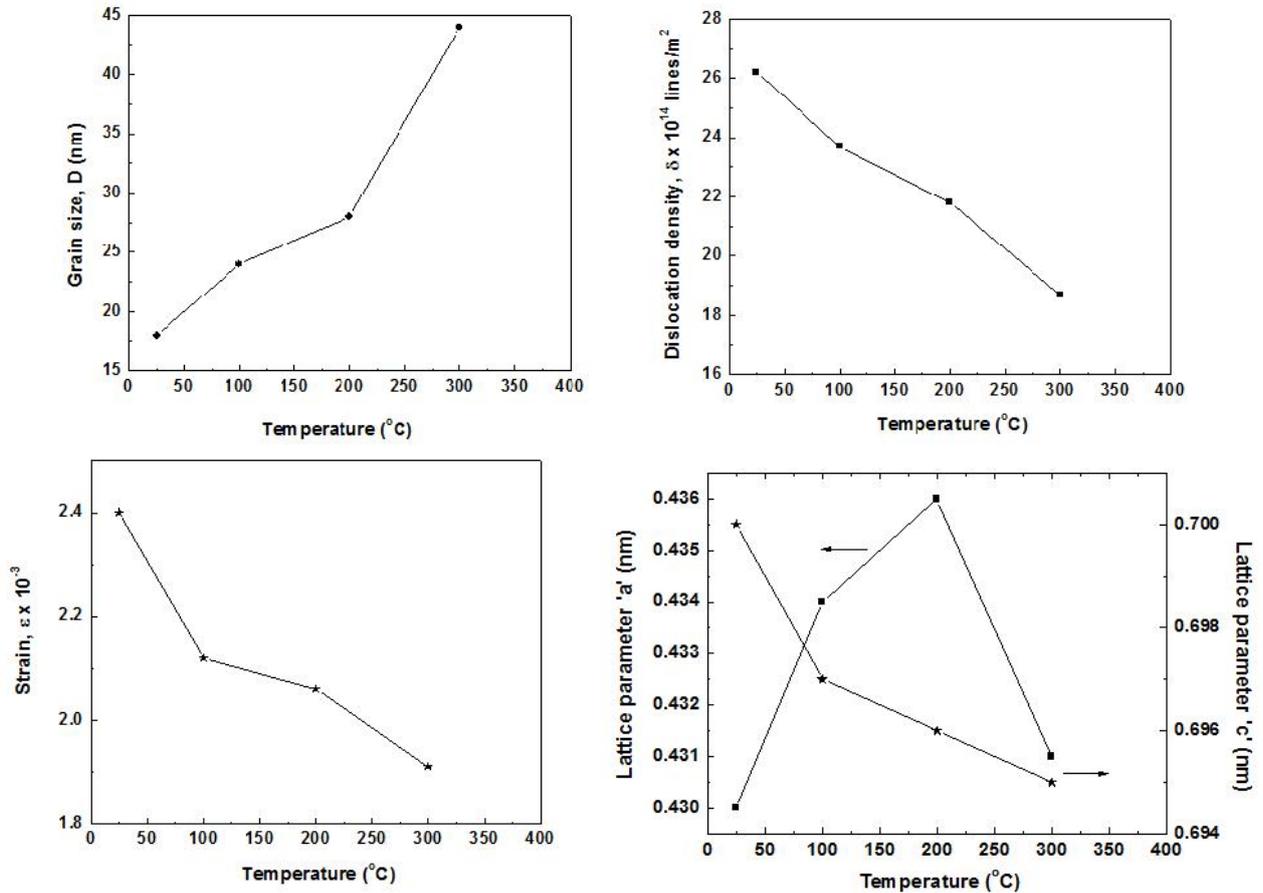


Fig. 2. Variation of micro structural parameters of CdSe films deposited at (a) RT and annealed at (b) 100, (c) 200 and (d) 300 °C

When the heat treatment temperature is increased to 100 °C, the films became highly orientated along (002) plane and the other peaks are found to be greatly suppressed. These results have been observed similar to the CdSe films deposited by molecular beam epitaxy technique (Patel *et al.*, 2008).

reduced, the extra free energy associated with these nano surface morphology tries to increase the fraction of the total free energy of these particles. It predicts that the available smaller particle can reduce this excess free energy by changing its lattice constant which has lead to an increased volume of the

**Table 1. Micro structural parameters of CdSe films deposited at various temperatures**

Temperature (°C)	Grain size D (nm)	Dislocation density (x 10 <sup>14</sup> ) lines/m <sup>2</sup>	Strain x 10 <sup>-3</sup>	No of crystallites n x 10 <sup>15</sup> /unit area	Lattice parameters a (nm) c (nm)	
100	24	23.7	2.12	20.7	0.434	0.697
200	28	21.8	2.06	16.2	0.436	0.696
300	44	18.7	1.91	9.5	0.431	0.695

Figure 2 shows the Variation of micro structural properties of CdSe films with different annealing temperatures and summarized in Table 1. The grain size of CdSe can be effectively tuned between 24 nm to 44 nm by varying the annealing temperature. The observed increase in grain size with increased heating temperature shows some improvement in crystallinity that reduces the grain boundary dislocations and discontinuities in the CdSe films. It has been a generally accepted and observed fact that strain and dislocation density in thin films are decreasing as the particle/grain size increases, which is a well-known physical and structural phenomena (Arif *et al.*, 2008). Strains are inherently seen and are the natural components of nano grained thin films and nano particle materials. Due to the large number of grain boundaries and the associated very short distance between them, the intrinsic strains accompanied with such interfaces are always present in nano structured thin films. Moreover, the increasing surface energy due to the presence of nano grains contributes to the varying magnitude of strains in thin films. Similar results have been reported/observed with increase of substrate temperature for vacuum evaporated CdSe films.

The calculated lattice parameter values ('a' and 'c') show in very close agreement with the standard values. The 'c' values are nearly the same as that of the standard value of 0.701 nm reported for the bulk material. However, the calculated 'a' values are found to be higher as compared to the 'a' value of 0.429 nm for the bulk material. Such deviations in the lattice constant values for the materials with nano grains may be attributed to an increased lattice strain. Strains create local distortion of the crystalline lattice leading to a change in lattice constant values from its bulk value, which is highly size dependent (Patidar *et al.*, 2008; Fitzpatrick 1989). In the present study, all the heat treated CdSe films show reduction in 'c' values which indicate that the nano crystallites are experiencing compressional force in the a-direction. These Electron Beam evaporated CdSe films show larger 'a' values compared to the standard value, which is indicating the action of tensile strength along the c-direction. These observations and the structural results from XRD analysis for the electron beam evaporated CdSe films are showing an opposite trend compared to the results reported for the CdSe thin films with nano crystalline lattice deposited by the wet electrochemical method (Fitzpatrick 1989). Further, it is stated that due to the presence of lattice with reduced grain size, almost all the nano grained materials are found to have different crystal lattice structure when compared to their polycrystalline or single crystalline counter parts (Hyugaji and Miura 1985) either in thin film form or powder form. This is mainly attributed to the inference that the number of atoms in nano grains/particles is

hexagonal crystal structure. This is consequently effected by the contraction or expansion, in the lattice atoms, in either of the 'a' or 'c' axis. Present structural studies on the electron beam evaporated and annealed CdSe films, show a reduction in 'c' values and an increase in the 'a' values, which justifies the discussion presented in the preceding sentences.

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