Multiscale simulations of ink-jet printed devices

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Introduction

In the last few years, the surge of modern portable technologies has boosted the demand for low-power and flexible devices. In this particular niche, printed electronics, raised by the recent advances in two-dimensional materials (2DMs) inks, have emerged as a major enabling technology. Although huge efforts have been made towards the characterization of the electrical properties of the networks of flakes of 2DMs comprising these devices [1], [2], a better theoretical understanding of the physical mechanisms controlling the transport at play in these structures is still needed. In this regard, we present a novel multiscale modeling approach able to simulate printed devices based on 2DMs inks (Fig. 1), and to capture both the microscopic physical mechanisms as well as to extract relevant measurable physical quantities such as the sheet resistance and mobility.

Method

The proposed approach consists of three main ingredients. First, the network of flakes of 2DMs forming the semiconducting region of the device is created by a Monte-Carlo algorithm setting the flakes' properties, e.g. lateral dimension, shape, orientation, etc, as well as the network properties, such as the filling factor (FF), i.e., the volume occupied by the flakes with respect to the overall channel volume (see Fig. 2). Second, by means of a precise multiscale methodology, which includes *ab-initio* calculations, we model the anisotropy between the micrometer transport along the flake (in-plane) and the nanometer vertical transport between partially overlapping flakes (inter-flake), as pictorially depicted in Fig. 3 and reported in Ref. [3]. Finally, we solve the transport in the network device by means of the self-consistent solution of the drift-diffusion and the Poisson equation.

Discussion

The model has been validated against graphene-printed structures realized in Refs. [1] and [2] . In Fig. 4 we report the experimental measurements of the sheet resistance versus thickness before (diamonds) and after (squares) annealing, which are compared with the multiscale simulations (circles and triangles), observing an excellent agreement and demonstrating the actual capabilities of the proposed approach [3]. Along with graphene, MoS_2-based devices have been studied [3] as well as printed devices of MoS_2–graphene composite inks [4]. This latter option has been proposed to optimize the performances of MoS_2-printed devices, which severely suffer of reduced mobility due to inter-flake transmissions [4]. In Fig. 5 we report the transfer characteristics of FET devices varying both the graphene ink concentration and the Schottky barrier between graphene and MoS_2, evidencing the impact of the ink mixing.

Conclusion

A simulation platform to study the electrical properties and behavior of 2DMs-based ink-printed devices is presented and validated against experimental results, which can constitute valuable support to guide experimental activity in printed electronics.

Acknowledgment

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References

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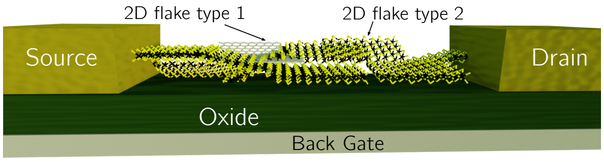

Fig. 1. Schematic depiction of an ink-jet printed network device with 2D materials. Figure adapted from Ref. [4].

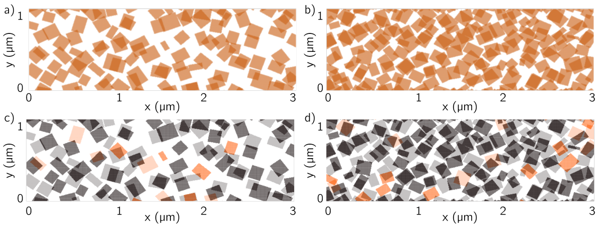

Fig. 2. Network structure sections in two adjacent planes perpendicular to the vertical direction. (a,b) Single material network FF = 0.4 (a) and FF = 0.7 (b). (c,d) Mixed material network, with 90% of material 1 (grey) and 10% of material 2 (orange), with FF = 0.4 (c) and FF = 0.7 (d). In the networks reported we have considered an average lateral size of 150 nm and random orientation. Figure adapted from Refs. [3] and [4].

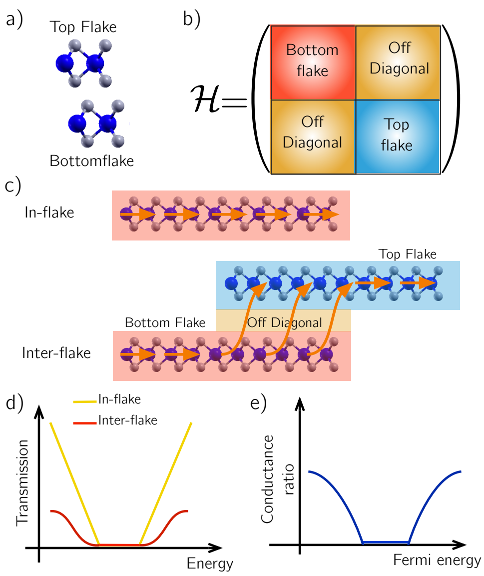

Fig. 3. (a) Bilayer structure used for ab-initio calculations. (b) Schematic wannier Hamiltonian, with indicated the sub-hamiltoanians for the bottom layer, top layer and the coupling between them (off-diagonal). (c) In-flake and inter-flake structures. (d) Pictorial depiction for the in-flake and inter-flake transmission coefficients. (e) Schematic depiction of the conductance ratio as a function of the Fermi energy

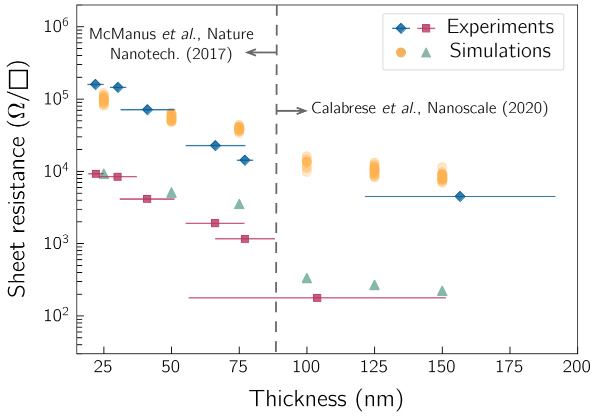

Fig. 4. Extracted sheet resistance for graphene as a function of the channel thickness compared with experimental results obtained in Refs. [1] and [2] before (diamonds) and after (squares) annealing. Two different filling factors FF = 0.35/0.3 for Refs. [1] and [2] and FF = 0.7 are considered in the simulations to reproduce the pre- and after-annealing scenarios. Figure from Ref. [3].

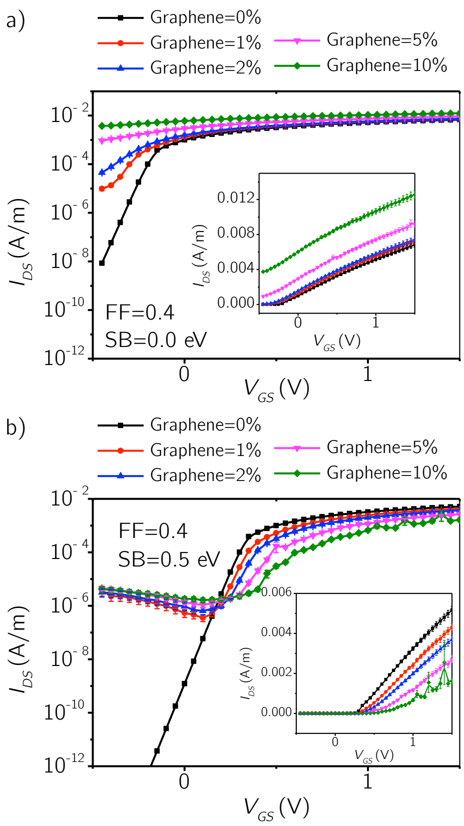

Fig. 5. Transfer characteristics of MoS_2-graphene composite ink-based printed network device with FF = 0.4 and with a Schottky barrier height of (a) 0.0 eV (b) 0.5 eV. Figure adapted from Ref. [4].