Hexagonal BN/graphene heterostructures as a technological option for next-generation devices

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The outstanding electrical properties of graphene are hard to be exploited in electronic applications. Indeed, the lack of a band gap prevents the possibility to properly switch off an FET with a graphene channel, as desired in digital electronics. The scenario would drastically change, if we could find a way to block one the flow of one type of charge carriers, either electrons or holes.

Triggered by a recent paper by Ci et al. [1], we propose a new device concept based on two-dimensional graphene intercalated with h-BCN (hexagonal boron carbon nitrogen), able to suppress the ambipolar behavior and to block one of the type carrier, as well as to fully modulate the current due to the carriers of the other type.

Recently, h-BCN has also been demonstrated to be as a good dielectric for graphene FET (G-FET) [2]. However, it is not clear how many h-BCN layers stacked one over the other have to be considered in order to suppress the undesired leakage towards the gate.

Within this work, we will address both two dimensional graphene/h-BCN based devices with in-plane transport, as well as vertical transport through graphene/h-BCN/graphene multilayers, in order to assess possible performance and limitations, against a silicon technology benchmark.

The followed approach is based on a multiscale method coupling density functional calculations (DFT) with the Non- equilibrium Green's functions (NEGF) formalism and the 3D Poisson equation. In particular, ab-initio calculations have been performed by means of the quantum ESPRESSO package [3], while transport along the channel has been computed through a tight-binding p_z-orbital Hamiltonian within the NEGF formalism. Tight-binding parameters have been extracted from DFT calculations and included in the NanoTCAD ViDES framework [4]. In Fig. 1, we show the longitudinal cross-section of a graphene-based FET, with an h-BCN barrier of thickness t_B in the graphene channel. The corresponding transfer characteristics for p-type FETs are shown in Fig. 2.

As a reference, the transfer characteristics of a graphene FET (GFET) is also shown. As can be seen, the introduction of a h-BCN barrier in the middle of the channel improves the I_{on}/I_{off} ratio with respect to that of a simple GFET, which is smaller than 10.

For the BC_2N case, an I_{on}/I_{off} ratio larger than 10^4 can be obtained, complying with ITRS requirements for next technological nodes. Such devices can manage to reach the THz range, if other parasitics are kept under control, as shown in Fig. 3.

In Fig. 4, we show the stacked graphene/h-BCN/graphene structure considered in order to compute transport in the vertical direction, while in Figs. 5 and 6, we show the computed transmission coefficient for a different numbers of stacked layers, both for a h-BN and h-BC_2N barrier. BN, due its larger energy bandgap, has better potential for gate dielectric, and already 4 BN layers can lead to a negligible leakage current.

In conclusion, we demonstrate through a multiscale approach that h-BCN/graphene heterostructures have high potential for application in next generation devices, both when applying h-BCN material as channel barrier, and as gate dielectric.

REFERENCES

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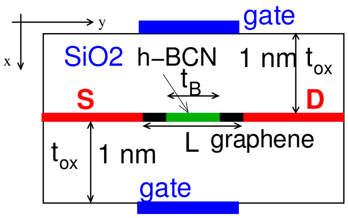

Fig. 1. Longitudinal section of the considered h-BCN based graphene transistor. Source and drain reservoirs are doped with a molar fraction f. Within the graphene channel, a h-BCN barrier t_B-thick has been considered.

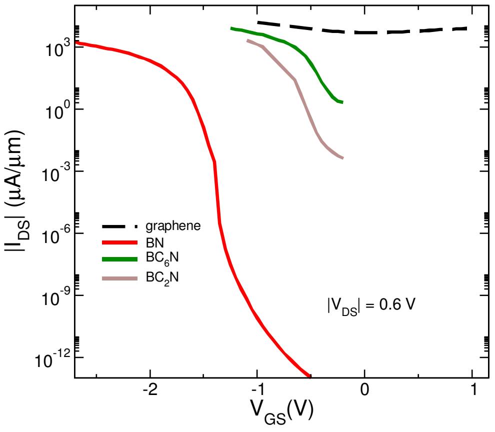

Fig. 2. Transfer characteristics for the different barrier materials. All the considered devices are p-MOS. $f = 10^{-2}$ for BC_2N and BC_6N. $f = 5 \times 10^{-2}$ for BN. t_B=5 nm.

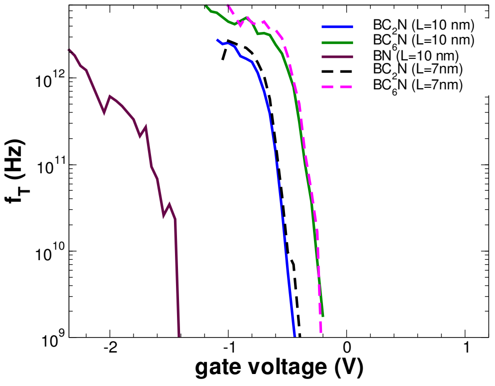

Fig. 3. Cut-off frequency defined as $f_T = g_m/2\pi C_G$, where g_m is the channel transconductance and C_G the gate capacitance, as a function of V_{GS} for the different h-BCN barriers.

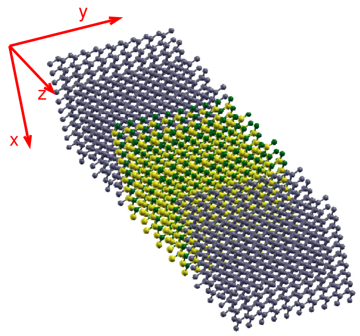

Fig. 4. Sketch of the graphene/h-BCN/graphene structure. Transport is computed along the z direction. Bloch periodic boundary conditions are imposed along the x and y directions.

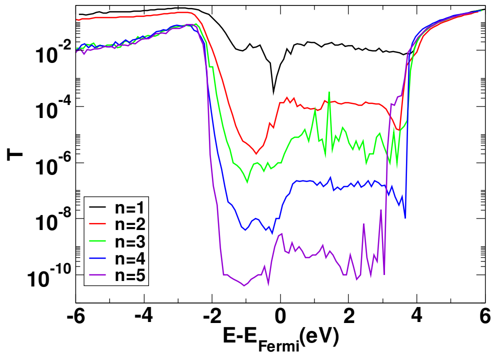

Fig. 5. Transmission coefficient as a function of energy, for different numbers of stacked BN layers.

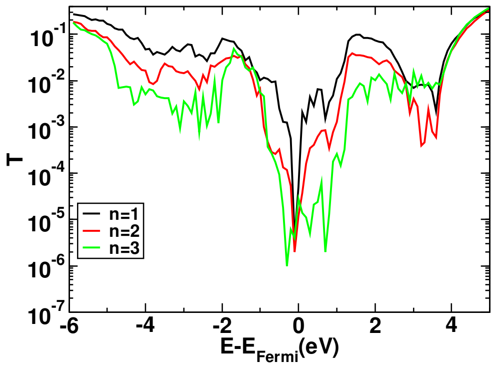

Fig. 6. Transmission coefficient as a function of energy, for different numbers of stacked BC_2N layers.