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Design and characterization of MoO_3/CdSe heterojunctions

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ABSTRACT

In this work, the morphological, compositional, structural, optical and dielectric properties of CdSe which are deposited onto glass and onto MoO_3 thin film substrates are investigated. The use of MoO_3 as substrate for the growth of CdSe is observed to increase the lattice parameters of the hexagonal unit cell of CdSe and decreases the values of grain size and strain. It also forms band tails of width of 0.20 eV in the band gap of CdSe. The optical analysis has shown that the MoO_3/CdSe interfacing results in blue shift in the energy band gap of CdSe and also result in large conduction and valence band of sets of values of 2.12 and 0.94 eV, respectively. The dielectric spectral analysis with the help of Drude-Lorentz approaches for optical conduction, revealed an enhancement in the drift mobility of charge carriers from 15.69 to 39.30 cm^2/V as a response to the incident electromagnetic field. The free carrier density of the MoO3/CdSe being of the order of 10^{17} cm^{-3} with the large valence and conduction band offsets and the sufficiently large drift mobility nominates the MoO_3/CdSe heterojunctions as an effective component of optoelectronic technology including thin film transistors.

1. Introduction

Recent investigations that take into account the performance of optoelectronic devices has reported the CdSe and MoO_3 as promising members of this technology [1]. In addition to their applications as solar cells, they are used as photodetectors [2]. Guided CdSe nanowires are reported to exhibit features presented by fast raise/fall times and high gain that nominate it for use as field effect transistors and photodetectors [2]. CdSe based films is observed to operate as a saturable absorber which can be used for Q-switched and mode-locked double-clad ytterbium-doped fiber lasers [3]. It was possible to generate a stable pulse of laser light within a power range of 0.97–1.20 mW. On the other hand, MoO_3 compound is regarded as materials suitable for use in solar cell production. High performance semitransparent organic solar cell that incorporates low bandgap polymer, in the photoactive layer and simple, non-patterned Dielectric/Metal/Dielectric anode composed of MoO_3/Ag/MoO_3 are found to display excellent photovoltaic properties with power conversion efficiency of 5% at 18.3% visible light transmission [4]. The one-dimensional α-MoO_3 nanorods are also found to exhibit high specific capacitance of 176 F/g with good cycle stability which make it favorable for use as supercapacitors [5].

The features of these two materials motivated us to design a heterojunction that comprises both of them as stacked layers. For this reason, here in this work we will study the MoO_3/CdSe interfaces as promising candidate for optoelectronic applications. Particularly, the structural, compositional, optical and dielectric properties of the CdSe, MoO_3 thin films which are deposited onto glass and CdSe deposited onto MoO_3 transparent dielectric substrate are investigated in details. The optical conductivity parameters will also be explored prior to technological applications.

2. Experimental details

Thin films of MoO_3 and CdSe are prepared by the physical vapor deposition technique from the MoO_3 powders (sigma-Aldrich 99.97%) and CdSe crystal lumps (Alfa-Aeser 99.99%), respectively. The films were prepared in a VCM 600 physical vapor deposition system under a vacuum pressure of 10^{-5} mbar onto ultrasonically cleaned glass substrates. The substrates were not subjected to any heating process during the growth cycles. Some of the produced MoO_3 films are used as substrates for the deposition of CdSe films to form the MoO_3/CdSe heterojunctions. The thicknesses of the films were monitored by an in situ INFICON (STM-2) thickness monitor which has rate resolution/measurement of 0.037Å. The Miniflex 600 X-ray diffraction unit (XRD), Coxem-200 scanning electron microscope (SEM), EDAX energy dispersion X-ray analyzer (EDS) and Thermoscientific Evolution 300

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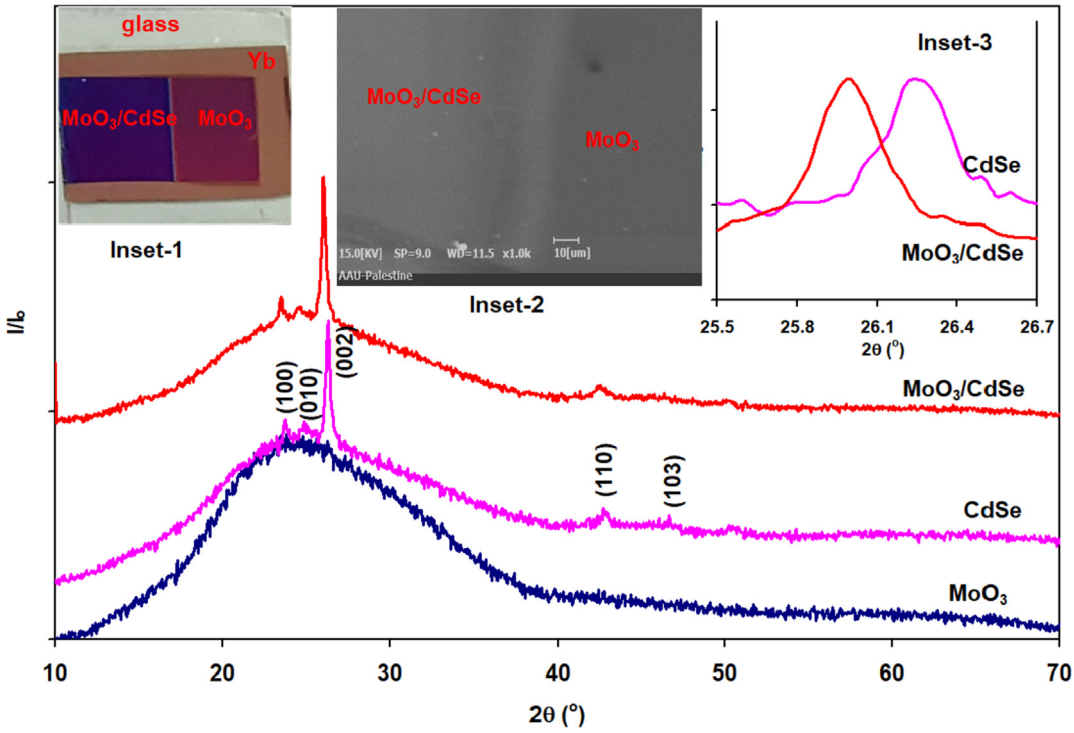

Fig. 1. The X-ray diffraction patterns for the MoO_3, CdSe and for MoO_3/CdSe films deposited onto glass substrates. Inset-1 show the optical image of the MoO_3/CdSe deposited onto metal substrate. Inset-2 show the scanning electron microscopy image for the interface deposited onto glass. inset-3 illustrate a comparison between the maximum peak of CdSe and MoO_3/CdSe.

ultraviolet–visible light spectrophotometer were used to study the structural, morphological, compositional and optical properties of the films. The scanning speed of the X-ray diffraction was 0.5 deg./min.

3. Results and discussion

The optical image of the designed MoO_3/CdSe heterojunction is shown as inset −1 of Fig. 1. The optical image is displayed for a sample deposited onto Yb metal surface because the MoO_3 has no color and it is appearance is very similar to that of glass. The respective enlargement of 1000 times for a similar heterojunction deposited onto glass substrate is shown in inset-2 of Fig. 1. The scanning electron microscopy image displayed very smooth surfaces with clearly observable interface boundaries. For the shown image, detailed energy dispersive X-ray analysis was carried out. The EDS measurements which were collected for different periods of scanning times and over more than 20 regions revealed an atomic content of 53.2% of Cd and 46.8% of Se for cadmium selenide ($Cd_{1.13}Se$). While the glass substrate is composed of SiO_2:Na_2O:$MgO_{0.6}$, the molybdenum oxide revealed the correct stoichiometry in accordance with the formula MoO_3. No other elements were detected in the EDS spectra of the samples indicating the high purity of the MoO_3 and CdSe. On the other hand, the X-ray diffraction patterns which are recorded for MoO_3, CdSe and MoO_3/CdSe thin films that are grown onto glass substrates are also shown in Fig. 1. While the XRD of MoO_3 displays no intensive patterns, the CdSe and MoO_3/CdSe shows one highly intensive peak and other four weak reflection peaks. The indexing of the peaks in accordance with the "TREOR 92" software packages reveal the lattice parameters which are displayed in Table 1. The lattice parameters of the hexagonal unit cell of CdSe are comparable to that reported in PDF card No 01-070-2554 as 4.298 and 6.767 Å along the $a-$ and $c-$axis of the crystalline unit cell, respectively. The deviation of the value of the lattice parameter along the $a-$axis from the standard value may be ascribed to the slight differences in the atomic stoichiometry [6] in CdSe. The deposition of the CdSe onto glass/MoO_3 caused a shift in the peaks positions indicating the strained nature of

Table 1
The structural parameters for the CdSe and MoO_3/CdSe heterojunctions.

	Lattice constant (Å)		D (nm)	$\in \times 10^{-3}$	δ ($\times 10^{11}$ lines/cm^2)	
	a	*c*			*a-axis*	*c-axis*
CdSe	3.743	6.784	37	4.68	5.06	2.79
MoO_3/CdSe	3.782	6.848	33	3.76	5.62	3.10

structural formation. The effect of the amorphous MoO_3 on the main reflection peak is displayed in inset-3 of Fig. 1. The inset clearly shows the shift toward lower angle values indicating larger lattice parameters. The calculated lattice parameters for CdSe deposited onto MoO_3 are also shown in Table 1. The table suggests a percentage increase in the lattice parameter of CdSe by 1.0% and by 0.94% along the $a-$ and $c-$axes, respectively. On the other hand, the calculated grain size (D), microstrain (ε) and dislocation density (δ) using the previously reported equations [6] are also displayed in Table 1. The data show a decrease in the value of grain size and strain and an increase in the dislocations densities when the MoO_3 substrate is used to grow CdSe in place of glass. Early works which targeted the preparation of ZnO:Mo films by the sputtering technique assigned the shift in the diffraction angle toward lower values to the ionic radiuses of the Zn and Mo [7]. The Mo ions which exhibit ionic radiuses value of 69.9 p.m. for Mo^{3+}, 65 p.m. for Mo^{4+}, 61 p.m. for $Mo^{5+}$and 59 p.m. for Mo^{6+} are less than that of Zn (74 p.m.). The substitution of Cd^{+2} (109 p.m. [6]) in sites of Mo is not possible, but un-bonded surface atoms of Mo can replace vacant sites of Cd. The bond lengths of Cd−Se, Mo−O, Mo−Se and Cd−O are 280.9, 169 [8], 250.4 [9] and 217.6 p.m. [10], respectively. The shortest bond length relates to Mo−O. It indicates strong interactions between the MoO_3 rings. However, because the bond length of Cd−O is less than that of Cd−Se, there is stronger interaction force between Cd and O atoms than Cd and Se atoms. Such forces usually lead to the strained structure which affects the grain size of CdSe and could also be regarded as a reason for the observed increased defect density upon