Contact Engineering in 2D-Material-Based Electrical Contacts

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Motivation and Background

- The undesirably large contact resistance between two-dimensional (2D) semiconductor and three-dimensional (3D) metallic electrodes represents one of the major obstacles towards the development of practical 2D electronic and optoelectronic devices [1].
- Extensive efforts have been made to improve current flow through contacts in 2D material-based devices [2,3,4,5].
- We develop a model that includes both, the material properties of 2D semiconductors and the geometrical electrostatic effect in mixed-dimensional nanostructures, which remains rarely studied in the literature so far.

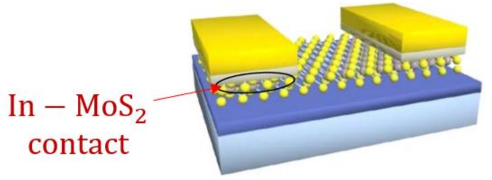

Fig. 1: Bottom-gate FET. The electrodes consist of 10-nm-thick In capped with 100-nm-thick Au. The ellipse under the contact indicates the interface region [5].

[1] Allain et al., Nat Mater **14**, 1195 (2015)
[2] Das et al., Nano Lett. **13**, 100 (2013)
[3] Xu et al., ACS Nano **10**, 4895 (2016)
[4] Liu et al., Nature **557**, 696 (2018)
[5] Wang et al., Nature **568**, 70 (2019)

Method

Self-consistent solutions are obtained by solving modified transmission line model [6] and thermionic emission model for 2D materials [6,7].

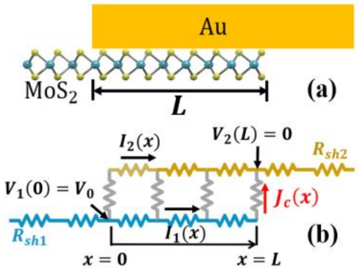

Fig. 2: (a) A typical parallel contact between Au and MoS_2. (b) its transmission line model. The width (transverse dimension) of the two contact members is w.

Applying Kirchoff's law in Fig. 2b,

$$\frac{\partial V_1(x)}{\partial x} = -\frac{I_1(x)R_{sh1}}{w}, \quad \frac{\partial V_2(x)}{\partial x} = -\frac{I_2(x)R_{sh2}}{w},$$

$$\frac{\partial I_1(x)}{\partial x} = -wJ_c(x), \quad \frac{\partial I_2(x)}{\partial x} = wJ_c(x) \qquad [6]$$

$$J_c(x) = J_{th}\left[\exp\left(\frac{eV}{k_BT}\right)-1\right], \quad V = V_1 - V_2$$

$$J_{th} = \frac{2e\Phi_{B0}k_BT}{\pi\tau\hbar^2 v_F^2}\left(1+\frac{k_BT}{\Phi_{B0}}\right)\exp\left(-\frac{\Phi_{B0}-\varepsilon_F}{k_BT}\right) \qquad [7]$$

$$I_1(x) + I_2(x) = constant = I_{tot}$$

Contact resistance $R_c = \frac{V_1(0)-V_2(L)}{I_{tot}}$

ϕ_{B0} = Intrinsic Schottky Barrier Height (SBH)
τ = carrier injection time
v_F = Fermi Velocity
ε_F = Fermi energy

[6] Banerjee et al., Sci. Rep., **9**, 14484 (2019)
[7] Ang et al., Phys. Rev. Lett., **121**, 056802 (2018)

Validation [8]

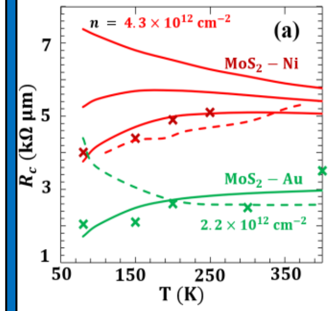

Fig. 3: R_c as a function of temperature T with (a) an increasing trend, and (b) a decreasing trend, for MoS_2 − metal contacts with different n. Crossed symbols are from experiments [9] ; solid lines are from our self-consistent Model, and dashed lines are extracted from model calculations in Ref. [9]

[9] English et al., Nano Lett. **16**, 3824 (2016)

Results [8]

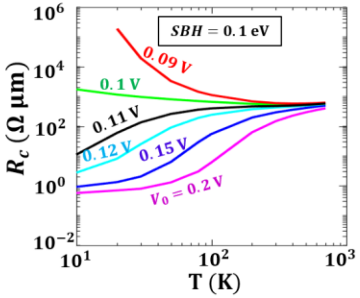

Fig. 4: R_c as a function of temperature T for different applied voltage V_0, for Schottky Barrier Height (SBH) = 0.1 eV. Here, the contact is between a monolayer MoS_2 and Au, with τ = 0.1 ps, and L = 50 nm.

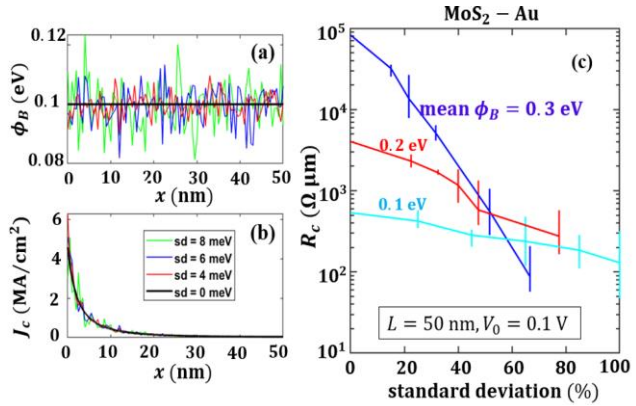

Fig. 5: (a) Roughness in Schottky barrier height ϕ_B, the resulting (b) current density $J_c(x)$, across the contact interface for a monolayer MoS_2-Au 2D/3D contact for different standard deviations (sd). (c) Contact resistance R_c as a function of surface roughness (standard deviation/ϕ_B) for different mean values of ϕ_B. Here, V_0 = 0.1 V, and L = 50 nm.

Conclusions [8]

- A self-consistent model to quantify the current distribution and contact resistance in 2D materials-based contacts is constructed and validated with existing experimental works.
- It is found that interface roughness can significantly reduce 2D/3D electrical contact resistance.

[8] Banerjee et al., Phys. Rev. Appl. **13**, 064021 (2020)

Acknowledgement

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