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# Magnetron sputtering fabrication and photoelectric properties of WSe<sub>2</sub> film solar cell device

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**ABSTRACT:** Tungsten diselenide (WSe<sub>2</sub>) films with different growing orientations exhibit diverse photoelectric properties. The WSe<sub>2</sub> film with C-axis  $\perp$  substrate texture has been prepared and applied to thin-film solar cells. W nanofilms with a thickness of 270 nm were deposited onto the Mo bottom electrode and then heat-treated in selenium vapor to synthesize WSe<sub>2</sub> films with a thickness of 1  $\mu$ m. ZnO films were deposited onto WSe<sub>2</sub> films to form a P-N junction and ITO films were deposited subsequently as the conductive layer. X-ray diffractometry, scanning electron microscopy and UV-VIS-NIR spectro-analysis instrument were employed to analyze the phase composition, optical absorptivity and micromorphology of WSe<sub>2</sub> films and the WSe<sub>2</sub> solar cell device. WSe<sub>2</sub> films exhibit excellent photoelectric performance with an optical absorption coefficient greater than  $10^5$  cm<sup>-1</sup> across the visible spectrum. The calculated direct and indirect band gap of the WSe<sub>2</sub> films is 1.48 eV and 1.25 eV, respectively. With the application of standard glass/Mo/WSe<sub>2</sub>/ZnO/ITO/Ag device structure, the open-circuit voltage of the battery device is 82 mV. The short-circuit current density is 2.98mA/cm<sup>2</sup> and the filling factor is 0.32. The photoelectric conversion efficiency of the WSe<sub>2</sub> film solar cell device is 0.79%.

**Key words:** tungsten diselenide, magnetron sputtering, solar cell device, layered structure, fabrication

## 1. Introduction

Compared with traditional silicon solar cells, thin-film solar cells have attracted great attention recently for their excellent features, such as low cost, relatively simple production process and high material utilization ratio [1]. However, the representative thin-film solar cells such as Cu(In,Ga)Se<sub>2</sub> and CdTe solar cells are either with complex composition or certain toxicity. So it is urgent and challenging to find an inexpensive and environmental-friendly absorption layer material with ordinary ingredients.

WSe<sub>2</sub> is a kind of transition metal dichalcogenides (TMDCs) with graphite-like layered microstructure [2]. W and Se only form one stable compound (WSe<sub>2</sub>) without any other stoichiometries [3]. So at room temperature, the crystalline structure of WSe<sub>2</sub> is highly stable, which makes the components of WSe<sub>2</sub> simple and controllable [4]. The band gap for WSe<sub>2</sub> lies between 1.16 and 1.54 eV, which is similar to the indirect band gap of visible light absorption [5]. WSe<sub>2</sub> films usually have two different kinds of growth texture (C-axis // substrate and C-axis  $\perp$  substrate) [6,7]. WSe<sub>2</sub> with C-axis // substrate texture can be employed in hydrogen evolution reaction, which has been studied in our former research [8], and the other can be used as the absorption layer of solar cells. The surface of WSe<sub>2</sub> crystal with C-axis  $\perp$  substrate texture is composed of selenium atomic layers without dangling bonds, which provides the potential for a non-surface-state heterojunction with highly mismatched lattice [9]. So WSe<sub>2</sub> is perfect to be used as the optical absorption layer of solar cells for its simple components and excellent photoelectric performance.

The existing synthetic methods of WSe<sub>2</sub> films include soft selenization [10], pulsed-laser deposition [11], chemical vapor deposition [12], electro-deposition [13], selenium-oxygen ion exchange [14], etc. A kind of environmental-friendly method should be favored for further development. Also, the application of WSe<sub>2</sub> films in thin-film solar cells is still a great challenge. Herein we present a WSe<sub>2</sub> solar cell device on the basis of the preparation methods of WSe<sub>2</sub> films reported before in our research group [15,16]. WSe<sub>2</sub> films with C-axis  $\perp$  substrate texture have been successfully synthesized and applied to thin-film solar cells.

## 2. Experimental

**Device Fabrication.** W films were DC-sputtered (direct-current) on molybdenum/glass substrates (20 mm $\times$ 15 mm $\times$ 4 mm) in an Ar (99.999%) atmosphere. The substrates were thoroughly cleaned employing a standard procedure, which included 15 min ultrasonic cleaning with the substrates immersed into acetone and ethanol respectively. The substrates were dried with Nitrogen (99.999%) prior to insertion into the sputtering system (JGP-450, Sky Technology Development). The deposition chamber was pumped down to a background pressure of  $5.0 \times 10^{-4}$  Pa and then washed with Ar (99.999%) for several times in order to reduce the oxygen content in the chamber. The substrates were fixed onto a rotating holder to ensure the homogeneity of the films. The distance between the substrate and W target (ZhongNuo Advanced Material Technology Co.,Ltd) was 153 mm. The W target was pre-sputtered for 5 min in order to remove the impurities on the surface. The specific deposition parameters for W films prepared on Mo/glass substrates are displayed in Table 1.

After that, the W films were exposed to selenium vapor to form WSe<sub>2</sub> films in a sliding tube furnace (Hefei Ke Jing Materials Technology Co., Ltd). The tube furnace was pumped down to a background pressure of 0.7 Pa and filled with N<sub>2</sub> (99.999%). This process was repeated for three times in order to remove the oxygen in the tube completely. 0.7 grams of selenium powder (bought from Aladdin) was put on one side of the tube and the heating system was on the other side. The furnace was pushed to the direction of W films and selenium powder when the temperature rose up to 600  $\square$  and was pushed away after 10 min of reaction.

ZnO films were deposited on WSe<sub>2</sub> films by radio-frequency (RF) magnetron sputtering in Ar (99.999%) atmosphere. Subsequently, ITO (indium tin oxide) films were DC-sputtered on the ZnO films. The experimental operation of sputtering ZnO films and ITO films was similar to that of W films. The distance between the substrates and the ZnO and ITO targets (ZhongNuo Advanced Material Technology Co., Ltd) were 75 mm and 153mm, respectively. ZnO and ITO films were both deposited after breaking the vacuum because the sputtering targets in the chamber had to be changed. WSe<sub>2</sub>, ZnO and ITO are all stable and the problem of oxidation does not exist. The specific deposition parameters for ZnO and ITO films are shown in Table 1. Finally, the surface of the device was evenly

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