

Vertical heterojunction of MoS₂ and WSe₂

Shudong Xiao, Mingda Li, Alan Seabaugh, Debjee Jena and Huili Grace Xing
Department of Electrical Engineering, University of Notre Dame
Notre Dame, Indiana 46556, USAEmail: sxiao1@nd.edu; hxing@nd.edu

The development of experimental methods¹ to create stacked structures of layered 2D materials with atomic-plane precision provides opportunities to study a variety of van der Waals heterojunctions that is difficult to fabricate with traditional growth methods. Here, we report the vertical integration of two 2D TMD materials, MoS₂ and WSe₂, to form van der Waals heterojunction. We show that the electrical properties of the heterojunction are controlled by gate voltage and rectification is observed with forward/reverse current ratio ~ 100 .

Vertically stacked MoS₂/WSe₂ heterostructure is fabricated with a dry transfer process similar to the method described in Ref. 2. Fig.1 shows the fabrication process. MoS₂ and WSe₂ flakes of few-layer thickness (<5nm) were first mechanically exfoliated on the transparent transfer mask and Si/SiO₂ (285 nm) substrate separately. Suitable thin flakes were identified by optical microscopy and transferred with our home-built transfer system to form stacked structure on Si/SiO₂. The alignment was controlled with a mechanical manipulator under long working distance objectives. After transfer, the polymer handling layer was removed by acetone. Cross-section TEM image of the heterojunction confirms that MoS₂ is in good contact with WSe₂ (Fig. 2). Metal contacts were patterned on the non-overlapping area by two steps of e-beam lithography and metal deposition: first Ti (5 nm)/Au (50 nm) on MoS₂, then Pd (50 nm) on WSe₂.

Current across the heterojunction was measured under two-probe configuration with back-gate voltage applied on the heavily doped Si substrate. The electrical measurement using the pair of electrodes on the non-overlapping region reveals the doping type of MoS₂ and WSe₂ as a function of the back gate voltage, as well as the nature of the top metal-semiconductor contacts. It is found that both the Ti/Au/MoS₂ and the Pd/WSe₂ junctions are Schottky like. Fig. 3(a) shows the transfer characteristics of MoS₂ and WSe₂ in non-overlapping region. At $V_g = -20V$, it is observed that MoS₂ is n-type and WSe₂ is p-type. Assuming MoS₂ in the overlapping region has the same residue charge with the non-overlapping MoS₂, the TCAD simulation (Fig. 4) shows the overlapping MoS₂ has a similar dependence on the back gate voltage since the thin WSe₂ underneath can not completely screen the gate field. It is found that in the overlapping region MoS₂/WSe₂ form an n-/p-junction at $V_g = -20V$. Fig. 3(b) shows the I-Vs measured across the stacked MoS₂/WSe₂ heterojunction under varying back gate voltages. At $V_g = -40$ and $0V$, very low current was observed since one of the TMD layers was fully depleted. At $V_g = -20, 20$ and $40V$, rectifying I-Vs were observed. Though the device behavior is complicated by the Schottky-like metal-TMD contacts, it is very likely that the rectification observed at $V_g = -20V$ stems from the vertical n-MoS₂/p-WSe₂ junction (i.e. the overlapping region). At $V_g = 20$ and $40V$, the rectifying behavior is likely a result of the n/n MoS₂/WSe₂ heterojunction together with the influence of the Schottky-like metal-TMD contacts.

In summary, we have observed rectifying behavior across heterojunction of 2D TMD crystals, which can be explained with simulated band diagrams. This represents the first steps toward achieving stacked p-n junctions using 2D layered materials to realize more advanced devices such as tunnel FETs³. This work was supported by the Center for Low Energy Systems Technology (LEAST), a STARnet center.

[1]C. R. Dean, A. F. Young, I. Meric, C. Lee, L. Wang, S. Sorgenfrei, K. Watanabe, T. Taniguchi, P. Kim, K. L. Shepard and J. Hone, *Nature Nanotechnology* 5, 722 (2010).

[2] P. J. Zomer, S. P. Dash, N. Tombros and B. J. van Wees, *Appl. Phys. Lett.* 99, 232104 (2011).

[3]M. Li, D. Esseni, G. Snider, D. Jena and H. G. Xing, *J. Appl. Phys.* 115, 074508 (2014)

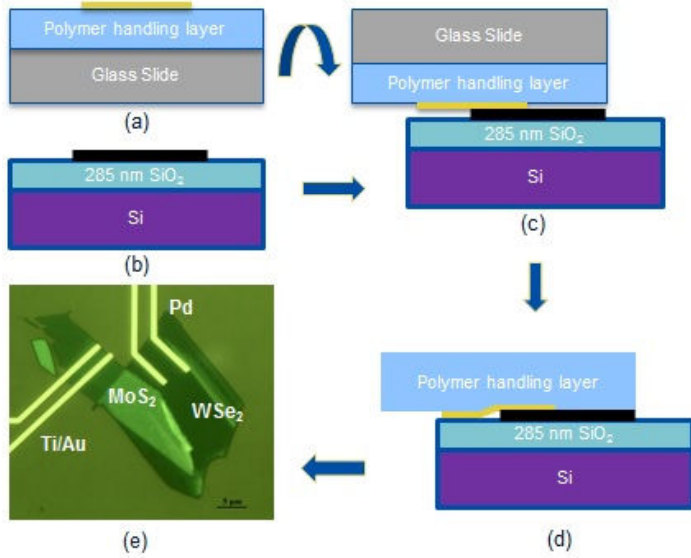


Fig. 1 Fabrication of MoS₂/WSe₂ heterojunction. (a) Exfoliation of MoS₂ on glass slide with polymer handling layer. (b) Exfoliation of WSe₂ on Si/SiO₂ substrate. (c) Alignment under optical microscope. (d) At 100 °C, polymer handling layer melts and leaves MoS₂ membrane on WSe₂. (e) Image of the device.

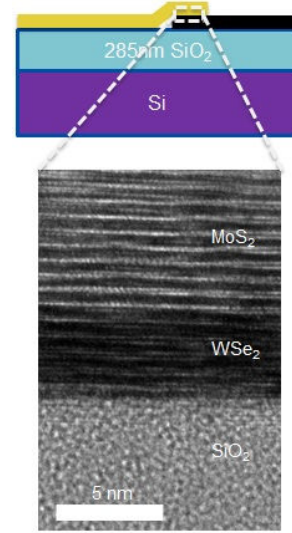


Fig. 2 Cross-section TEM image of MoS₂/WSe₂ heterojunction.

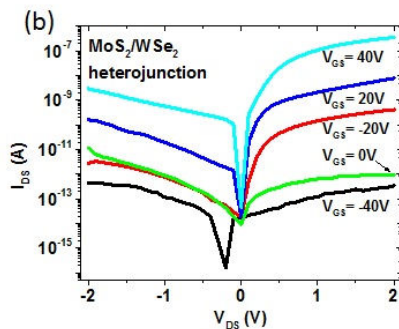
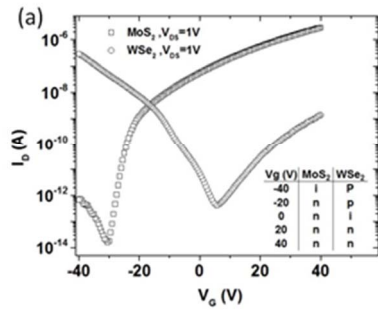


Fig. 3 (a) Transfer characteristics of MoS₂ and WSe₂ in non-overlapping region. The inset lists the type of carriers at different gate voltages. (b) IV characteristics of MoS₂/WSe₂ heterojunction.

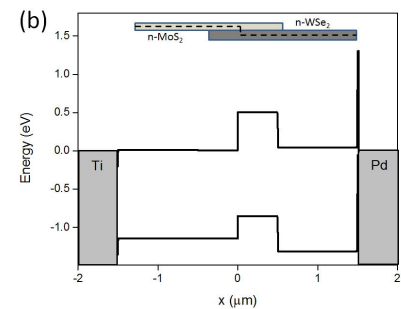
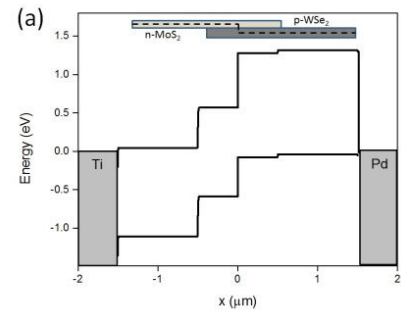


Fig. 4 Simulations of band diagrams: (a) n-type MoS₂ and p-type WSe₂ (b) n-type MoS₂ and n-type WSe₂.