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Article

Study of MoS₂ Deposited by ALD on c-Si, Towards the Development of MoS₂/c-Si Heterojunction Photovoltaics

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Abstract: Silicon-based heterojunction (SHJ) solar cells demonstrate high efficiencies over their homojunction counterparts, revealing the potential of such technologies. We present here the first steps towards the development of molybdenum disulfide (MoS₂)/c-silicon heterojunction solar cells, consisting of a preliminary study of the MoS₂ material and numerical device simulations of MoS₂/Si heterojunction solar cells, using SILVACO ATLAS. Through the optical and structural characterization of MoS₂/SiO₂/Si samples, we found a significant sensitivity of the MoS₂ to ambient oxidation. Optical ellipsometry showed a bandgap of 1.87 eV for a 7 monolayer thick MoS₂ sample, suitable for the targeted application. Finally, we briefly introduce a device simulation and show that the MoS₂/Si heterojunction could lead to a gain in quantum efficiency, especially in the region with short wavelengths, compared with a standard a-Si/c-Si solar cell.



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Keywords: 2D molybdenum disulfide; silicon heterojunctions; solar cells

1. Introduction

Among single-junction solar cells, gallium arsenide (GaAs) solar cells present the highest efficiencies, reaching up to 29.1% [1]. However, due to their high cost, their use is restricted to space applications. Thus, silicon technology is the most widespread, since it benefits from relatively low costs and high efficiencies. Particularly, the HIT (heterojunction with intrinsic thin layer) is the silicon technology exhibiting the highest efficiencies of about 26.7%, without concentration [1].

The principle of a heterojunction solar cells lies in a low surface recombination velocity through the separation of the crystalline (c-Si) absorber (<100 μm) from the highly recombination active metal contacts by a passivating and wide-bandgap emitter “buffer” layer. That buffer layer should be as “transparent” as possible to the majority carriers’ flow while reflecting that of the minority carriers and, therefore, should act as a selective contact for carrier extraction [2,3]. It is usually made of an hydrogenated amorphous a-Si:H layer, which displays a 1.7 eV quasi-bandgap, as compared to the smaller 1.1 eV bandgap of the c-Si, which leads to appropriate band offsets in both the conduction and valence bands, therefore giving the required barrier for minority charge carriers [4,5]. However, a-Si:H is a low conductivity material and displays a high recombination rate of electron–holes pairs. Moreover, the absorption coefficient of a-Si:H is large and leads to high optical losses, limiting the conversion of light at short wavelengths. Therefore, to overcome these limitations, a wider bandgap semiconductor could be a promising material to replace the a-Si:H.

Molybdenum disulfide (MoS₂) is a material that could meet such requirements for heterojunction solar cells with silicon, it can display a wider bandgap (up to 2.34 eV) than a-Si:H and a suitable electronic band line-up with the p-doped Si absorber [6]. It is a layered transition metal dichalcogenide (TMD), which is a material with an MX₂ structure, where

M is a transition metal and X is a chalcogen. Molybdenum disulfide is one of the most used TMDs, probably due to the natural abundance of Mo in the Earth's crust [7]. The bulk form of layered TMDs is made of a stack of 2D single(mono)-layers (ML), held together by weak Van der Waals bonds. For MoS₂, the monolayer is a stack of the S-Mo-S form, with a plane of Mo sandwiched between two planes of sulfur. Due to this structure, which consists of stacked monolayers, layered TMDs can be easily exfoliated to obtain 2D materials, and this gives rise to exceptional properties. For instance, due to the quantum confinement effect, the bandgap nature changes and goes from an indirect type for bulk MoS₂ to a direct bandgap for monolayer MoS₂ [8]. The bandgap value also increases with decreasing thickness, and while bulk MoS₂ has an indirect bandgap of 1.29 eV, the monolayer MoS₂ has a direct bandgap of 1.89 eV [8–11]. MoS₂ has three known polytypes, i.e., 1T-MoS₂, 2H-MoS₂, and 3R-MoS₂. 2H-MoS₂, the most common and stable form of MoS₂, has a hexagonal structure and has been found to be naturally a n-type semiconductor [12,13].

In 2013, Tsai and al. [6] demonstrated a power conversion efficiency (PCE) of 5.23% with a n-MoS₂ monolayer/p-Si heterojunction solar cell, which is to date, the best PCE for solar cells using monolayer TMD. Later, in 2019, Xu et al. [14] reduced the concentration of interface defects, observing a passivating effect of monolayer MoS₂ in a ITO/p-Si/Ag solar cell structure. The power conversion efficiency (PCE) was increased from 1.1% to 4.6% with the ITO/n-MoS₂/p-Si/Ag structure. Recently, Huang et al. [15] demonstrated 9.81% efficiency using thiourea doped few-layer MoS₂/Si heterojunction solar cells.

Regarding those interesting results, we present the optical and structural characterization of thin MoS₂ layers deposited on silicon dioxide/silicon substrates as a preliminary study to developing MoS₂/Si heterojunction solar cells. We also simulate an MoS₂/Si heterojunction solar cell device, using SILVACO ATLAS, showing the potentialities of such devices.

2. Materials and Methods

Chemical vapor deposition (CVD) of MoS₂ was performed employing Mo(CO)₆ (99.99%) (Versum Materials) and 1% H₂S (99.999%) in Ar (Air Products) utilizing a commercial 300 mm atomic layer deposition reactor modified with a showerhead inlet system. The reactor temperature was set at 550 °C, and the chamber pressure was maintained at ~2.2 Torr by an N₂ carrier flow of 150 standard cubic centimeters per minute (sccm). Precursor flux of the Mo source was determined by the source temperature (28 °C), and the H₂S flow was set at 10 sccm of the 1% gas mix. Growth was achieved on a selection of substrates including SiO₂ (80 nm) on HR Si and c-plane sapphire. Reproducibility and uniformity of the CVD process was found to be excellent, with a growth rate of approximately 4 nm/hour (~6 monolayer per hour). Nominal thicknesses of MoS₂ were achieved by assuming that the estimated growth rate was linear and by adjusting the growth time. Two-dimensional MoS₂ film samples with nominal thicknesses of 4, 5, and 7 monolayers (ML) were subsequently deposited on 80 nm SiO₂/Si substrates and 7 ML MoS₂ was deposited on a sapphire (Al₂O₃) transparent substrate.

Optical ellipsometry (O.E) measurements were performed on the 2D MoS₂ samples deposited on SiO₂/Si substrates at 70-degree angles of incidence using a Woollam M2000 Ellipsometer. The optical model used for spectroscopic ellipsometry analysis was MoS₂/SiO₂/Si using the CompleatEase software developed by Woollam.

UV-VIS-NIR normal incidence transmittance measurements were performed on the 7 ML MoS₂ deposited on sapphire using a Perkin Elmer Lambda 950 double-beam spectrophotometer.

Raman spectra were recorded using a Renishaw Invia Reflex micro-Raman spectrometer at room temperature. The Raman mapping was collected on several sites (50 nm × 50 nm, 1 nm step). The samples were excited using a CW Modu-Laser Stellar-REN laser emitting at 514.5 nm with a power of less than 0.4 mW. The reflecting microscope objective was 50× with NA = 0.75, and the excitation spot had a diameter of 1 μm. The back-scattered light was dispersed by a monochromator with a spectral resolution of 1.4 cm⁻¹, with the light being

detected by a charge-coupled device. The typical accumulation time was 20 s. Raman shifts were calibrated using the optical phonon frequency (520.5 cm^{-1}) of the silicon monocrystal. Surface roughness was also explored through Atomic Force Microscopy (AFM), using a Bruker Innova microscope in contact mode.

Chemical composition was confirmed through X-ray photoelectron spectroscopy (XPS) performed in a vacuum chamber with a non-monochromatized Mg $K\alpha_{1,2} = 1253.6\text{ eV}$ ray.

X-ray diffraction (XRD) measurements were performed using a 5-circles Smartlab Rigaku diffractometer with Cu $K\alpha_{1,2}$ radiation ($\lambda = 0.154184\text{ nm}$) and equipped with a HyPix-3000 detector.

Simulations were performed with the SILVACO ATLAS module, software from the TCAD (Technology Computed Aided Device) family, to solve the main semiconductor equations. Here, the Poisson's equation, continuity, and drift-diffusion models are used. Simulations of an-MoS₂/Si heterojunction solar cell device have also been performed to estimate the external quantum efficiency.

3. Results and Discussion

Raman spectroscopy results are shown in Figure 1. For all samples, in the A_{1g} and E_{2g} vibration modes, the distance between two modes have been found to be 24.3 cm^{-1} , 24.78 cm^{-1} and 24.8 cm^{-1} , respectively, for 4, 5, and 7 ML. Similarly, many studies have shown that the distance between the E_{2g} and A_{1g} Raman modes is reduced when the thickness of MoS₂ is reduced [16].

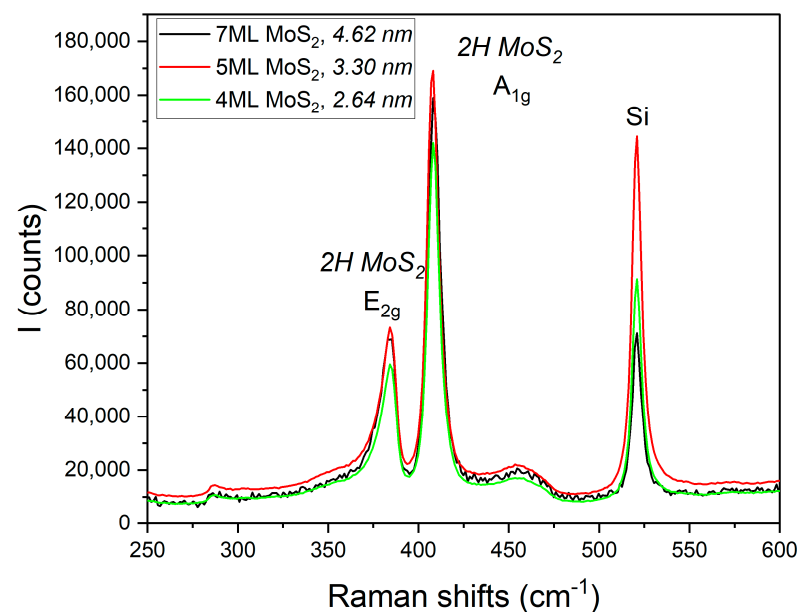


Figure 1. Raman spectra of the three samples with 4, 5, and 7 ML MoS₂.

Performing atomic force microscopy (Figures 2–4), we observe roughness in the region of 2 nm for all of the samples, which is significant relative to the thicknesses of the MoS₂ layers, which measure only a few nanometers. The AFM images also show outgrowths (yellow dots on the images), with some of them reaching about 10 nm. These outgrowths are representative of SO₂ outgassing that occur typically at MoS₂ defects and grain boundaries after prolonged exposure to air via the action of humidity to form MoS₂ MoO_{3-x}, as observed in the XPS results detailed in the next section.

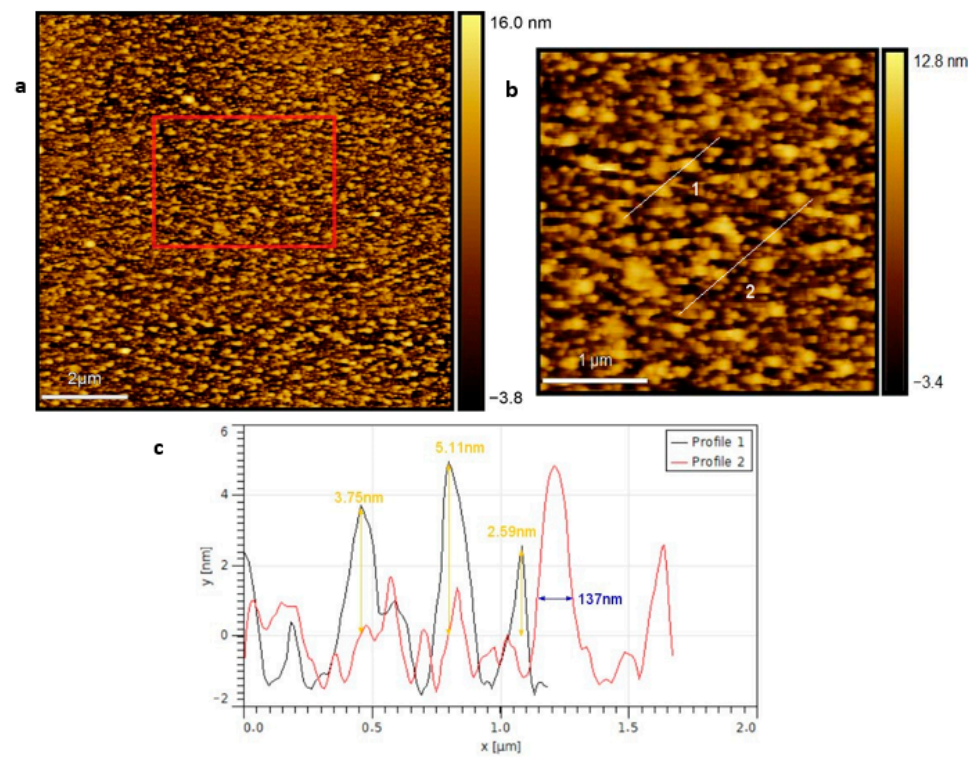


Figure 2. AFM images of 4 ML MoS₂: (a) 10 × 10 μm scan. (b) Magnified region from red box in (a). (c) Height profiles of magnified regions along lines 1 and 2 from (b).

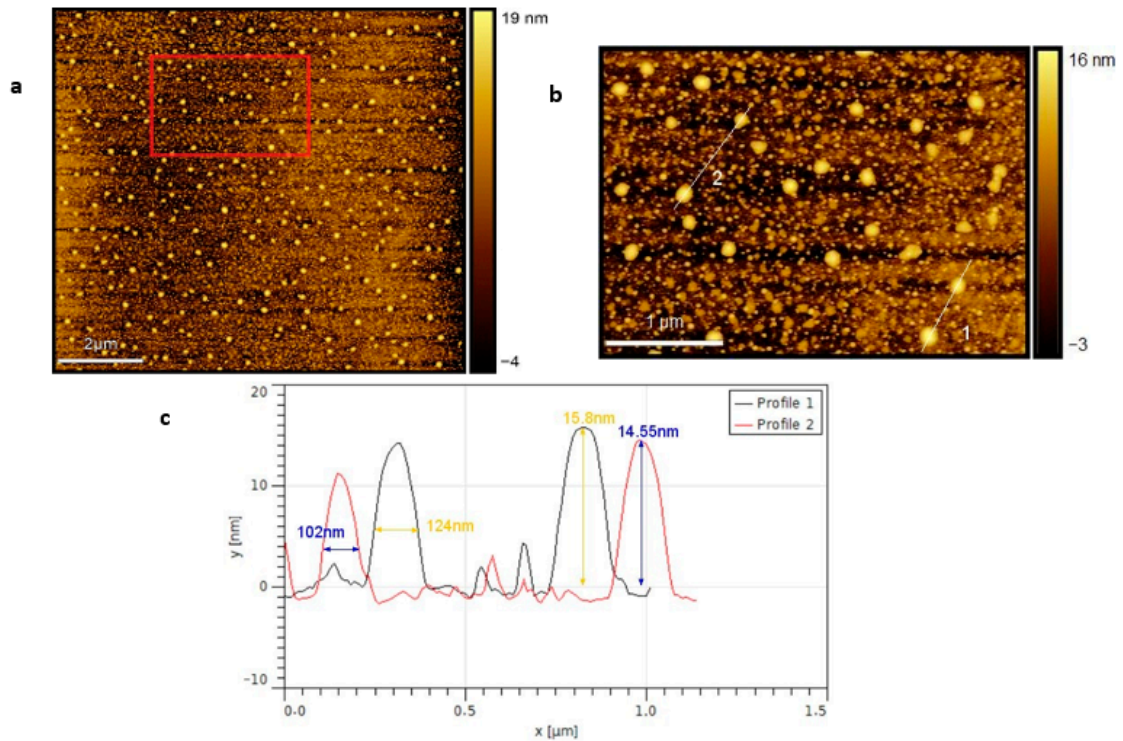


Figure 3. AFM images of 5 ML MoS₂: (a) 10 × 10 μm scan. (b) Magnified region from red box in (a). (c) Height profiles of magnified regions along lines 1 and 2 from (b).

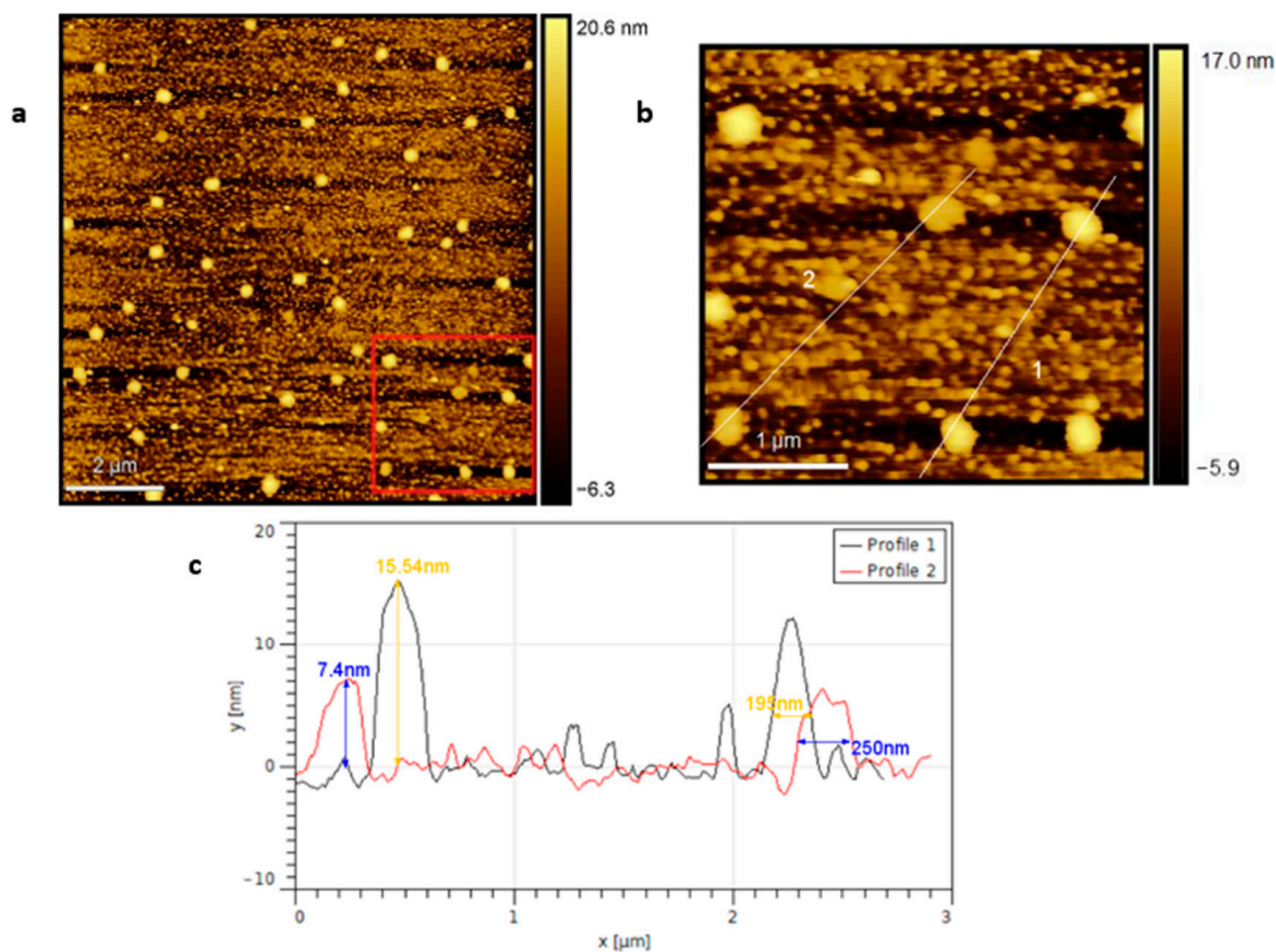


Figure 4. AFM images on 7 ML MoS₂: (a) 10 × 10 μm scan. (b) Magnified region from red box in (a). (c) Height profiles of magnified regions along lines 1 and 2 from (b).

We observe the core level of molybdenum 3d, through XPS measurements that reveal the presence of different oxidation states of molybdenum in the films (Figure 5). The peak at binding energy $E_b = 232.2$ eV is assigned to the Mo 3d_{3/2} core levels. The second peak at $E_b = 229.25$ corresponds to the Mo 3d_{5/2} core levels. The two peaks are consistent with the Mo⁴⁺ oxidation state of 2H-MoS₂, which corresponds to stoichiometric MoS₂. The Mo⁶⁺ (usually attributed to MoO₃)/Mo⁵⁺ oxidation states at $E_b = 235.5$ eV and $E_b = 232.15$ eV appear near the Mo⁴⁺ oxidation states. That would suppose that not only pure MoS₂ but also its oxidation products are present in the films. A similar phenomenon has already been described and explained in the literature [17–19]. The higher oxidation states being a consequence of exposure of MoS₂ to ambient air, such as oxidation, occurs preferentially at grain boundaries and in the defects of MoS₂, before extending throughout the film. Afanasev et al. [18] showed that MoS₂ is affected by ambient air, only after 10 min of exposure, after synthesis. The misfit between MoO₃ and MoS₂ lattices can subsequently lead to the formation of cracks [19] and outgrowths, which correspond to the AFM observations in this work. The ratio between Mo⁶⁺ oxidation states and the total signal of Mo 3d core levels is estimated to be about 8.1%, 12.8%, and 7.2%, respectively for 4, 5, and 7 ML MoS₂ films.

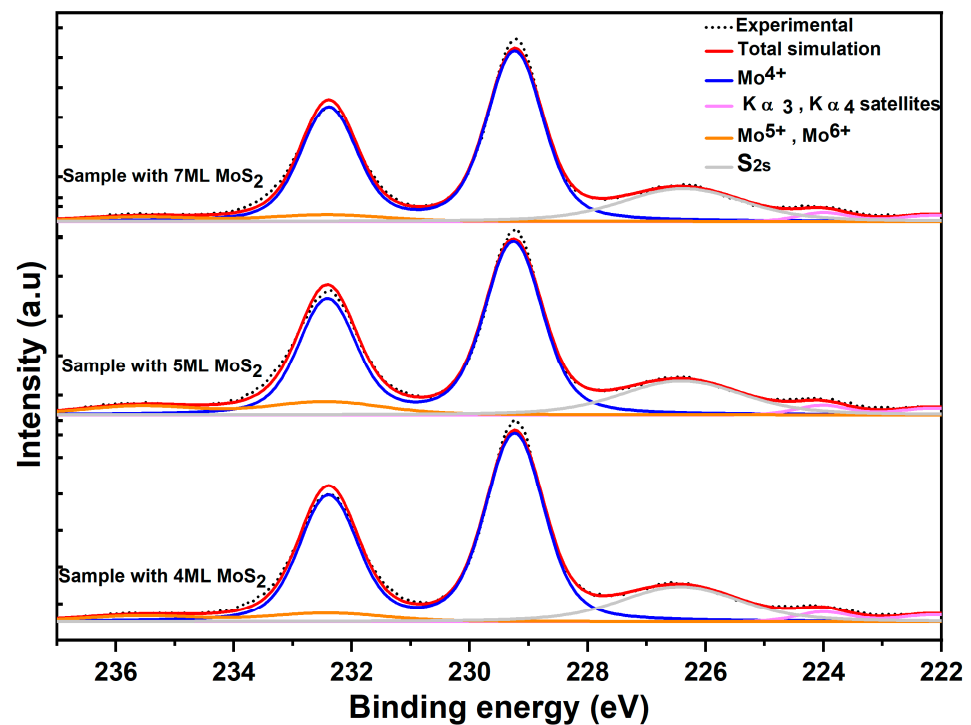


Figure 5. X-ray photoelectron spectroscopy (XPS) performed on samples with 4 ML, 5 ML and 7 ML MoS₂. The MoS₂ 3d core levels are shown.

The results of the XRD (Figure 6) $\theta/2\theta$ longitudinal scans reveal a very strong texture of the MoS₂, with a preferential orientation along the (002) planes of hexagonal MoS₂ (2H-MoS₂). That denotes a well-stacked layered structure [20]. The full width at half maximum (FWHM) values are, respectively, 4.7°, 5.1°, and 2.4° at the 2θ scale for 4, 5, and 7 ML. The (002) reflections occur at 2θ and are equal to 13.096°, 13.002°, and 13.812°, respectively, for 4, 5, and 7 ML. Pristine 2H-MoS₂ is expected to give (002) reflections at $2\theta = 14.4^\circ$ (interlayer spacing $d_{hkl} = 0.614$ nm) [21], showing larger interlayer spacing in our case (Table 1). Moreover, using the diffraction peak FWHM β and the 2θ positions, the crystallite sizes, D , are inferred through Scherrer's equation (Equation (1)) as follows:

$$D = \frac{K\lambda}{\beta \cos \theta} \quad (1)$$

where $K = 0.9$ is the crystallite shape factor and $\lambda = 0.154184$ nm. The crystallite sizes are about a few nanometers, which is consistent with the thickness of the films.

Table 1. X-ray diffraction results on MoS₂ layers.

Film	2θ (°)	Inter-Reticular Spacing d (nm)	Crystallite Size (nm)
4 ML	13.096	0.676	1.7
5 ML	13.002	0.68	1.7
7 ML	13.812	0.641	3.34

However, the crystallites sizes are smaller than the film thicknesses for all samples, indicating that the deposited MoS₂ contain some structural defects that limit the size of the coherent domain of diffraction along the growth axis.

Since the optical properties of the MoS₂ layer are critical for the performance of the solar cell, we have measured the optical transmission of 7 ML MoS₂ (Figure 7) deposited on blank sapphire (Al₂O₃). From the transmission curve, we identify two absorption edges.

The first one is located at 611 nm, corresponding to an energy of 2.03 eV (B exciton), and the second absorption edge is located at 1.87 eV (A exciton).

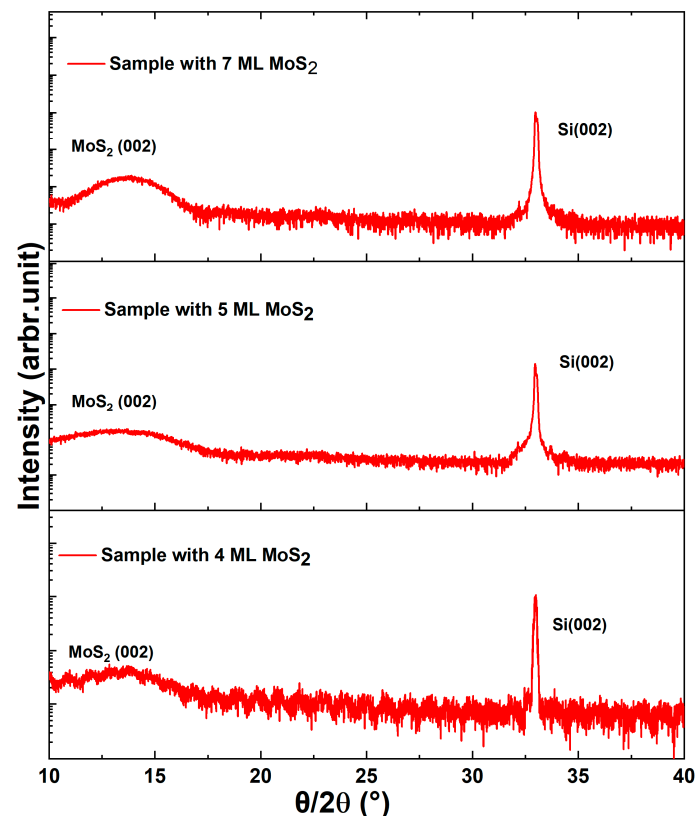


Figure 6. X-ray diffraction on MoS₂/SiO₂/Si samples.

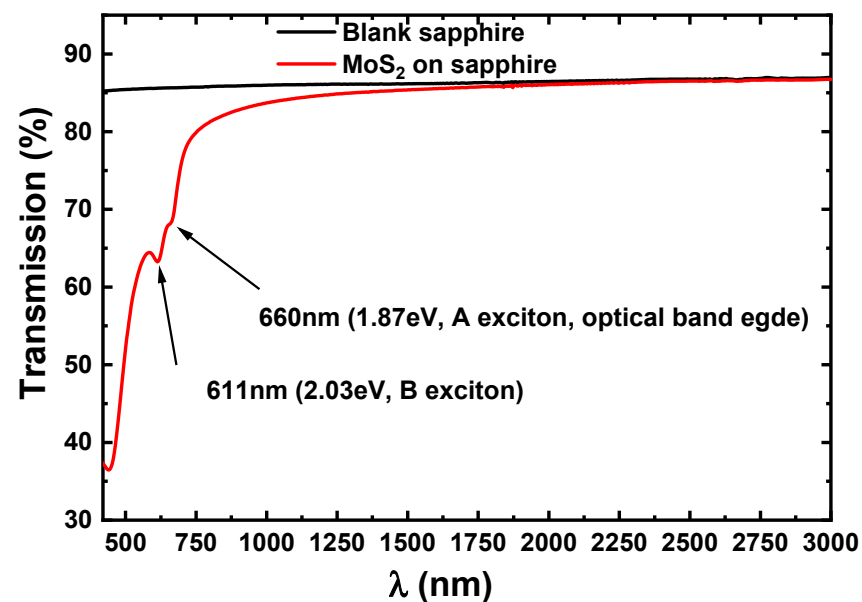


Figure 7. Transmission of 7 ML MoS₂ deposited on sapphire.

These two excitons have already been reported in the literature for very thin to monolayer MoS₂ [8,10,22,23]. The A exciton corresponds to the optical bandgap of MoS₂. In addition to confirming the high bandgap character of MoS₂, the transmission curve

shows that MoS₂ would transmit most of the incoming light to the silicon substrate, even for a 7 ML-thick MoS₂.

The optical constants deduced from O.E. are implemented in device simulation. Most details about the implemented parameters are given in Table 2.

The simulated device architectures are kept basic since the aim of the present study is to show a proof-of-concept. For both n-MoS₂/p-Si and n-Si/p-Si solar cells, we assume perfect ohmic contacts. We also assume a standard AM1.5G incident light beam. Neither Intraband tunnelling nor trap-assisted tunnelling transport was taken into account. An interface recombination velocity $S_q = 1.10^3$ cm/s is also introduced between the MoS₂ emitter and the Si absorber [24], and other parameters used for the calculation are given in Table 2.

We present the simulated device in Figure 8 and band alignments between n-MoS₂ and p-Si in Figure 9. The band alignments are shown under dark (no illumination in simulated conditions) and under light (AM 1.5 illumination). E_c is the energy level of the conduction band and E_v the energy level of the valence band. The Fermi level is referred to as E_F , in dark condition. Under illumination, the Fermi energy level splits with one for holes and one for electrons, referred to as hole quasi-fermi level (Hole QFL) and electron quasi-fermi level (Electron QFL), respectively. As one can see, the simulation shows that a type 2 heterojunction is obtained, which is favorable to carrier separation. Tsai et al. [6] have experimentally demonstrated such an heterojunction type between monolayer MoS₂ and Si.

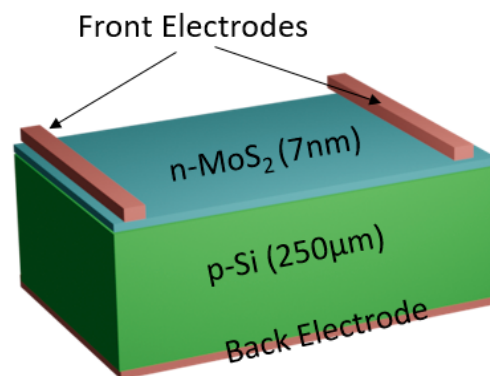


Figure 8. Simulated n-MoS₂/Si heterojunction solar cell.

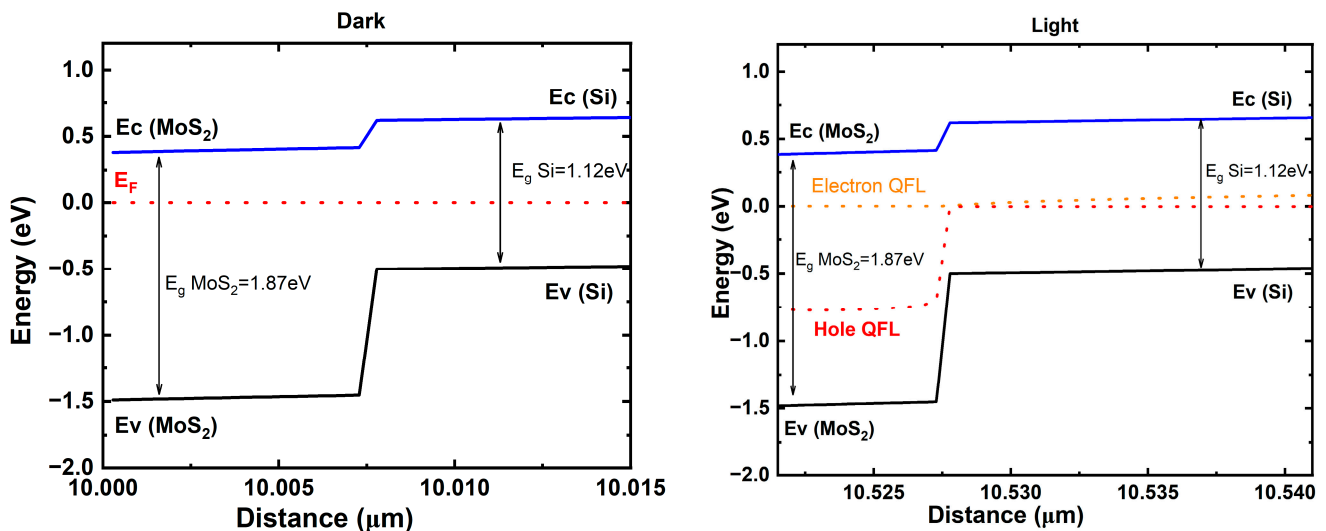


Figure 9. Simulated band diagram of MoS₂/Si heterojunction solar cell in the vicinity of the MoS₂/Si interface (dark and AM 1.5 light illumination, 0 Volt bias).

Figure 10 shows the results of the simulated external quantum efficiency (EQE) of MoS₂/Si solar cell. The EQE gives the number of carriers that is effectively collected over the number of incident photons, assuming that each photon produces one carrier. In Silvaco software, we calculate EQE as follows:

$$\text{EQE} = \frac{I_{\text{electrode}}}{I_s} \quad (2)$$

where $I_{\text{electrode}}$ is the current collected at the electrode and I_s is the source photocurrent given as follows:

$$I_s = q \frac{B\lambda}{hc} W \quad (3)$$

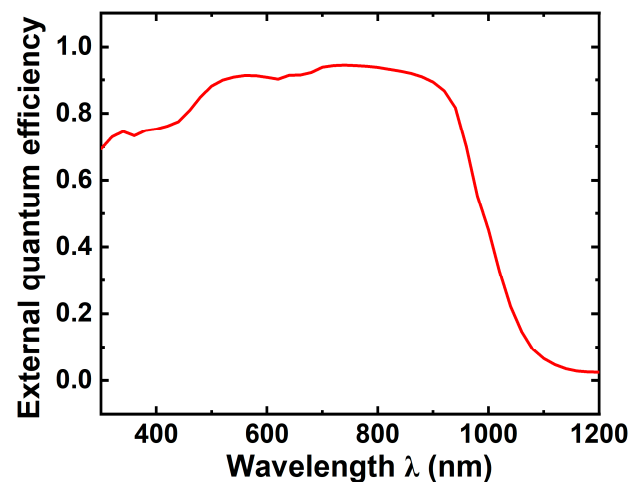


Figure 10. Simulated external quantum efficiency of MoS₂/Si heterojunction solar cell.

With B as the incident beam intensity, λ as the wavelength, h as the Planck constant, c as the speed of light in a vacuum, and W as the beam width that could be defined as the rate of incident photons on the device in terms of current density.

In the short-wavelength region, the MoS₂/Si heterojunction appears to lead to a gain in EQE, as compared with standard devices [4,25]. We attribute that gain to the high bandgap of MoS₂, which limits parasitic absorption.

Table 2. Simulation parameters of n-MoS₂/p-Si heterojunction solar cell.

Material	p-Si	n-MoS ₂
Thickness (μm)	250	7×10^{-3}
Bandgap (eV)	1.12	1.87
Electron affinity (eV)	4.05	4.25 [26,27]
Doping level (cm^{-3})	1×10^{16}	1×10^{14}
Permittivity	11.9	7 [28]
Electron Mobility ($\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{S}^{-1}$)	1350	44 [29]
Hole mobility	500	86 [29]
Effective conduction band density N_c (cm^{-3})	2.8×10^{19}	2.5×10^{20}

4. Conclusions

We have investigated the optical and structural properties of thin 2H-MoS₂ and performed a device simulation for a MoS₂/Si heterojunction solar cell. Through AFM measurements, we have shown the rough morphology of the sample surface, with the presence of grains, holes, and outgrowths, which we attribute to the consequences of

ambient oxidation, as confirmed by XPS. Raman spectroscopy measurements have shown the multi-layer character of the samples. Regarding XRD measurements, the interlayer spacing is higher than what is reported in the literature, which we could also attribute to the presence of oxides resulting from ambient oxidation. Optical ellipsometry (O.E) measurements show the high bandgap character of MoS₂, which would make it suitable for heterojunction solar cells with silicon. O.E also provided optical constants that were integrated into a simple device simulation that indicated that using n-MoS₂ would permit a potential gain in quantum efficiency, due to the high bandgap of ~1.87 eV MoS₂, for a MoS₂/Si heterojunction solar cell, with the formation of type 2 heterojunction. Due to the observations in this work, we plan to use MoS₂ samples with an ITO capping layer to prevent the oxidation and degradation of MoS₂ and, consequently, to improve the viability of MoS₂/Si heterojunction solar cells.

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