

Photovoltaic Devices Made from Plasma-Doped Two-Dimensional Layered Semiconductors

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Abstract:

Two-dimensional (2D) layered transition metal dichalcogenides (LTMDs, especially WSe_2 and MoS_2) exhibit a high absorption of visible light. For example, a LTMD monolayer (~ 0.5 nm) can absorb as much sunlight as 50-nm-thick silicon (Si) films [1]. Therefore, they are suitable for making next-generation ultrathin, flexible photovoltaic (PV) devices. However, society lacks the device physics knowledge and skills for generating built-in potentials in such emerging layered materials, which are required to separate photo-generated electron-hole pairs and create photocurrents. This REU project sought to leverage the plasma-doping method and vertically stacked LTMD heterostructures developed by Prof. Liang's group to create and optimize PV devices made from multilayer WSe_2 films with plasma-doping-induced p-n junctions. To achieve this goal, we fabricated PV devices with a vertically stacked indium tin oxide (ITO)/ WSe_2 /Au structure, using 2D layer printing, photolithography, thin-film deposition/lift-off, and plasma etching/doping. Our results provide critical information for identifying the band diagram of WSe_2 PV devices as well as optimizing their PV performance. This work provides scientific insights of the unique optoelectronic properties of 2D LTMDs at the backbone of emerging atomically layered PV devices.

Introduction:

LTMDs have a potential for making ultrathin photovoltaic (PV) devices that have great flexibility, high light-absorbing efficiency, long lifetime and low manufacturing cost. Molybdenum disulfide (MoS_2), a semiconducting LTMD, has recently been observed by Liang's group as a photovoltaic material. Tungsten diselenide (WSe_2) is another LTMD that has a similar layered structure to MoS_2 but has been anticipated to have the higher light absorption coefficients over a broader wavelength range in comparison with MoS_2 . However, the PV

response characteristics of WSe_2 -based devices still remain poorly studied. Especially, the research society needs new scientific and technical schemes to form reliable p-n junctions (or built-in potentials) in such layered semiconductors, which is expected to be very different from the junction formation schemes for conventional semiconductors.

The goal of our project was to fabricate and characterize WSe_2 -based photovoltaic cells with plasma-formed p-n junctions. In a PV process, the incident photons excite electrons from the valence band to the conduction band, creating electron-hole (e-h) pairs. The built-in field of the p-n junction can separate e-h pairs and result in a splitting of quasi-Fermi levels of electrons and holes as well as a photocurrent in the external circuit.

Experimental Procedure:

The schematic diagram of the device fabrication process is illustrated in Figure 1. Adhesive tape squares were used to exfoliate pristine WSe_2 flakes from a bulk WSe_2 ingot (1a). The exfoliated WSe_2 flakes were then thinned by repeatedly applying them to multiple adhesive tape squares. The tape squares containing the pristine WSe_2 flakes were treated with fluoroform (CHF_3) by reactive-ion etching (1b). These flakes were subsequently bonded onto wafers containing gold

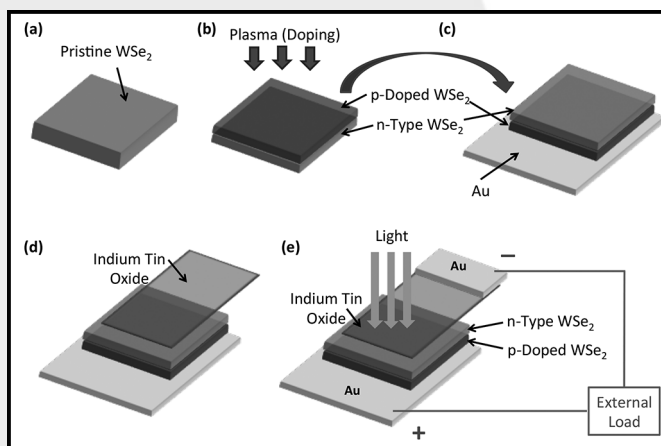


Figure 1: Schematic of the fabrication process.

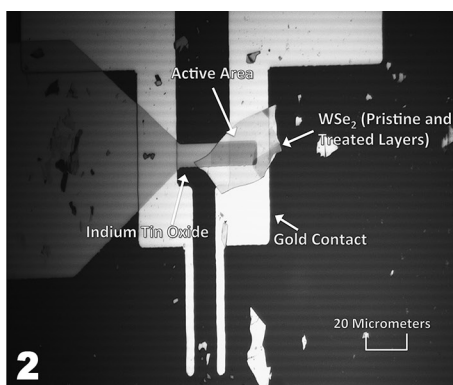


Figure 2: Completed photovoltaic cell diagram.

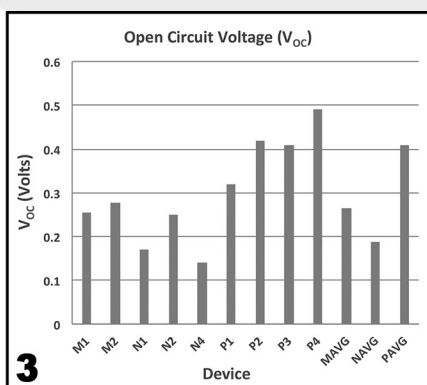


Figure 3: Open-circuit voltages for each device and averages of each device type.

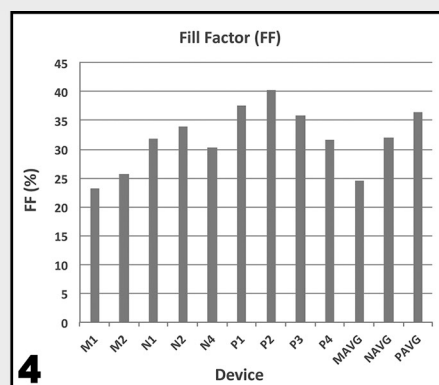


Figure 4: Fill factors for each device and averages of each device type.

(Au) contacts. Heating the wafers removed the tape residue and transferred the WSe₂ flakes onto the Au contacts of the wafers (1c). Four samples were treated with fluoroform after exfoliation and not before. Photolithography techniques were used to create a trench into which a thin film of ITO was sputtered (1d). The optical micrograph of an as-fabricated photovoltaic device made using this process is displayed in (1e) and in Figure 2.

Results and Conclusions:

A semiconductor-parameter analyzer is used for the I-V characterization of all PV devices under the illumination of 532 nm laser light. From the measured I-V characteristics, critical PV performance parameters of all devices, including open-circuit voltages (V_{OC}) (Figure 3) and fill factors (FF) (Figure 4) were determined.

“M devices” refers to MoS₂ cells previously fabricated by Liang’s group, while “N devices” refers to n-type-WSe₂/Au structured cells, and “P devices” refers to p-type-WSe₂/Au structured cells. While M cells exhibited a higher average V_{OC} (0.266 V) than N devices (0.187 V), P cells have a higher average V_{OC} (0.410 V) than both M and N devices. Furthermore, P samples exhibit the highest average FF (36.4%), followed by N samples (32.0%) and M samples (24.5%).

From these data, we can conclude that P devices (i.e., p-type-WSe₂/Au structured cells) exhibit significantly higher V_{OC} and FF parameters in comparison with M and N devices, which are crucial to ultimately obtain unprecedented PCE parameters in the future.

Future Work:

After removing the area of WSe₂ above the gold contact and not below the ITO (i.e., marginal area), power conversion efficiency (PCE), external quantum efficiency (EQE) and short circuit photocurrent density (J_{SC}) data can be obtained for further analysis and comparison. Texturing the surfaces of silicon photovoltaic cells helps contain the light in the P-N junction for a longer time and reduces surface reflections, leading to more generated carriers and a greater photocurrent [2]. This process could significantly enhance the efficiencies of the WSe₂ photovoltaic cells. Also, some LTMDs have not been examined for their efficiencies in the p-n junction of the photovoltaic cell. The same fabrication and testing processes used in this project could be employed for future investigations of newly studied LTMDs.

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References:

- [1] Wi, S., et al.; “Enhancement of Photovoltaic Response in Multilayer MoS₂ Induced by Plasma Doping”; ACS Nano, 8, 5270-5281 (2014).
- [2] Edwards, M., et al.; “Effect of texturing and surface preparation on lifetime and cell performance in heterojunction silicon solar cells”; Solar Energy Materials and Solar Cells, 92, 1373-1377 (2008).

