Photoelectronic Properties of MoS_2/CdS Thin Film Heterojunction

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Abstract—We report the photoelectronic properties of MoS2/CdS heterojunction films fabricated via rapid chemical vapor deposition (CVD) and chemical bath deposition (CBD). Silver-doped MoS2 thin films were deposited on prepared indium tin oxide substrates via CVD, and then CdS films were prepared on the surfaces of the MoS2 thin films via CBD. The MoS2/CdS heterojunction has strong optical electronic properties. It shows an open-circuit voltage of 0.66 V and a short-circuit current density of 0.227 × 10-6 A/cm2 under illumination by a 100 mW light source, indicating that the device has good current–voltage (I–V) characteristics and pronounced photovoltaic behavior and can be used to fabricate high-quality heterojunction thin film solar cells.

Keywords-MoS2/CdS heterojunction film; optical absorption; I-V; photovoltaic effect

I. INTRODUCTION

Molybdenum disulfide (MoS2) has a hexagonal crystalline layered "sandwich" structure [1–3]. The special "sandwich" structure and narrow band gap give it unique optoelectronic properties that can be applied for lubrication, energy storage [4, 5], catalysis [6–8], and many other purposes [9, 10]. Similar to that of graphite, the layered structure has a weak van der Waals force and can be easily stripped to a single layer or a few layers [11–13]. Also similar to graphene, single-layer MoS2 has high electron mobility and can be used to fabricate optoelectronic devices. In fact, single- and multilayer MoS2 transistors have been proven to have a high current on/off ratio of ~105 and a carrier mobility of 80 cm2/Vs [14, 15]. Moreover, single-layer MoS2 has a large direct band gap, which enhances its optical absorption by 103–104 times compared to that of bulk MoS2, suggesting that MoS2 is suitable for photovoltaic solar cells [16, 17].

CdS has a large direct band gap of 2.5 eV and can often be used as an optical absorption and window material for solar cells. It is known that hexagonal CdS is better for use as the n-type window layer of solar cells owing to its high transmission and electrical conductivity. Some experiments suggest that CdS and MoS2 can form a p-n junction at the contact surface [18]. Therefore, we designed MoS2/CdS to form a heterojunction solar cell, where CdS acts as an n-type film, whereas MoS2 is doped with Ag to form a p-type film. The CdS film was prepared by chemical bath deposition (CBD), which is simple and low-cost, and easily produces large-area CdS thin films [20]. Then MoS2 films were deposited via chemical vapor deposition (CVD). We studied the structures, photoelectric features, and optoelectronic conversion efficiency of the MoS2/CdS films and heterojunction solar cells.

II. EXPERIMENTS

The MoS_2/CdS heterojunction solar cells were fabricated by initial deposition of a MoS_2 film on an indium tin oxide (ITO) transparent conductive glass substrate by CVD technology, on which a CdS film was prepared by CBD. First, the ITO conductive glass substrates were cleaned in acetone solution and then in anhydrous ethanol for 10 min each and then rinsed with deionized water. Finally, the ITO substrates were dried with flowing N_2. The CVD equipment consists of a quartz tube furnace, a vacuum system, an air inlet system, a temperature control system, and a water bath heating system. The ITO substrates were placed exactly at the center of the quartz tube furnace. Pure MoS_2 and pure $AgNO_3$ powders (1 g each) were mixed in a beaker, and 200 ml of diluted sulfuric acid (H_2SO_4) was added and stirred evenly. Then the solution was placed in a water bath heating box and heated to 70 °C. During the experiment, the tube furnace was evacuated to 10^{-2} Pa and heated to 550 °C. Ar gas with a flow rate of 20 sccm was initially introduced into the solution and carried the MoS_2 molecules and Ag ions into the tube furnace. The MoS_2 thin film was deposited for 10 min and then annealed at 600 ℃ for 20 min in an Ar atmosphere.

Next, CdS films were prepared on the surfaces of the MoS_2 films via CBD. Similarly, 0.007 mol cadmium acetate [$Cd(CH_3COO)_2$ $2H_2O$] and 0.05 mol thiourea (H_2NCSNH_2) were mixed, hydrolyzed, and heated to 80 ℃. The MoS_2 film substrates were drenched in a reaction tank for 60 min and cleaned in deionized water. To improve the characteristics of the MoS_2/CdS heterojunction solar cells, a saturated $CdCl_2$ methanol solution was coated on the surface of the CdS thin films and annealed at 400 °C for 30 min in the atmospheric environment.

Finally, Au electrodes were plated by magnetron sputtering on the surface of pre-existing MoS_2/CdS thin films. The structures and surface morphologies of the MoS_2 and CdS thin films were characterized by atomic force microscopy (AFM) and X-ray diffraction (XRD). The electrical properties were measured via total Hall effect measurement (HMS-3000). Furthermore, the photon response characteristics of the MoS_2/CdS heterojunction solar cells were assessed by a Keithley 4200 semiconductor characterization system.

III. RESULTS AND DISSCUSION

A. AFM images of the CdS and MoS_2 films

Fig .1 shows AFM images of the CdS and MoS_2 films on a quartz crystalline slide. The surface of the MoS_2 film shown in Fig .1(a) is continuous and compact, and some nanoparticles are present on the top layer, which can effectively promote light absorption. Additionally, many CdS quantum dots around 100 nm in diameter, as shown in Fig .1(b), are uniformly deposited on the surface of the MoS_2 film. Under the quantum dots, the MoS_2 film is homogeneous and continuous, with a uniform color and a thickness of about 10 nm, which is equal to a few layers of MoS_2. This growth mode, called the layer–quantum dot mode, corresponds to the hexagonal crystalline structure of MoS_2.

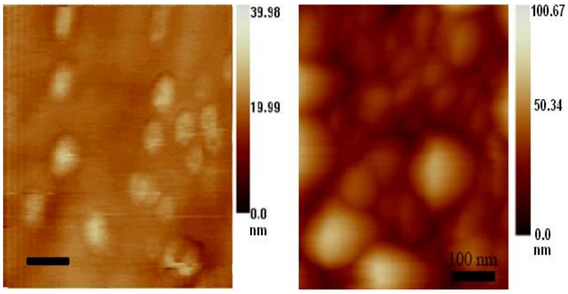

Figure 1. The AFM images of the and the CdS film on a quartz crystalline slide.

B. Crystalline structure of the MoS_2 and CdS film samples

The crystalline structure of the MoS_2 and CdS film samples were analyzed by XRD, as shown in Fig .2. The red line is the spectrum of the Ag-doped MoS_2

film, and the black line is that of the CdS film. Seven diffraction peaks located at 14.7°, 29.3°, 33.1°, 45.1°, 47.8°, 54.6°, and 56.4° are attributed to the (002), (004), (100), (104), (105), (106), and (110) crystal planes of MoS_2, respectively, which reveal various types of crystal structures. No diffraction peaks of silver are observed, indicating that the crystal structure of MoS_2 was not changed by the doped Ag ions. For the CdS film, the diffraction peak at 26.2° belongs to the (111) plane of the cubic phase; the other peaks, which appear at 24.8°, 28.2°, 43.7°, and 50.8°, correspond to the (100), (101), (110), and (112) diffraction planes of hexagonal CdS, respectively. In addition, these diffraction peaks are somewhat sharper, especially the (111) and (101) peaks, which reflects the high crystallinity of the CdS film.

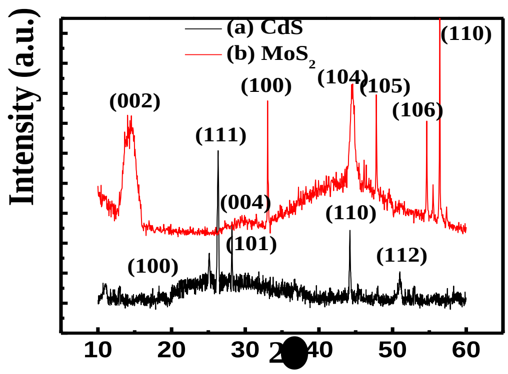

Figure 2. The XRD spectra of the MoS_2 and CdS films.

C. The surface I–V behavior of the MoS_2 and CdS films

The surface I–V behavior of the MoS2 and CdS films was measured by a Hall effect instrument

(HMS-3000), as shown in Fig .3(a) and Fig .3(b), respectively. The surface I–V behavior was measured at four points, a, b, c, and d, arranged in a square on the surface of the MoS2 and CdS films. The I–V

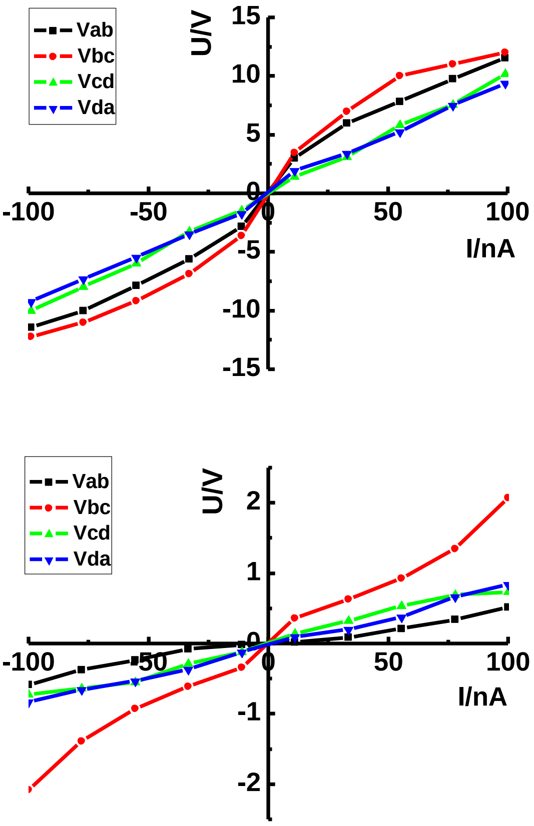

Figure 3. The surface I-V behaviors of the MoS_2 film (a) and of the CdS film (b) samples measured by the MS-3000 Hall effect instrument.

characteristics of the films between a and b, b and c, c and d, and d and a exhibit mostly linear relationships except for some small waves in the b–c curve in the CdS film resulting from the large size difference and boundaries between the particles in the film. The linear relationship shows that both the MoS2 and CdS films have good surface conductivity.

D. The optoelectronic characteristics of the MoS_2/CdS p-n junction solar cell

The optoelectronic characteristics of the MoS_2/CdS p-n junction solar cell were investigated in the dark and under illumination by a 100 mW light source. Fig .4(a) shows the *I–V* properties of the MoS_2/CdS p-n junction with Au electrodes on the MoS_2 film and the back side of the CdS film in the dark. The current passing through the junction increases exponentially under a positive

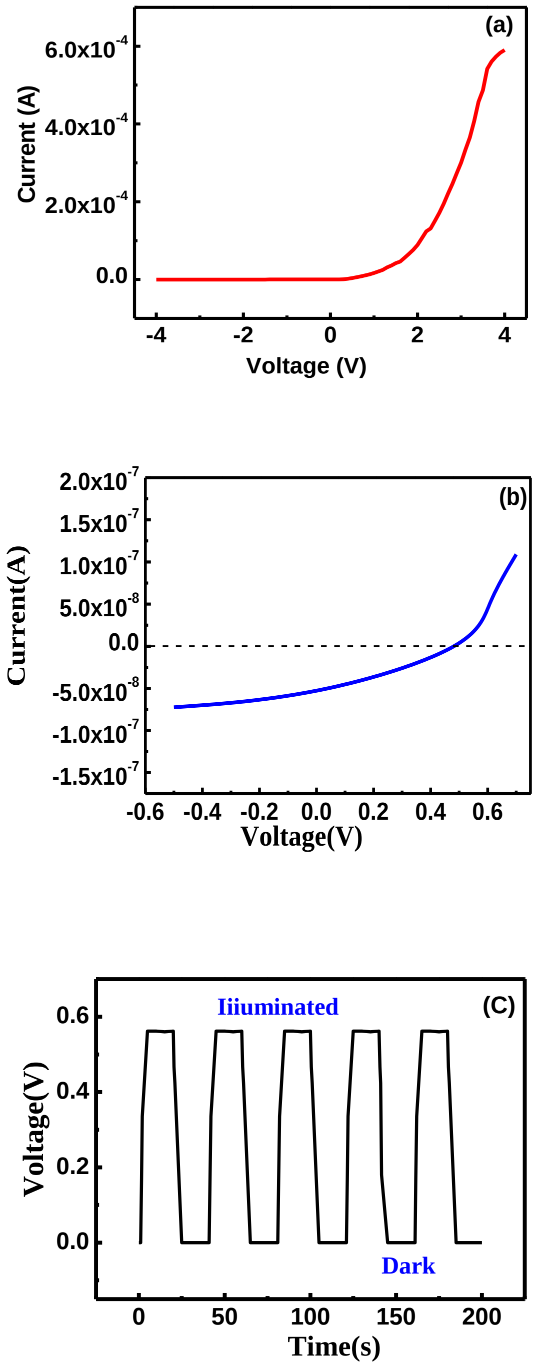

Figure 4. (a) The I-V behaviors of the MoS_2/CdS heterojunction illumination by 100 mW simulation light source.
(b) the I-V behaviors of the MoS_2/CdS heterojunction at dark case.
(c) the light response of the MoS_2/CdS heterojunction illuminated by 100 mW.voltage. It falls to zero when a reversed voltage is applied, suggesting that the p-n junction has good unilateral conductivity and rectification characteristics. Fig .4(b) shows the photocurrent characteristics of the MoS_2/CdS solar cell. We can see that the short-circuit current (I_{sc}) is approximately 7.5 × 10^{-8} A, and the open-circuit voltage (V_{oc}) is about 5.0 × 10^{-8} V. Fig .4(c) shows the light response properties of the MoS_2/CdS heterojunction solar cells with illumination and

darkness applied alternately in a 25 s cycle. For several cycles' measurement, the open-circuit voltage of the MoS_2/CdS heterojunction solar cells is about 0.6 V under illumination. The open-circuit voltage obviously rises and drops sharply. According to the data analysis, this result clearly proves the good repeatability and sensitivity to light of the MoS_2/CdS heterojunction solar cells.

IV. CONCLUSIONS

MoS_2/CdS heterojunction solar cells were fabricated using CVD and CBD processes. Both films have high-quality surface topography, crystallinity, and surface conductivity properties. Moreover, the heterojunction solar cell has a large short-circuit current (I_{sc}) of 0.227 × 10^{-6} A/cm^2 under illumination and an open-circuit voltage (V_{oc}) of 0.66 V. The results demonstrate that a MoS_2 film can be used to fabricate heterojunction solar cells. Optimization of the growing conditions is expected to further improve the performance of MoS_2/CdS heterojunction solar cells.

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