Subband Structure and Ballistic Conductance of a Molybdenum Disulfide Nanoribbon in Topological 1T' Phase: A k·p Study

Viktor Sverdlov
Christian Doppler Laboratory
for Nonvolatile Magnetoresistive Memory and Logic
at the Insitute for Microelectronics
Technische Universität Wien
Vienna, Austria
sverdlov@iue.tuwien.ac.at

Al-Moatasem Bellah El-Sayed, Siegfried Selberherr
Institute for Microelectronics
Technische Universität Wien
Vienna, Austria
el-sayed@iue.tuwien.ac.at, Selberherr@TUWien.ac.at

EXTENDED ABSTRACT

Edge states in a sheet of MoS_2 in its 1T' phase, a two-dimensional topological insulator [1], propagate without backscattering, and are attractive for designing highly conductive transistor channels. The dispersion of edge states lies within an inverted gap of a topological insulator. By applying a vertical electric field E_z, the inverted gap can be reduced, closed, and opened again as a direct dielectric gap in the "bulk" of the sheet [1]. As no propagating edge states are allowed within the direct gap, the current is dramatically reduced [2].

In order to enhance the on-current through the channel it is beneficiary to have many edges by stacking several narrow nanoribbons. We evaluate the subband structure in a narrow nanoribbon of 1T' molybdenum disulfide by employing an effective **k·p** Hamiltonian [3], [4]. Highly conductive topologically protected edge states whose energies lie within the bulk band gap are investigated. Due to the interaction of the edge modes located at the opposite edges, a small gap in their linear spectrum opens in a narrow nanoribbon (Fig.1, circles)). This gap is shown to sharply increase with the perpendicular out-of-plane electric field, in contrast to the behavior in a wide nanoribbon. The gaps between the electron and hole bulk subbands (Fig.1, diamonds and squares) also increase with the electric field. The increase of the gaps between the subbands leads to a rapid decrease of the ballistic nanoribbon conductance and current with the electric field, which can be used for designing molybdenum disulfide nanoribbon-based current switches.

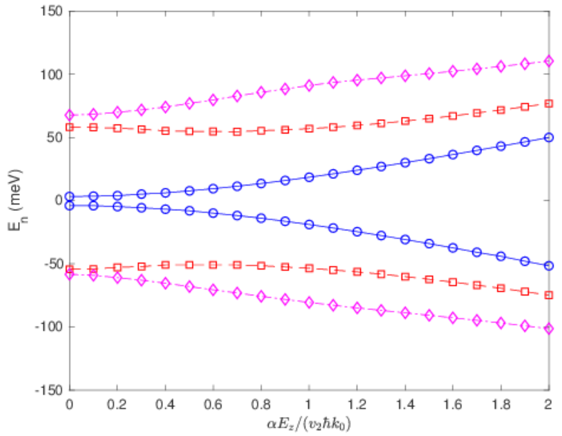

Fig. 1. Dependence of electron (hole) subbands minima (maxima) on the electric field E_z for the first three subbands. In contrast to the bulk case, the gap never closes and keeps increasing with E_z

The increasing gap between the edge-like subbands is reflected in the sharp decrease of the corresponding nanoribbon ballistic conductance shown in Fig.2 (diamonds). Although the edge-like subbands give the leading contribution in the conductance (Fig.2, circles) the role of other subbands shown in Fig.2 by squares is non-negligible. First two electron (hole) bulk-like subbands (Fig.1, diamonds and squares) give similar contributions to the ballistic conductance totaling to 30%. However, all contributions to the total conductance G rapidly decrease as a function of E_z (Fig.2). This makes 1T'-MoS_2 potentially suitable for switching applications.

ACKNOWLEDGMENT

Financial support by the Austrian Federal Ministry for Digital and Economic Affairs and the National Foundation for Research, Technology and Development is gratefully acknowledged.

REFERENCES

[1] X. Qian et al., Science, vol. 346 (6215), p.1344, 2014.
[2] L. Liu and J. Guo, J.Appl.Phys., vol.118, 124502, 2015.
[3] V. Sverdlov et al., EUROSOI-ULIS 2020, accepted.
[4] V. Sverdlov and S. Selberherr, Phys.Rep., vol.585, p.1, 2015

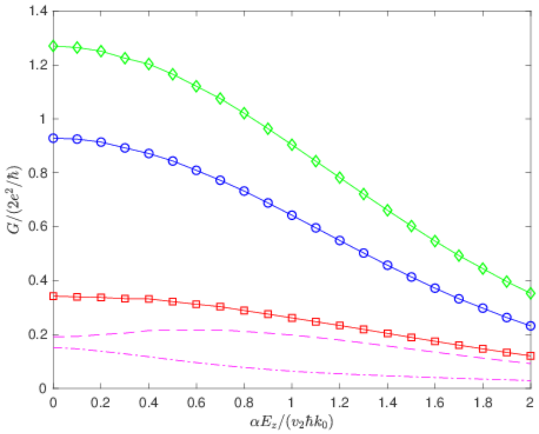

Fig. 2. Ballistic conductance (diamonds) of a 1T'-MoS_2 nanoribbon, with the contributions from the edge-like states (circles), and the remaining bulk-like subbands (squares). Dashed line from subbands shown in Fig.1 by squares; dot-dashed line- from Fig.1 by diamonds.