Materials Chemistry and Physics xxx (2016) 1–6

Contents lists available at ScienceDirect

Materials Chemistry and Physics

journal homepage: www.elsevier.com/locate/matchemphys

Effect of deposition temperature on the structural, morphological and optical band gap of lead selenide thin films synthesized by chemical bath deposition method

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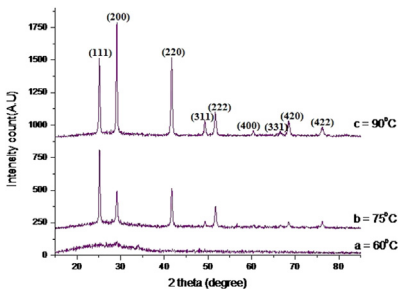
HIGHLIGHTS

- The crystallinety of the films improved as the deposition temperature increased.
- The deposition temperature strongly influenced the preferred orientations.
- Microstrain and dislocation density are decreased linearly with deposition temperature.
- Band gap decreased from 2.26 eV to 1.13 eV as the deposition temperature increased.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 29 October 2015
Received in revised form
28 June 2016
Accepted 14 August 2016
Available online xxx

Keywords:
Thin film
Chemical bath deposition
Microstrain
Preferred orientation
X-ray diffraction

ABSTRACT

Lead selenide (PbSe) nanocrystalline thin films have been deposited on silica glass substrates by the chemical bath deposition technique. The samples were deposited at the bath temperatures of 60, 75 and 90 °C respectively and characterized by a variety of techniques. The XRD results revealed that the PbSe thin film deposited at 60 °C was amorphous in nature. Films deposited at higher temperatures exhibited sharp and intense diffraction peaks, indicating an improvement in crystallinety. The deposition temperature also had a strong influence on the preferred orientation of the crystallites as well as other structural parameters such as microstrain and dislocation density. From the SEM study it was observed that film deposited at 90 °C had well defined crystallites, uniformly distributed over the entire surface of the substrate. The EDAX study confirmed that the samples deposited at the higher temperature had a better stoichiometric ratio. The optical band gap varied from 2.26 eV to 1.13 eV with increasing deposition temperature.

1. Introduction

Semiconductor selenides have attracted considerable attention due to their interesting properties and potential applications [1]. Lead selenide (PbSe) is a group IV–VI compound semiconductor, possessing excellent optoelectronic properties and abundance in nature. It exhibits the cubic structure with face centered phase [2,3]. The interest in lead selenide is due to its narrow band gap, which is employed to produce photoresistors, photodetectors, and photoemitters in the IR range, as well as injection lasers [4]. PbSe has a direct optical band gap of 0.27 eV at room temperature [3] but

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http://dx.doi.org/10.1016/j.matchemphys.2016.08.034
0254-0584/

it exhibits strong quantum size effects [5] hence the energy band gap of its nanocrystals can be tuned to anywhere between 0.27 eV and 4.5 eV [6] by changing various deposition conditions [7]. Quantum confinement effects begin to appear at relatively large particle dimension owing to its large Bohr exciton radius (46 nm). This results a strong confinement of electron-hole pair and larger optical nonlinearity [8].

PbSe thin film can be synthesized by several deposition techniques such as co-evaporated [9], pulse sonoelectrochemical [4], thermal evaporation [3], pulsed laser deposition [10] and chemical bath deposition [11,12]. Among these techniques, the chemical bath deposition (CBD) method is currently attracting considerable attention as it is relatively inexpensive, simple and convenient for large area deposition [13]. Properties of thin films such as film thickness, crystalline size and band gap can be controlled by varying the CBD growth parameters that include bath temperature, pH and deposition time [14]. Among these parameters, the deposition temperature is suggested to be the most important parameter which strongly influences the thin film structure over a narrow temperature range [15]. In this work, we investigated the effect of deposition temperature on the structural, morphological, and optical band gap of nanocrystalline PbSe thin films deposited by CBD technique from chemical bath containing lead acetate, sodium hydroxide, ammonia and sodium selenosulphate at a pH of 12.

2. Deposition and characterization of the thin film

The PbSe thin films were deposited on silica glass substrates using the deposition condition described in our previous report [16]. Three different samples were prepared at deposition temperatures of 60 °C, 75 °C and 90 °C respectively. After deposition, the samples were removed from the solution, rinsed with deionized water and dried under ambient conditions before film characterization. All the deposited PbSe thin films were mirror-like and well adherent. The crystal structure of PbSe thin films were characterized by a PANalytical Empyrean X-ray diffractometer with a Cu-k_α radiation ($\lambda_{\alpha 1} = 1.5406$ Å). The machine was operated at 40 mA and 45 kV. The elemental composition and surface morphology of the samples were determined using energy dispersive X-ray analysis (EDAX) attached to high resolution JEOL JSM-7600F scanning electron microscope (SEM). The optical absorption spectra of the samples were measured at room temperature, using a Shimadzu UV/Vis mini-1240 Spectrophotometer within the wavelength range of 200 nm–1100 nm.

3. Results and discussion

3.1. X-ray diffraction analysis

Fig. 1 shows the X-ray diffraction patterns of PbSe thin films at different deposition temperature.

The lack of discernible diffraction peaks in the XRD pattern of the PbSe thin film deposited at 60 °C (Fig. 1a) is an indication of the poorly crystalline nature of the film. This may be attributed to the low migration activity of the Pb and Se atoms on the substrate surface, resulting the crystal atoms may have a random distribution with short range order [15,17]. The films deposited at 75 °C and 90 °C exhibited sharp diffraction peaks corresponding to reflections from the (111), (200), (220), (311), (222), (400), (420) and (422) planes. The diffraction pattern was well matched with the standard JCPDS data file reference code: 01-077-0245 of the face centered cubic structure. The intensity and number of diffraction peaks increased with the deposition temperature, indicating a considerable improvement in the crystalline nature of the PbSe thin film. The deposition temperature also had a significant effect on the preferred orientations of the crystallites. For the films deposited at 75 °C, the crystallites had a preferred orientation along the (111) plane, whilst for the deposition temperature of 90 °C, the crystallites had a preferred orientation along the (200) plane. This indicates that the orientation of the grains growth along different directions depending on the deposition temperature. On the basis of the thermodynamics principle, [18], have suggested that the basic reason for variation of preferred orientation is the change of the total system free energy during the film growth. The total free energy variation during the film growth is affected by the interface, surface, and strain energy contributions. Moreover, the degree of these three energy contributions may be different under certain preparation conditions, which consequently leads to different preferred orientations [18]. The growth mechanism of PbSe thin films is mainly dominated by the surface and the strain energy contributions. Hence, the differences of the surface and the strain energy density is responsible for variation of preferred orientation [15,19].

Lattice constant (a_{hkl}) for the cubic structure was calculated using Equation (1) and the results are presented in Table 1.

$$a_{hkl} = d_{hkl}h^2 + k^2 + l^2 \quad (1)$$

The average crystallite size was calculated from a full width at half maximum of the diffraction peaks using the Debye-Scherrer formula [13]. The average crystallite size of the films increased almost linearly from 18.21 nm to 23.11 nm as the deposition temperature increased from 60 °C to 90 °C. Similarly the average thickness of the films increased from 65.32 nm to 438.90 nm as the deposition temperature increased from 60 °C to 90 °C. This result indicated that at low deposition temperature, the film formed was very thin. This may be attributed to the fact that the required number of ionic species is not available in the solution to get better quality film. The film thickness was measured by weight difference method [20]. The deviation of the calculated lattice constant from the bulk sample value shows that the crystallites may be under some strain [21]. The microstrain value (ε) of the as-deposited PbSe thin films were calculated using the following mathematical relation [22]:

$$\varepsilon = \frac{\beta\, Cos\, \theta}{4} \quad (2)$$

where, θ is the diffraction angle and β is the full width at half maximum. The other structural parameter calculated was the dislocation density (δ) which is a measure of the defects in the film [21], and this was calculated using Williamson and Smallman's formula [23]. Strain and dislocation density were calculated from the (200) plane and the results are tabulated in Table 1. From Table 1, it can be observed that the dislocation density and strain decreased with increasing deposition temperature. This indicates the formation of high quality of thin films [22]. In addition the dislocation density decreased with increasing crystallite size. This may be due to a decrease in the occurrence of grain boundaries because of an increase in the crystallite size of the film with increasing deposition temperature.

3.2. Elemental analysis and morphological studies

The compositional analyses of the synthesized PbSe thin films were studied by EDAX measurement without elemental restriction. Figs. 2 and 3 show the EDX patterns of PbSe thin films deposited at 60 °C and 90 °C respectively. The EDAX pattern of the PbSe thin film deposited at 60 °C showed the presence of Pb and Se peaks but the strong peak is due to silicon. The average atomic percentage of Pb and Se at 60 °C was 76:24, which showed that the sample was

Please cite this article in press as: F.G. Hone, F.K. Ampong, Effect of deposition temperature on the structural, morphological and optical band gap of lead selenide thin films synthesized by chemical bath deposition method, Materials Chemistry and Physics (2016), http://dx.doi.org/10.1016/j.matchemphys.2016.08.034