Electronic Supplementary Material (ESI) for Nanoscale.

Sulfur Vacancy Activated Field Effect Transistors Based on ReS_2 Nanosheets

Kai Xu,[1] Hui-Xiong Deng,[2] Zhenxing Wang,[1] Yun Huang,[1] Feng Wang,[1] Shu-Shen Li,[2,3] Jun-Wei Luo[2,3] and Jun He[1*]*

**To whom correspondence should be addressed: hej@nanoctr.cn & jwluo@semi.ac.cn*

1. National Center for Nanoscience and Technology, Beijing 100190, P. R. China

2. State Key Laboratory for Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Science, Beijing 100083, P. R. China

3. Synergetic Innovation Center of Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

Experimental Section:

Synthesis of ReS_2NSs on SiO_2/Si and carbon fibers: The ReS_2 NSs were grown on SiO_2/Si substrates and carbon fibers in a horizontal two-zone tube furnace. In the typical synthesis process, S (0.3 g, 99.5% Alfa) powder as precursor was placed at front zone, while high purity ReO_3 (1 mg, 99.9% Alfa Aesar) powder was located at back zone. Substrates were faced down and placed on the upper side of ReO_3 powder. Before increasing the temperature, the tube was pumped and flushed with Ar gas several times. When the front zone temperature reach to 130-150 ^oC at a rate of 10 $^oCmin^{-1}$, the back zone was raised to 500 ^oC at a heating rate of 20 $^oCmin^{-1}$ and held for 30 min. Finally, the furnace was allowed to cool down to room temperature and the whole synthesis process was under Ar (50 sccm) gas flow.

Material Characterizations and electrical measurements: The microstructure and morphologies of ReS_2 NSs were conducted by transmission electron microscopy (TEM, Tecnai F20) and by field emission scanning electron microscopy (FESEM, Hitach S-4800). The Raman spectrum was characterized on a confocal microscope based Raman spectrometer (RenishawInVia, 532 nm excitation laser). The slit width and instrument broadening are ~65 μm and 2 wave numbers, respectively. Chemical configurations were performed by XPS (ESCALAB250Xi). The electrical measurements were conducted on a probe station (Lakershore TTP4), which are equipped with semiconductor system (Keithley 4200), a vacuum pump, and temperature controller.

First-principles calculations of the formation energy of defects: The formation energie of defects are calculated as follows:[1, 2]

$$\Delta H_f(\alpha,q) = \Delta E(\alpha,q) + \sum n_i\mu_i + qE_F \quad (1)$$

where $$\Delta E(\alpha,q) = E(\alpha,q) - E(host) + \sum n_i E(i) + q\epsilon_{VBM}(host). \quad (2)$$

E (host) is the total energy of host material and *E (α,q)* is the total energy of the host material containing defect α in charge state q. The Fermi level E_F is referenced to the valence band maximum (VBM) of the host material and μ_i, determinedby experimental conditions, is the chemical potential of element *i,* which is referenced to total energy E_i of its elemental solid/gas. n_i is the number of atoms of element *i* removed from or added to the host materials and q is the number of electrons transferred from the supercell to the reservoirs in forming the defect cell.

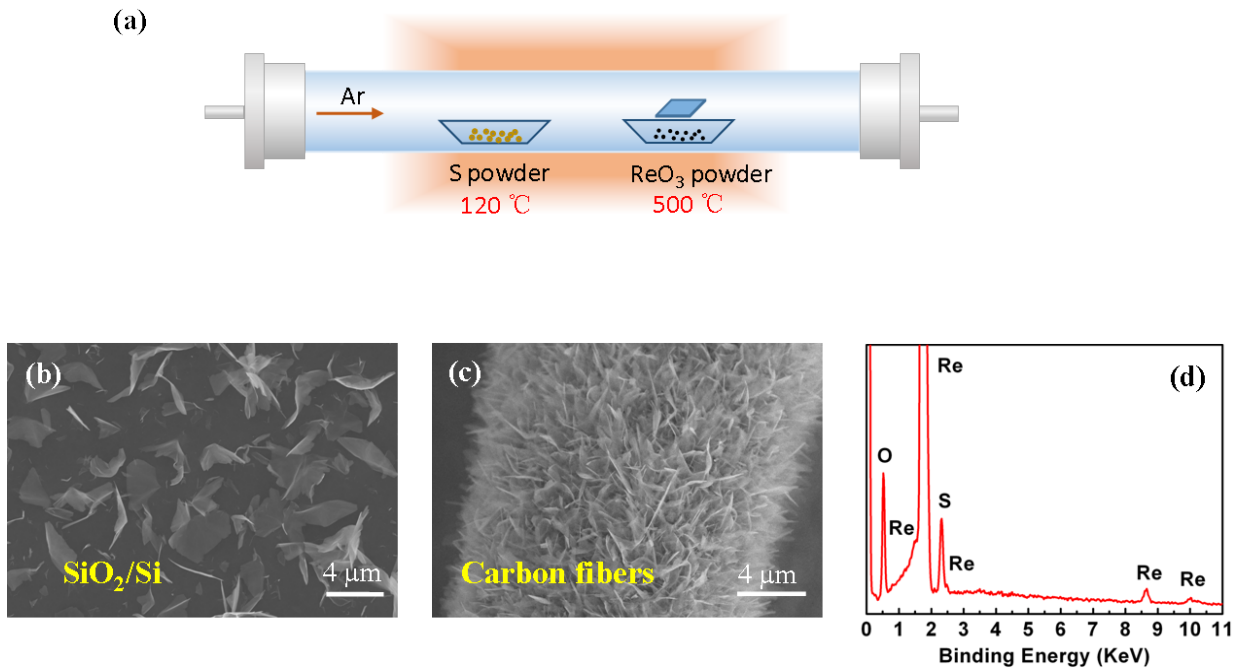

Figure 1. (a) schematic experimental setup for synthesizing ReS_2 NSs. (b), (c) SEM image of ReS_2 NSs grown on SiO_2/Si and carbon fibers. (d) The corresponding SEM-EDS confirmed atomic percent of Re and S is exactly 1:2.

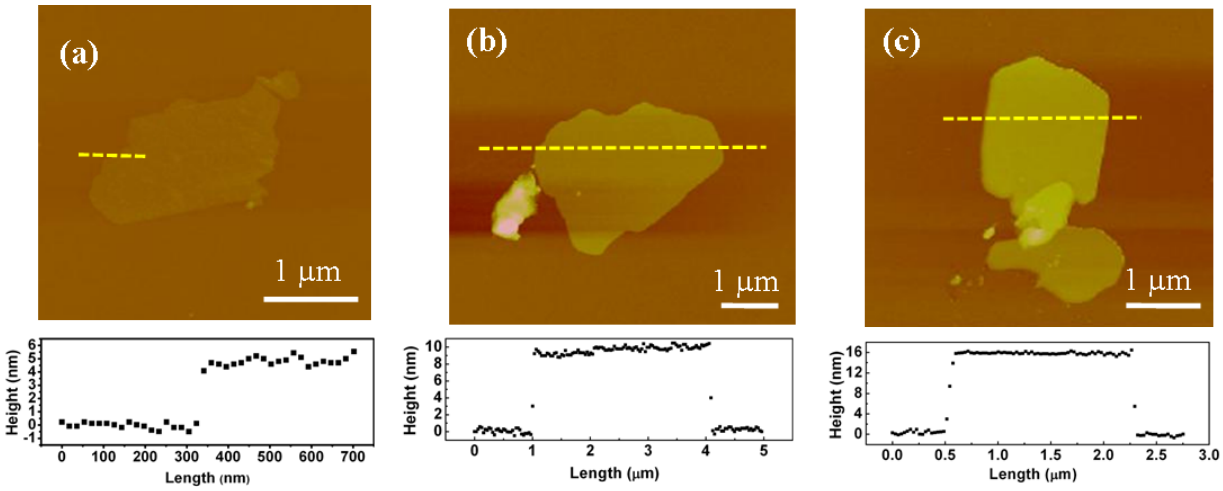

Figure 2. (a), (b), (c) AFM image of ReS_2 NSs grown on SiO_2/Si. The thicknesses were found to be 4~15 nm.

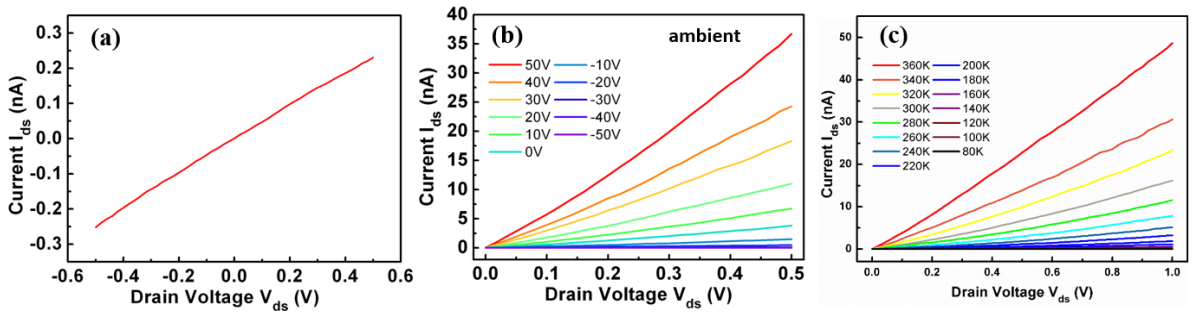

Figure 3. (a) The linearity of I-V curves indicates the ohmic contacts between ReS_2 NSs and Cr/Au electrodes. (b) Output characteristics in ambient. (V_g = -50V~50V, V_d = 3V) (c) The I-V curves at variable temperature (80 K ~ 360 K, V_g = 0V)

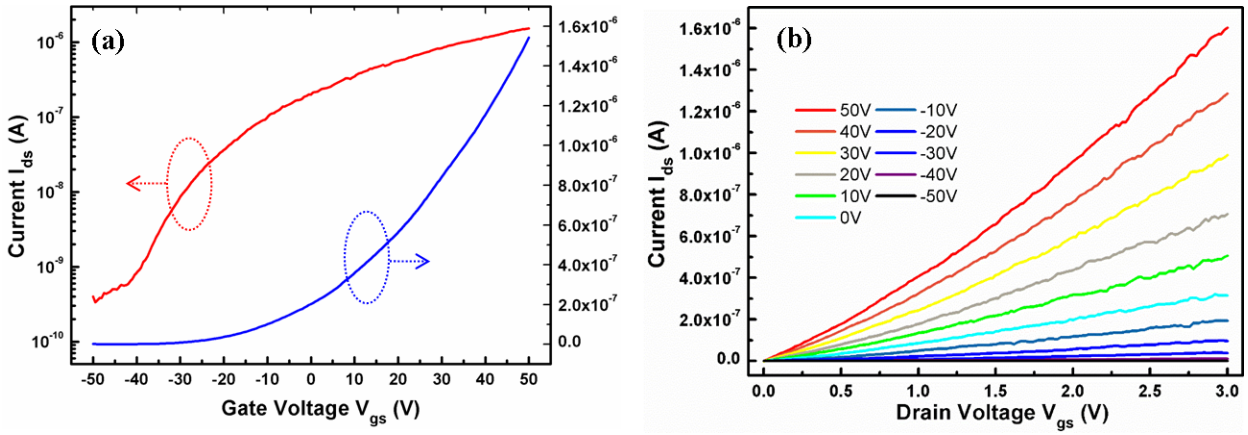

Figure 4. (a) The transfer and output characteristics of ReS_2 NSs FET were conducted before device was annealed at 300 ^oC for 3 hours. The on/off ratio is ~10^3, less than the value of annealed device.

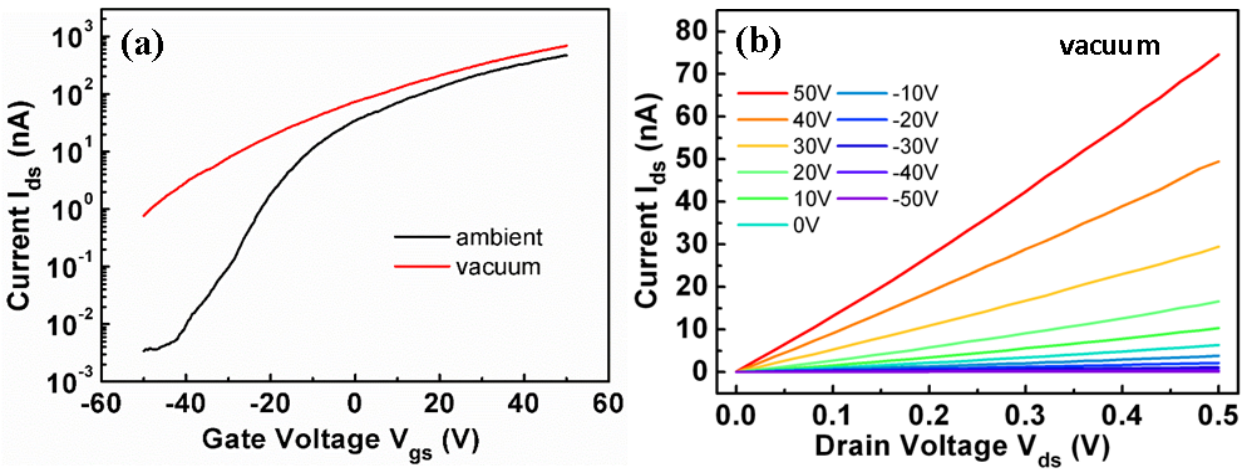

Figure 5.(a), (b) Transfer and output characteristics in vacuum. (V_g = -50V~50V, V_d = 3V). A relatively large increase of the drain currents of transfer characteristics happened, especially off-state current

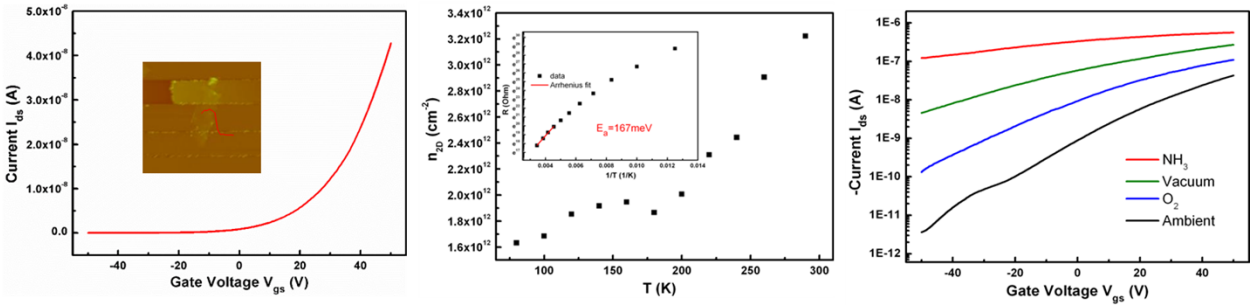

Figure 6. ReS_2 NSs device with thickness ~15nm. (a) Transfer characteristics in ambient. (V_g = -50V~50V, V_d = 3V). The relationship between n_{2D} and temperature was plotted in (b). Activation energy ~167 meV was obtained, similar with 175 meV. (c) Vacuum, O_2 and NH_3 atmosphere dependence of electronic measures were conducted.

1 S. H. Wei, *Comput. Mater. Sci.,* 2004, **30**, 337-48.
2 S. H. Wei and S. Zhang, *Phys. Rev. B,* 2002, **66**, 155211.