2D Materials-based Optoelectronic Devices

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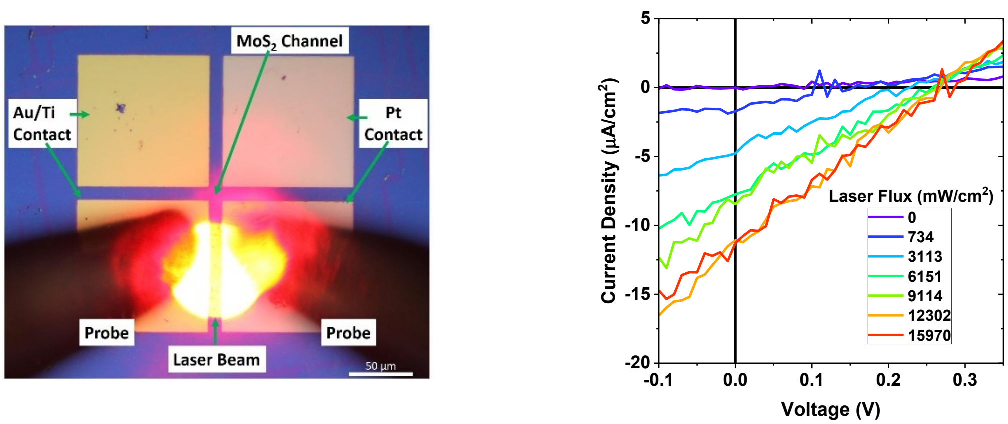
Abstract: Optical properties of 2D MoS_2 have been investigated and used to design optoelectronic devices. Photodetectors and photovoltaic devices, fabricated with symmetric and asymmetric metal contacts, show high photoresponsivity and open-circuit voltage, respectively.

The strong light-matter interaction in two-dimensional (2D) transition metal dichalcogenides (TMDCs) such as molybdenum disulfide (MoS_2) results in a very high absorptance in these materials, making them promising materials for flexible and transparent photovoltaics[1]. However, doping these materials to form high-quality p-n junctions has, to date, been a challenging task. Here, we present photodetectors and photovoltaic devices using large-area 2D MoS_2 with carrier-selective contacts.

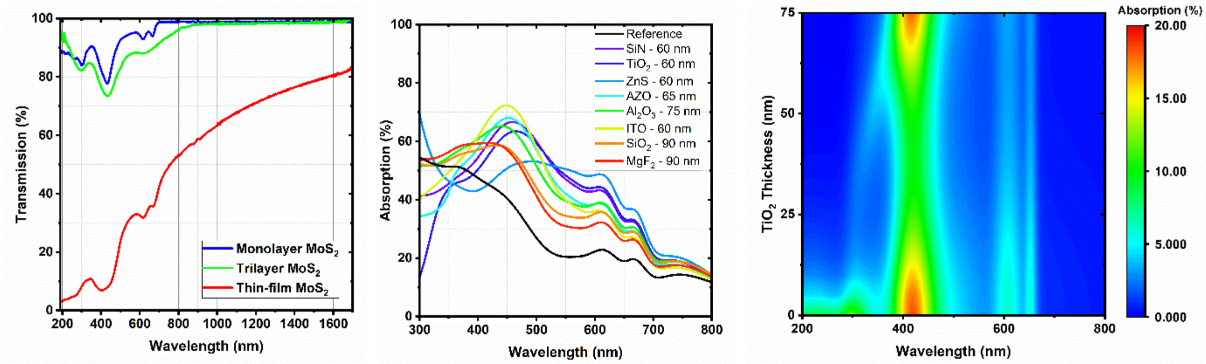
2D MoS_2 is synthesized on a sapphire substrate using a standard chemical vapor deposition (CVD) process using MoO_3 and S precursors with Ar carrier gas under vacuum in a tube furnace[2]. The films are then transferred to SiO_2-on-Si substrates for device fabrication. The grown films show a combination of monolayer and bilayer thickness. To create differing Schottky junctions, Ti and Pt are chosen as the contact metals because of their low (4.33 eV) and high (5.64 eV) work-functions, respectively. These asymmetric contacts create band offsets at the metal-MoS_2 interface between the Fermi levels of these metals and that of MoS_2 - 0.9 eV at the Ti-MoS_2 interface and 0.41 eV at the Pt-MoS_2 interface - thus driving the electrons toward Ti and holes toward Pt and separating the photo-generated carriers. On the other hand, symmetric contacts (Ti-Ti or Pt-Pt) can effectively detect photons for transistor-type photodetector applications.



(a) (b)

Figure 1: (a) Optical micrograph of Ti-Pt asymmetric and Ti-Ti/Pt-Pt symmetric contact monolayer MoS_2 optoelectronic devices; (b) Illuminated I-V curve of a monolayer MoS_2 Schottky-junction photovoltaic device with Ti and Pt as contact metals under 660 nm excitation wavelengths.

A Schottky-type photovoltaic device with lateral current flow between asymmetric contacts is successfully fabricated with an active area of 10 µm X 100 µm, as shown in Fig. 1. Since this is on CVD-grown materials, device active area can be easily scaled up with contact engineering. As shown in Fig. 2 (a), the initial devices show a V_{OC} of >270 mV under 660 nm monochromatic laser illumination, which is state-of-the-art for 2D materials photovoltaics. However, the initial photocurrent in the asymmetric contact devices is low and exhibit poor I_{SC}. Symmetric contact Ti-Ti transistor-type photodetector devices have also been fabricated that shows 25% external quantum efficiency (EQE) at 620 nm monochromatic illumination and a carrier mobility of 3.3 cm^2/V.s. Combining the relatively high V_{OC} of the asymmetric contact devices and relatively high EQE and carrier mobility of the symmetric contact devices paves the path toward improved efficiency photovoltaic devices, realization of which is currently underway.



(a) (b) (c)

Figure 2: (a) Transmittance vs. wavelength in monolayer, Trilayer, and thin-film (33.5 nm) MoS_2; (b) Optical modeling showing broadband absorption enhancement in thin-film MoS_2 using thin-film optical coatings; (c) Optical modeling showing confinement of absorption in a narrow spectral band using a thin layer of TiO_2 on trilayer MoS_2 film.

In parallel, an optical/semiconductor device model is developed using COMSOL Multiphysics to better understand the photon absorption and generation, and carrier transport in the devices and to help design future devices. The model takes the electronic and optical properties of 2D MoS_2 and work-functions of metal contacts as parameters and calculates the band bending, dark current, generation and recombination of carriers upon illumination, and generates an IV plot with V_{oc} and J_{sc}, among other characteristics.

Optical modeling is also used to enhance absorption in the devices and to design devices that only absorb certain bandwidth of the spectrum. Fig. 2 (a) shows the measured transmittance through different thicknesses of MoS_2 and Fig. 2 (b) and (c) shows the results of an optical model where thin layer of optical coatings are placed on top of MoS_2 films and how that effects the broadband/narrow-band absorption. These models help design photovoltaics for higher absorption and photodetectors/sensors that only absorbs light of a narrow bandwidth.

Other ongoing efforts to improve device performance include density functional theory analysis of metal-semiconductor interfaces, experimental measurement of Schottky barrier heights, use of passivating surface treatments, exploration of other contact metals, device contact pattern engineering over large areas, and investigation of nanostructures for enhanced photon capture. We will also transfer the CVD grown MoS_2 on to a flexible substrate, such as PDMS, for fabricating flexible 2D photovoltaics.

[1]Bernardi, M., Palummo, M., & Grossman, J. C. (2013). Extraordinary sunlight absorption and one-nanometer thick photovoltaics using two-dimensional monolayer materials. *Nano letters*, *13*(8), 3664-3670.

[2]Wang, S., Rong, Y., Fan, Y., Pacios, M., Bhaskaran, H., He, K., & Warner, J. H. (2014). Shape evolution of monolayer MoS2 crystals grown by chemical vapor deposition. *Chemistry of Materials*, *26*(22), 6371-6379.