



Modulation of the band gap of tungsten oxide thin films through mixing with cadmium telluride towards photovoltaic applications



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ABSTRACT

Tungsten oxide (WO_3) is a wide band gap semiconductor that has received extensive interest in optoelectronic applications. However, its band gap is too large for applications based on the absorption of visible light. To that end, we have modulated the band gap of WO_3 thin films through mixing it with cadmium telluride (CdTe). The films were prepared by thermal evaporation of WO_3 containing controlled concentrations of CdTe (0–25%). The obtained films showed a continuous reduction in the band gap from 3.30 eV (0% CdTe) to 2.47 eV (25% CdTe). Photocurrent response increased significantly with the increase of CdTe concentration due to the enhancement of the light absorption in the long wavelength region. The results obtained support the potential of these alloyed films for photovoltaic applications.

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1. Introduction

Wide band gap semiconductors exhibit emission and absorption wavelengths in the green, blue, and ultraviolet (UV) regions of the electromagnetic (EM) spectrum [1]. Among these, wide band gap metal oxide semiconductors have drawn growing interest, due to their unique optical, electrical, chemical and mechanical properties. Besides non toxicity, they are also of low cost and easy to fabricate [2]. These unique properties make them candidates for a variety of applications, including gas sensing [3], solar cells [4], water splitting [5], transparent conductors [6], as well as photocatalysis [7]. Although the large band gaps make metal oxides suitable for short wavelength optoelectronics [8], they are of limited applicability in the fabrication of photovoltaic devices. Among metal oxide semiconductors, tungsten oxide (WO_3) is an *n*-type semiconductor which possesses different polymorphs including monoclinic (17–330 °C), orthorhombic (330–740 °C), and tetragonal (>740 °C) [9]. Thin films of WO_3 have been extensively investigated for electrochromic devices [10], gas sensing [11], photoelectrochemical [12], photocatalytic [12], and optoelectronic applications [13]. Amorphous WO_3 thin films have a

wide band gap value of 3.4 eV, while crystalline films have a smaller band gap of 2.6 eV [8]. Consequently, these band gap values limit photo-absorption to the near UV and blue regions of the EM spectrum. Thus, the ability to extend light harvesting further into the whole visible region (1.7–3.1 eV) requires the modification of the band gap.

Various routes were developed to engineer the band gap of WO_3 . These include: (i) doping or mixing with additives of elements or metal oxides such as silver [14], titania [15], nitrogen [16], vanadium [17] and iron oxide (Fe_2O_3) [18]. The reduction of the band gap by this route was attributed to the increase of the grain size, lattice disorder of the WO_3 matrix, or creation of impurity levels below the conduction band of WO_3 [14–18], (ii) fabrication of core/shell nanostructures (called type II alignment) based on alloying of core semiconductor quantum dots with shell nanostructures [19–21]. This leads to the formation of core/shell semiconductor heterostructures in which the conduction and valence bands of the core semiconductor are higher or lower than those of the shell. The band gaps of the two materials (core and shell) overlap but no one totally encloses the other, leading to the separation of the two carriers (electrons and holes) between the core and the shell materials [21,22]. As a consequence, type II alignment has reduced band gaps compared to those of the constituent core and shell components, which leads to the tunability of the band gap of the core semiconductor [21,23,24].

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For instance, the reduction of the band gap of WO_3 by fabrication of WO_3/CdS core/shell nanowires has been reported [25], and (iii) fabrication of WO_3 quantum dots in which the band gap of WO_3 is blue-shifted due to the narrowing of both the conduction and valence bands with decreasing the size of the nanostructures [19,26]. A widely-used technique for modifying the properties of materials is the fabrication of an alloy or a solid solution [27–31]. Alloys may be formed by mixing two or more solid materials [32]. In this technique, the band gap is engineered by alloying multiple semiconductors [33]. An alloy of two semiconductors is termed a binary alloy; one with three is a ternary alloy; and one with four is a quaternary alloy [34]. Binary semiconductors have fixed band gaps and lattice constants [35], and fabrication of a binary alloy results in the tuning of the band gap to take intermediate values between those of the parent compounds. Motivated by a necessity of extending the optoelectronics applications of WO_3 over a wide spectral range for energy conversion and photovoltaic devices, we aim to achieve band gap modulation of WO_3 thin films by alloying with the narrow-band-gap II–VI compound semiconductor cadmium telluride (CdTe), which possesses an optimum band gap of 1.44 eV for solar absorption and high optical absorption coefficient [36,37]. To the best of our knowledge, mixing of these two materials has not been investigated. This field of research is expected to provide an opportunity for numerous applications of other wide band gap metal oxide semiconductors in the visible region. In this work, we investigate the effect of CdTe concentration on the structural, chemical, and optical properties of WO_3 thin films, as well as the suitability of the CdTe-alloyed WO_3 thin films for photovoltaic applications.

2. Experimental details

The source materials were powders of WO_3 (Alfa, 99.999% purity) and CdTe (Blazers, 99.999% purity). The mass of the WO_3 powder was 2 g in all depositions. Various concentrations of CdTe, specifically 5%, 10%, 15%, 20% and 25% were added to WO_3 powder. These concentrations were the ratio of the CdTe mass to that of WO_3 . The mixture was then thermally evaporated in a Leybold L560 box coater using a molybdenum boat. The films were deposited on unheated tantalum and fused silica substrates. The evaporation rate (0.2 nm/s) was monitored by a rate controller. The thickness of the films was fixed by a quartz crystal to be 300 nm. However, the real thickness was estimated optically and verified by a stylus profilometer and was found to be 270 ± 20 nm. Prior to evaporation, the thermal evaporation system was pumped down to a base pressure of 2×10^{-5} mbar, and the starting material was slowly out-gassed. During deposition, the substrate holder was rotating to obtain uniform films. The structural properties of the films were studied using X-ray diffraction (XRD), which was performed in a Rigaku Ultima IV diffractometer, employing $\text{Cu K}\alpha$ radiation (1.54 Å). The 2θ range scanned was $10\text{--}80^\circ$, the 2θ step was 0.02° , and the step acquisition time was 1 s. A contact-mode atomic force microscopy system (AFM; Veeco Innova diSPM) was utilized for the investigation of the surface morphology of the films. A silicon tip of 10 nm radius oscillating at its resonant frequency of 300 kHz was used to probe the surface of samples. The scan area was $2 \times 2 \mu\text{m}^2$. The chemical analysis of the films was carried out using X-ray photoelectron spectroscopy (XPS) performed in a Thermo Scientific ESCALAB 250 Xi spectrometer equipped with an $\text{Al K}\alpha$ (1486.6 eV) X-ray source. The analysis spot diameter was 600 μm . The base pressure inside the spectrometer was 7×10^{-10} mbar. The binding energies of the XPS spectra were calibrated with adventitious C 1s peak positioned at 284.5 eV. Elemental depth profiles of the alloyed thin film samples were accomplished by a sequence of 60 s Ar^+ ion etching followed by XPS analysis. Etching was achieved with a 3 keV Ar^+ ion beam with a

medium ion current over a $1 \times 1 \text{ mm}^2$ area of the sample surface. During depth profile process, the pressure inside XPS chamber was 5×10^{-8} mbar. To eliminate charging of film surface during XPS analysis, all films were deposited on tantalum substrates. The transmittance measurements were conducted in a Jasco V-570 double beam spectrophotometer over the wavelength range 200 to 800 nm. Photocurrent was measured in a standard three electrode configuration with WO_3/CdTe thin films on indium-tin oxide as a working electrode, Ag/AgCl as a reference electrode, and a Pt foil as a counter electrode, respectively. Photoelectrochemical measurements were conducted in 0.5 M Na_2SO_4 (Sigma Aldrich) electrolyte. The samples were illuminated by an artificial sunlight simulator ($300 \text{ mW}/\text{cm}^2$) using a Xenon lamp. The bias voltage was kept at 0.23 V for chronoamperometric study.

3. Results and discussion

3.1. Structural analysis

Fig. 1 shows the XRD patterns of the films. The XRD patterns of pure WO_3 thin films exhibited the amorphous nature of the films. The pure CdTe films had a poly-crystalline nature with a dominant XRD peak at $2\theta = 23.80^\circ$, corresponding to the (111) plane of the cubic structure of CdTe, and two other weak peaks centered at $2\theta = 39.21^\circ$ and $2\theta = 46.34^\circ$, corresponding to the (220) and (311) planes. A similar polycrystalline growth of thermally evaporated CdTe film under the same conditions was previously reported [38]. Addition of CdTe into WO_3 did not improve the structure of WO_3 up to a CdTe concentration of 15%, as evidenced from the absence of XRD peaks. However, at higher CdTe concentrations ($\geq 20\%$), there was still no improvement in the structure of WO_3 , but a polycrystalline form of CdTe was observed. This indicates the presence of an amorphous WO_3 and a polycrystalline CdTe form of phase, and hence, a two-phase mixture was formed.

3.2. Morphological analysis

Fig. 2 shows representative three-dimensional AFM images for the pure and alloyed thin films. The surface roughness of the investigated films was characterized by evaluating the root-mean-square roughness (R_{rms}). Pure WO_3 displayed a columnar structure, while granular and columnar structures were formed in the pure CdTe thin films as shown in Fig. 2a and b, respectively. The columnar structures of the pure WO_3 were transferred into granular structures when alloying with CdTe as shown in Fig. 2c.

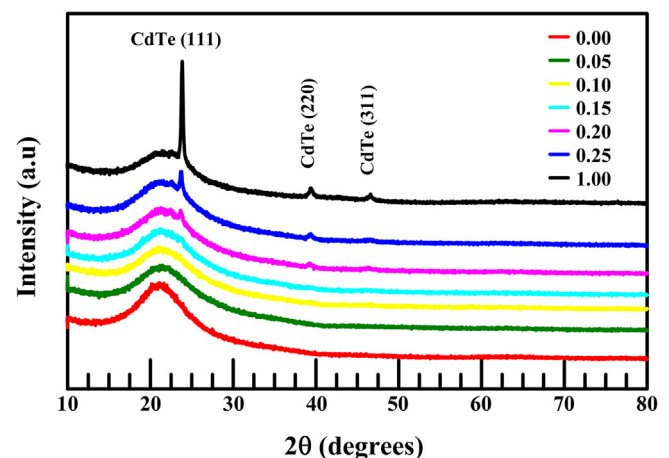


Fig. 1. XRD patterns of WO_3 , CdTe and CdTe-alloyed WO_3 thin films. CdTe mass concentration relative to WO_3 is indicated on the spectra of the alloyed films.

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