Local Conduction in Transition Metal Dichalcogenides: The Role of Stacking Faults, Defects and Alloying

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2D materials

Modification of the Band-structure:
- Charge
- Strain
- Mixing
- Defects
- Stacking
2D materials
Defects in MoS$_2$

Nano Lett., 2013, 13 (6), pp 2615–2622
MoS$_2$-metal contacts
Unpredictable behavior

ACS Nano, 2014, 8 (3), 2880–2888

ACS Appl. Mater. Interfaces, 2015, 7 (22), 11921–11929
Conductive AFM as a nanoscopic tool for electrical characterization
Overview

1. Schottky barrier heights in MoS$_2$/metal contacts
Schottky barrier heights in MoS$_2$/metal contacts

Visualization of Defects

Topography

200 nm
Defects located in the Mo-layer

STM

S-vacancies

5 nm

Metal-like defects

S-vacancy
Charge transport
Metal-Semiconductor contacts

Thermionic emission:

\[ I = I_0 \left[ \exp\left( \frac{qV}{\eta k_B T} \right) - 1 \right] \]

\[ \phi_B = \frac{k_B T}{q} \ln\left( \frac{A^* A T^2}{I_0} \right) \]

\[ I_0 = AA^* T^2 \exp\left( -\frac{q\phi_B}{k_B T} \right) \]
Charge transport

Metal-Semiconductor contacts

![Graph showing charge transport characteristics with SBH]
Charge transport
Fermi level pinning

\[ \Phi_B = \Phi_M - x \]

\( S \approx 0.3 \)
\( S \approx 0.1 \)

Bampoulis et al., ACS Appl. Mater. Interfaces 9, 22, 19278-19286, 2017
Stacking faults
Overview

2. Local conduction in MoWSe$_2$ alloys
WSe$_2$

Atomic Periodicity with C-AFM
Local conduction in MoWSe$_2$ alloys

Segregation

Mo$_{0.3}$W$_{0.7}$Se$_2$ 6.4 nA

Mo$_{0.7}$W$_{0.3}$Se$_2$ 7.1 nA

Mo$_{0.3}$W$_{0.7}$Se$_2$ 3.2 nA

Mo$_{0.7}$W$_{0.3}$Se$_2$ 3.8 nA
Local conduction in MoWSe$_2$ alloys

Segregation

Topography

2 nm
Local conduction in MoWSe$_2$ alloys

Segregation

(i) W-rich
(ii) Mo-rich

Bampoulis et al., ACS Appl. Mater. Interfaces 10, 15, 13218-13225, 2018
Conclusions

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Thank you for your attention