Calculation of the Ballistic Current of Few-Layer MoS_2 Field-Effect Transistors

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MoS_2-based field effect transistors (FETs) are promising candidates to replace Silicon in future technology nodes. In this work, we evaluate the ballistic current of MoS_2 FETs with different thicknesses as a function of the number of layers. The electronic structure calculations have been performed using the SIESTA code [1], within the GGA and the pseudopotential approaches. Our DZP basis has been optimized under the SIMPLEX algorithm. This procedure has been employed to calculate the band structure of MoS_2 channels with 3 to 6 layers. The band structure for the 4 and 6 layer cases are shown in Fig. 1(a). The effective mass is evaluated at the conduction band minima, located along the $\Gamma \rightarrow K$ direction, at the so-called Λ point, marked in the figure. First, for each number of layers, a quadratic fit of the DFT conduction band profile provides the in-plane effective mass m^{ip}, which is assumed to be isotropic. Therefore, m^{ip} determines both the density of states and the transport effective masses. Then, the confinement effective mass, m^{c}, is found from the separation between the first two conduction band minima at the Λ point. The values we have achieved are almost independent of the number of layers for both effective masses, and therefore we have opted for their average: $m^{\mathrm{ip}} = 0.58m_0$ and $m^{\mathrm{c}} = 0.77m_0$. The calculated in-plane effective mass is similar to other values found in the literature [3].

The top-of-the-barrier (ToB) approach [2] is employed to simulate double-gated few-layer MoS_2 FETs, using the effective mass values obtained from DFT for the six degenerate Λ valleys. For the sake of simplicity, we just assume heavily-doped MoS_2 as source and drain. Al_2O_3 is used as gate insulator, and a metal with work function $\Phi_{\mathrm{m}} = 4.61\mathrm{eV}$ is employed as the gate contact. The channel length is L=30nm. The electrostatics are evaluated by solving the 2D Poisson equation in the confinement and transport directions, while the charge distribution is calculated using the 1D effective mass Schrödinger equation at each point of the transport grid. The results are depicted in Fig 1(b), where $I_{\mathrm{ds}} - V_{\mathrm{ds}}$ curves are plotted for various V_{gs} values and for 4 and 6 MoS_2 layers. As can be seen, the devices show a good saturation behavior, as no significant short channel effects appear for the considered gate length. The results also demonstrate that reducing the device thickness does not provoke a strong reduction of the drain current. In particular, as the applied V_{gs} is increased, the differences between the number of layers are reduced, and I_{ds} becomes almost independent on the channel thickness.

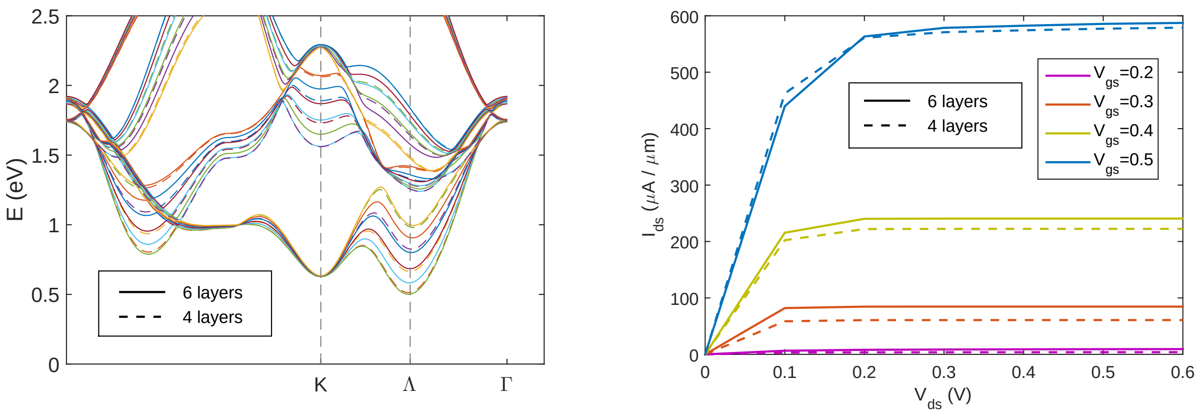

Fig. 1. (a) Band structure for 4-layer and 6-layer MoS_2. The Λ point, around which the effective mass is evaluated, is disclosed. (b) Ballistic I_{ds} vs. V_{ds} for different values of the gate bias, for 4-layer and 6-layer devices.

References

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Acknowledgment: This work has been supported by the MINECO under the FIS-2011-26005 project. B. Biel also acknowledges funding by the RYC-2012-10381 contract from the Ramón y Cajal Program (MINECO). A. Toral and J. M. González-Medina are grateful to the University of Granada for its support through the "Iniciación a la Investigación" Program. E. G. Marin acknowledges CEI-BioTIC funding under Project TIC7-2015.