Quantum simulation of tunnel field-effect transistors based on transition metal dichalcogenides

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Abstract

The tunnel field-effect transistors (TFETs) may enable a more aggressive reduction of the supply voltage than the MOSFETs, by lowering the sub-threshold swing (SS) under the thermionic limit of 60mV/dec at room temperature. Promising experimental results were reported for TFETs based on silicon and III-V semiconductors. However, in nanoscale devices, quantum confinement widens the band gaps and precludes the implementation of truly broken band gap alignments in 3D semiconductors [1], while interface states degrade the SS [2]. The use of semiconducting transition metal dichalcogenides (TMDs) may represent an extremely advantageous alternative thanks to their intrinsic 2D geometry and thinness, the absence of dangling bonds, and the variety of available materials, which results in a large range of energy band gaps and band alignments.

In this contribution, we predict an extremely steep sub-threshold swing for inter-layer TFETs based on WTe_2 and MoS_2 layers with a 1 nm thick *h*-BN interlayer [3]. Figure 1 shows a sketch of the device and its equivalent 2D structure. Our full-quantum simulations are based on the non-equilibrium Green's function formalism and accurately account for the device electrostatics by a self-consistent coupling to the Poisson equation. Electron-phonon scattering is calibrated to make the simulations consistent with available mobility experiments. By means of this numerical apparatus, we investigate the role of several relevant design parameters such as chemical doping, top gate geometrical alignment and back-gate biasing (see Fig.2). Our analysis reveals that carefully designed TMD TFETs can offer excellent SS values (<30 mV/dec) and represent a promising technology for future low-power nanoelectronics.

References

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[3] M. Li *et al.*, J. Appl. Phys. **115** (2014) 074508 .

Figures

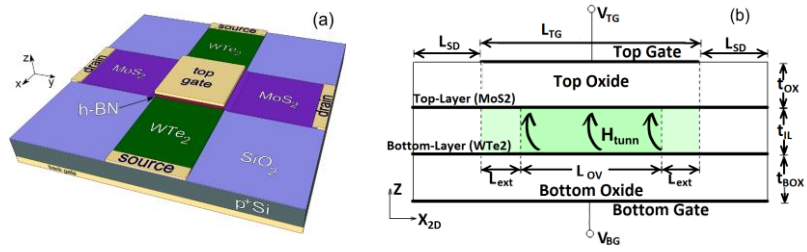

Fig1: (a) Sketch of the TFET under study. (b) Equivalent 2D model used in the simulations. The x_{2D} axis corresponds to the *y*-direction for MoS_2 and to *x*-direction for WTe_2.

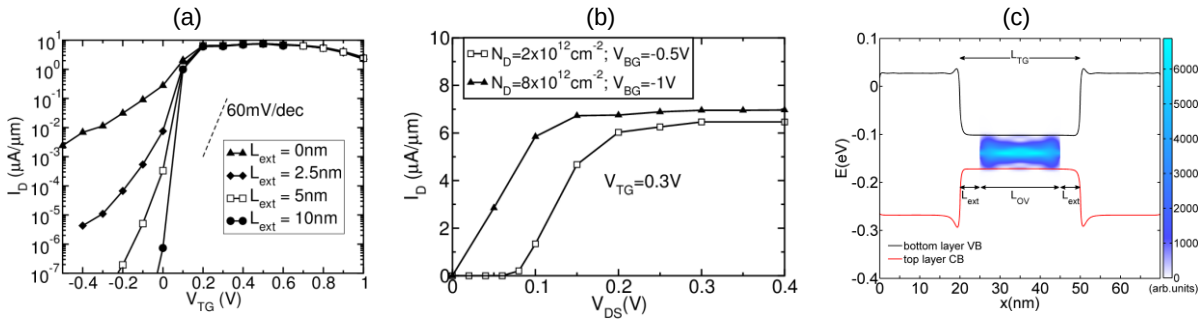

Fig.2: (a) Transfer characteristics as a function of the top-gate voltage V_{TG} for different values of the gate extension in the contact regions. The SS is 100, 27 and 17 mV/dec for L_{ext} = 0, 5 and 10nm, respectively. (b) Output characteristics for different top-layer dopant concentration N_D and back-gate voltage V_{BG}. (c) Band profile and energy spectrum of the inter-layer current density in the transistor on-state (V_{TG}=0.3V).