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Structural and the optical dispersion parameters of nano-CdTe thin film/flexible substrate

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ABSTRACT

CdTe thin films of different thicknesses were deposited on polymer substrates for flexible optical devices applications. X-ray diffractogram of different thicknesses for CdTe films are measured and their patterns exhibit polycrystalline nature with a preferential orientation along the (111) plane. The optical constants of CdTe films were calculated based on the measured transmittance spectral data using Swanepoel's method in the wavelength range 400–2500 nm. The refractive index n and absorption index k were calculated and the refractive index exhibits a normal dispersion. The refractive index dispersion data followed the Wemple–DiDomenico model based on single oscillator. The oscillator dispersion parameters and the refractive index no. at zero photon energy were determined. The possible optical transition in these films is found to be allowed direct transition with energy gap increase from 1.46 to 1.60 eV with the increase in the film thickness. CdTe/flexible substrates are good candidates in optoelectronic devices

1. Introduction

Cadmium telluride is considered at present one of the most promising materials, for device applications. It has a high absorption coefficient in the visible range of the solar spectrum and its band gap is close to the optimum value for efficient solar energy conversion [1,2]. CdTe/CdS solar cells are one of the prospective candidates for widespread commercial success in solar energy conversion [3–6]. They can be produced at low price with good efficiency and excellent stability. Thin film polycrystalline photovoltaics have been aimed at the lower cost market where lower efficiency is acceptable [7,8]. The conventional cells are usually manufactured on glass substrates and offer no weight advantage over single crystal cells. Producing thin film cells on thin foil substrates (0.05 mm or less thick), however, offers several advantages for space as well as terrestrial applications. Since the substrate material can be as thin as 0.05 mm, the weight savings are significant in the case of thin film devices on flexible substrates. Furthermore, the photovoltaic devices on flexible substrates can be folded in any shape, and the supporting structure requirements are minimum compared to the heavy glass substrates. One of the major obstacles in the development of low cost and high efficiency solar cells is the use of glass substrates. The poor thermal conductivity of glass makes it extremely difficult to maintain a constant annealing temperature across a large area panel and to avoid thermal stresses which cause breakage during fabrication. Thus, panel efficiency is much lower than would be expected from the efficiency of small devices. Hence metal foil mounted cells can both reduce weight and promise efficient cheaper cells.

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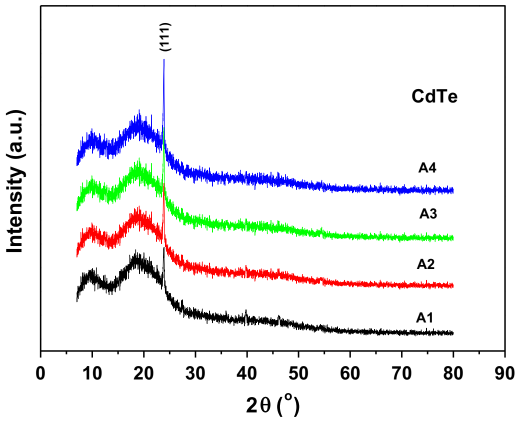

Fig. 1. The XRD patterns of CdTe films/flexible substrates of different thicknesses.

High efficiency can be achieved due to the high optical absorption coefficient. For example, in CdTe, light is absorbed within 2 mm and crystalline defects are relatively less important than in single crystal cells. Since the cells are so thin actual damage per unit radiation flux is less. Hence, thin film solar cells should be less susceptible to radiation degradation than single crystal solar cells. The interest in CdTe-based devices on light weight and flexible substrates gained interest in mid-90s and there are large number of reports on the film growth [9–24], post deposition treatments [10–12], structural characterization [19–24] and optoelectronic characterization [25–31]. We can concluded that CdTe thin film on flexible substrates still requires more studies to optimize its optical and electrical characterizations for high efficiency solar cell absorbed materials. The thermal conductivity and melting point T_m of utilized flexible substrate (polymer acetate sheet) is 0.16–0.36 $W\,m^{-1}\,K^{-1}$ [32] and 564 K [33] respectively.

In the present work, CdTe/flexible polymer substrates were prepared and characterized by XRD and optical spectroscopy measurements. XRD parameters such as crystallite size, microstrain were calculated and interpreted as a function of film thickness. Optical constants were calculated on the basis of Swanepoel's method for the first time. The relation between the structure of the studied CdTe thin films and their optical constants parameters were described in details. Optical dispersion parameters were calculated and interpreted.

2. Experimental techniques

CdTe single crystal was grown by the Bridgman technique in the Institute of Physics, Warsaw, Poland. Different thickness of CdTe thin films were deposited by thermal evaporation from a resistance heating quartz glass crucible onto transparent polymer acetate sheets as flexible substrates using high vacuum coating unit type Edward 306 A. Film thicknesses and the rate of evaporation were monitored with a quartz crystal monitor FTM4 attached to the vacuum system. Films were grown at a pressure of 10^{-6} Pa. The mechanical rotation of the substrate holder ($\approx$30 rpm) during deposition produced homogeneous film. The distance between the source heater and substrates holder is 21 cm to avoid any heat flow from the source to the substrates.

The elemental composition of the films was analyzed by an energy dispersive X-ray spectrometer (EDXS) unit interfaced to scanning electron microscope (SEM) (Philips XL) operating at an accelerating voltage of 30 kV. The relative error of determining the indicated elements does not exceed 3.2%. The structure of the as-deposited films were measured at room temperature by an analytical X′Pert Diffractometer System, which has CuK_α as a radiation source of wavelength $\lambda = 1.540598$ Å. The X-ray tube voltage and current were 40 kV and 30 mA, respectively. The 2θ range is 4–80° with a step size of 0.02 and scanning time of 0.4 second.

The transmittance $T(\lambda)$ and reflectance $R(\lambda)$ spectra of the as-deposited CdTe thin films of different thicknesses were measured at normal incidence of light in the spectral range of 400–2600 nm using a double-beam spectrophotometer (JASCO model V-670 UV–vis–NIR).

3. Results and discussion

3.1. X-ray diffraction analysis

The thickness of the four CdTe thin films deposited on flexible substrates as calculated in terms of Swanepoel's method was found to be 701 nm, 1052 nm, 1328 nm and 1691 nm. Effect of the change in thickness of the film on the structural using the X-ray diffractogram are shown in Fig. 1. XRD patterns exhibit polycrystalline nature and a major diffraction peak is observed at $2\theta = 23.80°$ along with few weak peaks. The presence of the predominant peak at $2\theta = 23.80°$ suggests that the CdTe films are of zinc blende (cubic) structure (JCPDS Data file: 1-75-2086-cubic) with lattice parameters $a = b = c = 6.41$ Å and a preferential orientation along the (111) plane. The (111) direction is the close-packing direction of the zinc blende (cubic) structure and this type of textured growth has often been observed in polycrystalline CdTe films grown on the flexible substrate. It can be seen that the film thickness affects the XRD pattern of CdTe thin films i.e. the peak intensity increases with increasing film thickness. Each X-ray diffraction line profile obtained in a diffractometer is broadened due to instrumental and physical factors (crystallite size and lattice strains). The microstructure parameters of the CdTe films such as crystallites size (D_v) and microstrain (e) were calculated by analyzing the XRD data using the Scherrer's formula

$$D = \frac{0.9\lambda}{\beta \cos \theta}, \quad (1)$$

and Wilson formula

$$e = \frac{\beta}{4 \tan \theta}, \quad (2)$$

where β describes the structural broadening, which is the difference in integral X-ray peak profile width between the sample and a standard (silicon) and is given by $\beta = \sqrt{\beta_{obs}^2 - \beta_{std}^2}$. Table 2 shows a comparative look of microstructure parameters (D_v and e) of the CdTe films of