Schottky Barrier Reduction on Optoelectronic Responses in Heavy Ion Irradiated WSe_2 Memtransistors

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1. Raman spectra of the pristine and irradiated samples

We found a number of features below and above the first-order mode in 5L-WSe_2 prepared by mechanical exfoliation method, as shown in Fig.S1. The two features located at 246.8 and 255 cm^{-1} might correspond, respectively, to the first order E^1_{2g} and A_{1g} modes. The peaks at 116cm^{-1}, 137 cm^{-1}, 352 cm^{-1}, 370 cm^{-1}, and 392 cm^{-1} have been assigned as second-order Raman modes involving phonons at the M point. For most monolayer TMDC, B^1_{2g} is the optically inactive mode. Its origin has been recently reported as an acoustic (A)-symmetry first-order mode corresponding to an interlayer vibration, which can be used to distinguish monolayer and multilayer WSe_2.

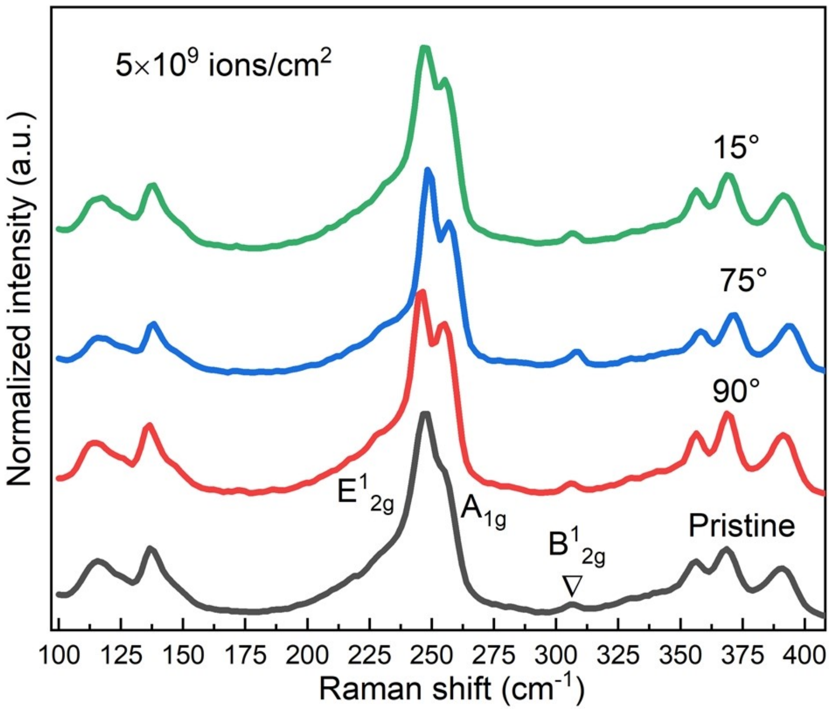

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Fig.S1 Demonstration of the Raman peaks of the pristine and irradiated WSe_2 devices.

2. Microstructure of the tracks

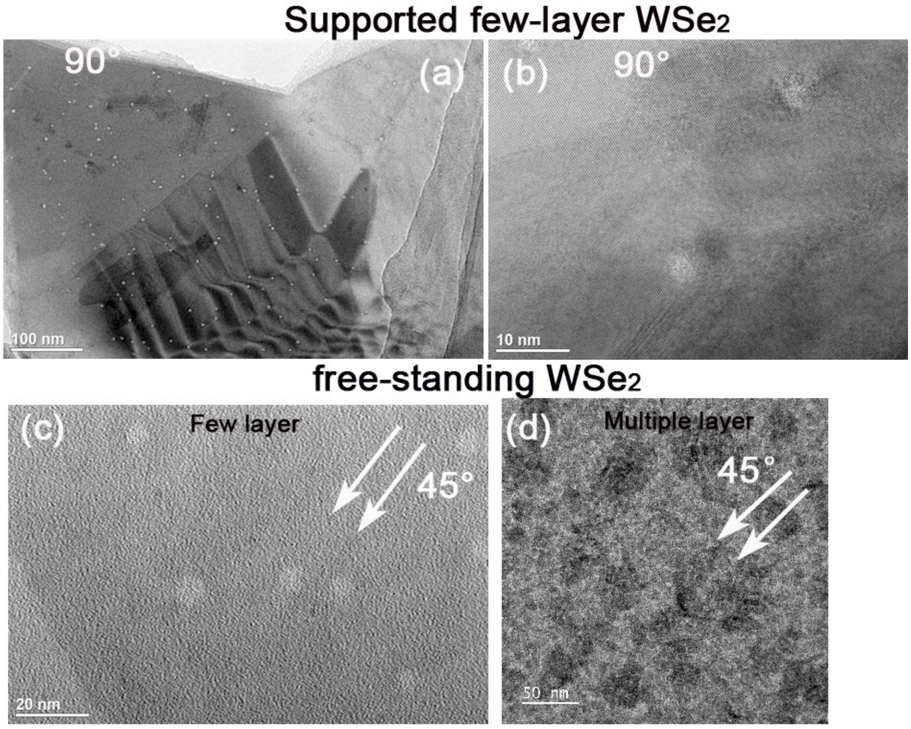

Fig.S2 (a) Averagely distributed tracks induced by Ta ion irradiation, The applied fluence is 5×10^{10} ions/cm^2. (b),(c) TEM images of the carbon-film supported few-layer WSe_2 film irradiated by Ta ions with an angle of 90° and 45°. The applied fluence is 5×10^{10} ions/cm^2. (d) TEM images of the free standing WSe_2 film irradiated by Ta ions with angles of 45°. The applied fluence was 5×10^{10} ions/cm^2.

3. I-V scanning loops of the pristine devices

Fig.S3 depicted the 20-turn *I-V* curve characteristics of the pristine devices under electrical signal stimulation with light excitation (P_{in}=100 mW/cm^2). The *I-V* curves of the pristine devices showed typical *I-V* characteristics without RS behaviors. Particularly, the value of current under dark conditions was slightly greater than that under light excitation.

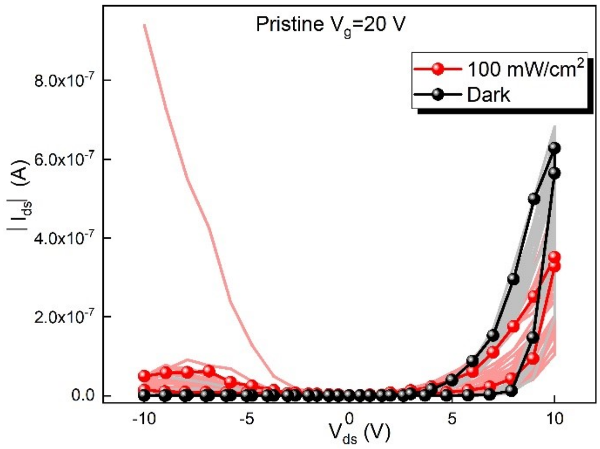

Fig.S3 *I-V* scanning loops of the pristine devices with and without illuminance. The backgate voltage is kept as 20 V.

4. I-V scanning loops of the irradiated devices

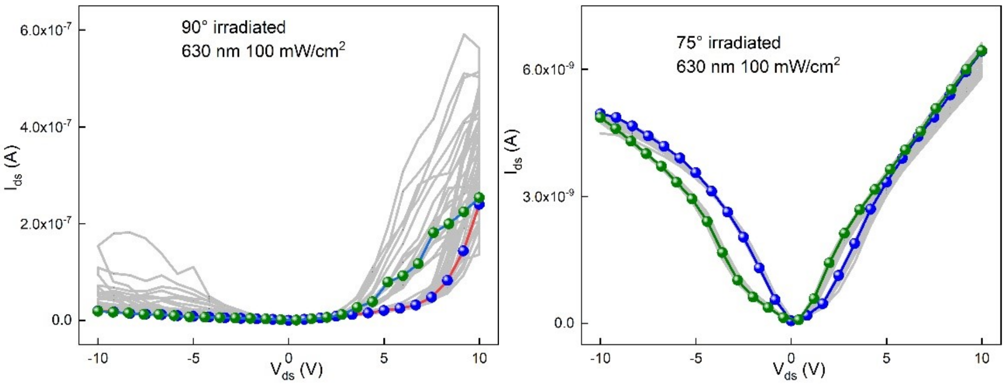

Fig.S4 *I-V* scanning loops of the WSe_2-based devices irradiates by SHIs with angles of 90° and 75°. The backgate voltage is kept as 20 V.

5. Simulation details

Self-consistent periodic DFT calculations were carried out using the Vienna ab initio simulation package 'VASP'. Briefly, the exchange-correlation effects were treated within the generalized gradient approximation using the PBE functional. The ionic cores were described using the projected augmented wave (PAW) method, and the Kohn-Sham one-electron valence states were expanded in a basis of plane waves. Simplify processes of melting and quenching were setup to simulate the density of states (DOS) of heterostructure Cr (3 layers)/ WSe_2(3 layers). The molten structure was quenched at a rate of 10^{14} K/s, which was in a similar timescale according to the spike model. Complex defects were introduced in the system. The spin-up and spin-down total DOS shown in Fig.S5(a) and (b) were symmetric, which indicated that these systems exhibit the non-magnetic ground states. An obviously reduced DOS at E_F was depicted for Cr in the defective heterostructure, resulting from strong chemical interactions between the metal electrodes and WSe_2 flakes, as seen in Fig.S5(c). Considering the computation and time consuming, the heterostructure model of Cr (3 layers)/ WSe_2(3 layers) including 672 atoms were setup in this work. Combined with actual experimental conditions, high-energy heavy ions can completely penetrate 5 layers or 3 layers of WSe_2. Therefore, the conclusion related with irradiation induced interfacial mixing will not be affected when the model is smaller to 3 layers WSe_2.

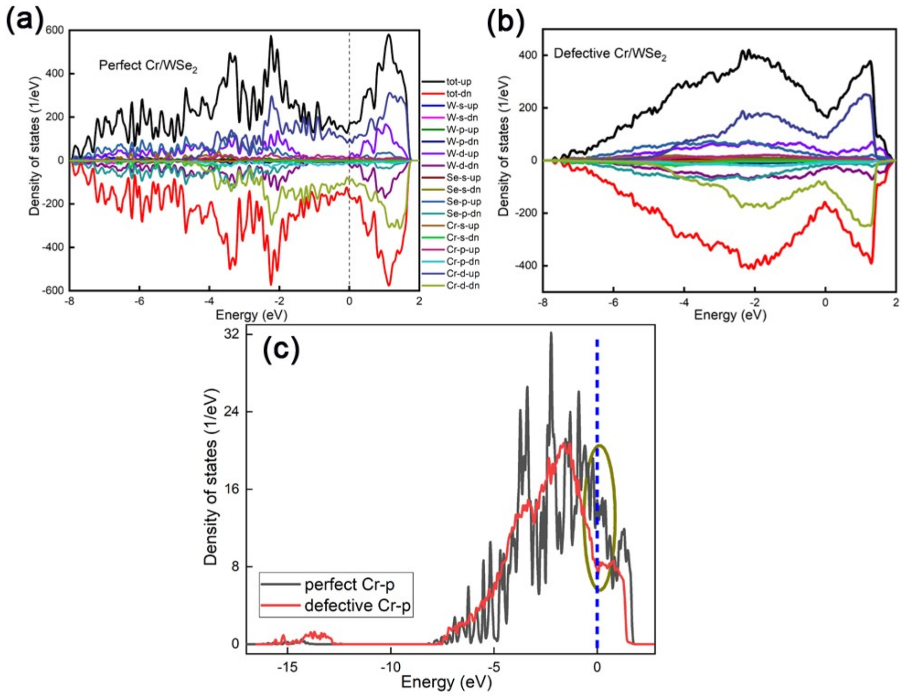

Fig.S5 (a) Total DOS patterns of the pristine heterostructure Cr/WSe_2. (b) Total DOS patterns of the defective heterostructure Cr/WSe_2. (c) Comparison of the partial DOS of Cr *d* states in the perfect and defective heterostructure.

6. Sweep loops of the transfer characteristic of SHI irradiated devices

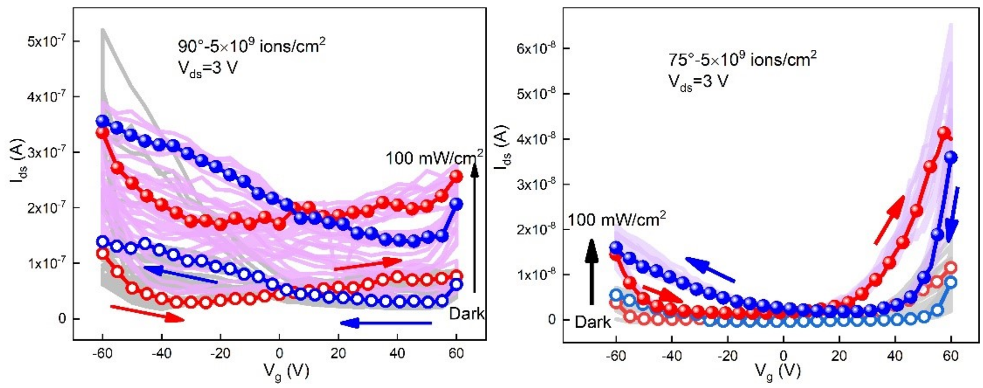

Fig.S6 The sweep loops of the transfer characteristic of SHI irradiated devices. The transfer characteristics were measured under dark and illumination with power density of 100 mW/cm^2, which were labelled by hollow and solid circles in the figures. The swept directions were marked by red and blue arrows.

7. I-T curves of the devices irradiated with angles of 90° and 75°

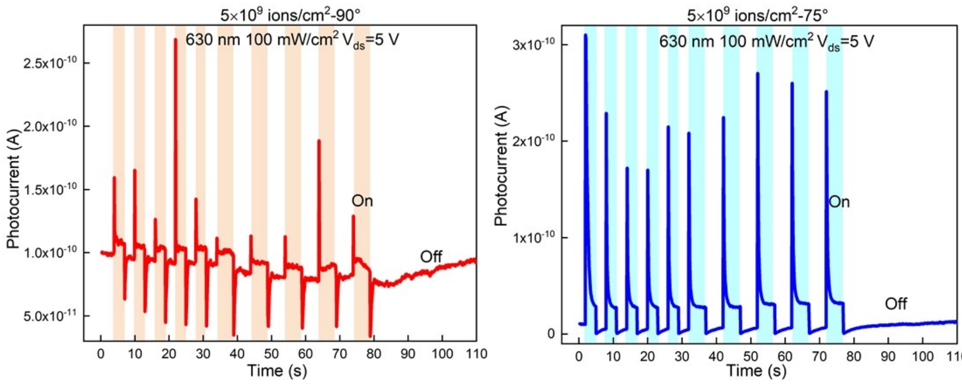

Fig.S7 *I-T* curves of the devices irradiated with an angle of 90° and 75° under 630 nm pulses with intensity of 100 mW/cm^2. The width and intervals were increased from 3 s to 5 s. The applied voltage V_{ds} was 5 V at V_g = 0 V.