Solar Energy 159 (2018) 88–96

Contents lists available at ScienceDirect

Solar Energy

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

Effect of growth temperature on large surface area, ultrathin MoS_2 nanofilms fabrication and photovoltaic efficiency

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ARTICLE INFO

Keywords:
Two-dimensional transition metal dichalcogenides
Molybdenum disulfide nanofilms
Growth temperature
Schottky junction solar cells

ABSTRACT

Monolayer and few-layer two-dimensional (2-D) transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS_2) demonstrate excellent semiconducting and optical properties that have made them promising candidates for optoelectronic applications. However, fabricating high-quality and highly uniform MoS_2 nanofilms on a large surface area remains a challenge. In this study, an effective synthesis method for large surface area of 2 cm by 2 cm, ultrathin MoS_2 nanofilms using direct sulfurization of annealed molybdenum (Mo) foil was tested. Because of the unique band structure, the MoS_2 layer not only serves as a carrier transport layer but also as an effective blocking layer for the diffusion of photo-generated holes. By optimizing the structural characteristics of MoS_2 nanofilms, a dramatic increase in photovoltaic performance was measured as high as 11.2% in the novel graphene/MoS_2/n-Si (G/MoS_2/n-Si) Schottky junction solar cells. Our approach offers guidance to the synthesis of large surface area, ultrathin MoS_2 nanofilms and furthers their appeal for use in highly efficient solar cell technologies.

1. Introduction

The unique physical properties of carbon-based allotropic graphene have piqued a recent interest in the field of optoelectonics. Graphene-based transparent conductive electrodes have been widely utilized in optoelectronic devices because of this materials high electrical conductivity, optical transmittance and excellent physical stability (Feng et al., 2011; Miao et al., 2012; Wu et al., 2013; Cruz et al., 2012; Phan et al., 2012; Vakili et al., 2016; Li et al., 2014; Ramachandran et al., 2015). However, extensive research has gone into increasing the sub-optimal light harvesting performance of graphene-based solar cells (Fang et al., 2014). The graphene/crystal silicon (G/Si) Schottky junction solar cells have been found to have light harvesting potential, decent power conversion efficiency (PCE) and an advantageous low input cost (Lee et al., 2008; Kim et al., 2009; Diao et al., 2017). Graphene-derived solar cells were initially studied in 2011 by Zhu et al., where graphene served as a transparent electrode for introducing an electric field near the interface of the graphene/n-type silicon (G/n-Si) to collect photo-generated carriers. This G/n-Si Schottky junction based solar cell reached an initial photovoltaic efficiency of 1.5% (Li et al., 2010). A variety of methods have been explored to further increase the light harvesting efficiency of G/Si solar cells. This includes chemical doping, a graphene modification resulting in reduced graphene sheet resistance (Shi et al., 2010; Fan et al., 2011). Graphene/*n*-silicon solar cells exhibited a 10% PCE for chemically doped graphene. The PCE further increases to 12.4% with oxide thickness of 15 Å, and to 15.6% after applying an antireflective coating (Wang et al., 2014; Song et al., 2015; Bonaccorso et al., 2015; Singh et al., 2017). Additionally, the development of the crystalline silicon (c-Si) solar cell has also increased the light-to-electric PCE via surface oxidation control (Shi et al., 2010). Despite the attempts at increasing the efficiency of the G/n-Si Schottky junction solar cells, its efficiency has remained lower than that of the conventional c-Si solar cells. This limitation has shown to be due to bandgap defects and the relatively low carrier mobility of graphene on c-Si (Yavuz et al., 2016; Kuang et al., 2015). Furthermore, the G/n-Si interface recombination results in low built-in potential due to the low G/n-Si Schottky barrier height that consequently decreases the open circuit voltage (Ding et al., 2017).

Optoelectronic applications of graphene may be limited considering the zero band gap in monolayer graphene that is needed as a charge carrier to conduct electric currents (Umrao et al., 2017; Singh and Nalwa, 2015; Castellanos-Gomez et al., 2012). Our aim in this study was to further improve the performance of the graphene-based solar cells using transition metal dichalcogenides (TMDs). These TMD

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http://dx.doi.org/10.1016/j.solener.2017.10.048
Received 4 September 2017; Received in revised form 3 October 2017; Accepted 12 October 2017

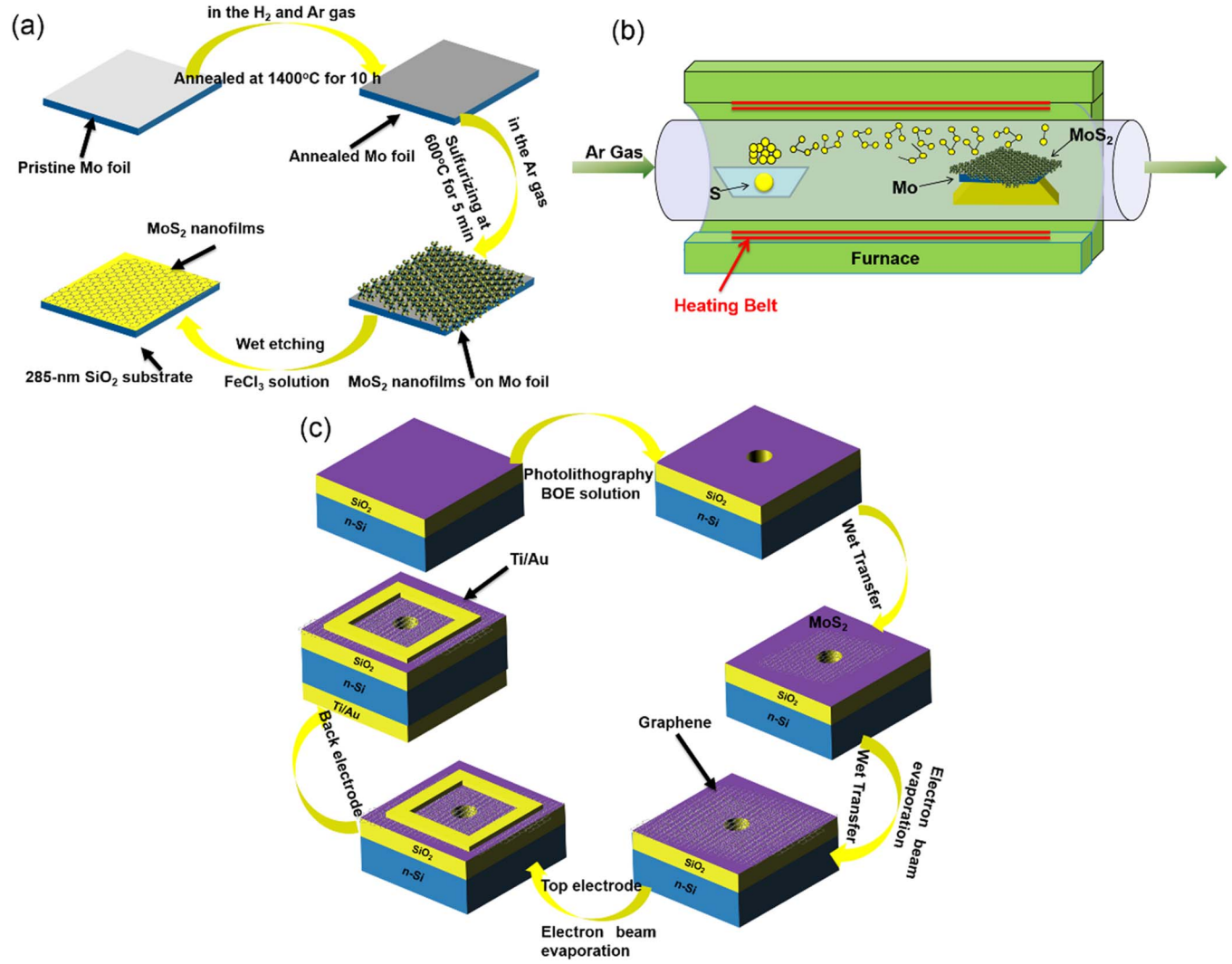

Fig. 1. (a) Flowchart depicting the Mo foil transference and the subsequent MoS_2 nanofilm fabrication; (b) Schematic illustration the MoS_2 nanofilm synthesis; (c) Flowchart of the fabrication process of the graphene/MoS_2/n-Si solar cells.

materials have a layered structure (Kumar et al., 2015) and can have metallic, semiconducting or superconducting properties (Deokar et al., 2017). Compared to graphene, TMDs such as MoS_2 have outstanding photoelectrical properties and offer the option of band gap engineering (Ponraj et al., 2016; Xu et al., 2017; Butler et al., 2013; Kim et al., 2016; Hsiao et al., 2017). For instance, MoS_2 can compensate for the band gap deficiency of graphene. It has been shown that a MoS_2-based band gaps can be engineered to as high as 1.8 eV in a monolayer and as high as 1.2 eV in bulk layer MoS_2 with direct-to-indirect band gap variation (Radisavljevic et al., 2011; Choi et al., 2014). In addition, strong light-matter coupling and band nesting have been demonstrated using MoS_2, allowing for the development of extremely flexible photovoltaic devices (Li et al., 2015; Bonaccorso et al., 2015; Britnell et al., 2013; Li et al., 2015). The MoS_2 layer functions as an effective passivation and electron-blocking layer in the G/MoS_2/n-Si solar cells (Tsuboi et al., 2015). Currently, two-source chemical vapor deposition (CVD) methods and mechanical exfoliation are widely utilized for MoS_2 synthesis via various substrates (Singh et al., 2017), including sulfurizing MoO_3 at high temperatures (Lee et al., 2012; Najmaei et al., 2013). These methods are not only difficult to control, but also result in triangular islands, random MoS_2 domain orientations, and skewed scale MoS_2 films (van der Zande et al., 2013). Thus, fabricating high-quality, uniform MoS_2 nanofilms with a large surface area is essential to improve solar cell performance.

In this study, the CVD method was employed to fabricate large surface area of 2 cm by 2 cm, ultrathin MoS_2 nanofilms by sulfurizing annealed Mo foils. We investigated the structural characteristics and the effect of growth temperature on MoS_2 nanofilms. Additionally, we analyzed the Mo foil annealing process and confirmed that our method enabled the production of uniform and continuous MoS_2 nanofilms. To demonstrate the crystalline structure of the MoS_2 nanofilms, we created G/MoS_2/n-Si solar cells. The photovoltaic (*PV*) properties of the G/MoS_2/n-Si solar cells exhibited a dramatic performance enhancement in comparison with G/n-Si Schottky junction solar cells. A high PCE of 11.2% was recorded from the G/MoS_2/n-Si solar cells after optimizing the MoS_2 nanofilms, demonstrating the considerable potential application of TMCs in improving the PCE of the G/n-Si Schottky junction solar cells.

2. Experimental methods

2.1. One-source CVD method for fabricating MoS_2 nanofilms

A 3 cm × 3 cm Mo foil (25 μm, Alfa, 99.95%) was treated with ethanol, acetone, IPA, then deionized water for 5 min. The Mo foil was then dried using a nitrogen gas gun and annealed at 1400 °C for 10 h under a 150 sccm argon (Ar) and 50 sccm hydrogen (H_2) atmosphere inducing recrystallization. Large surface area MoS_2 nanofilms were fabricated using the CVD process at atmospheric pressure and room