Materials for spintronics: electronic and transport properties of the zigzag graphene nanoribbon/hexagonal boron nitride heterostructures

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Abstract

High charge carrier mobility in graphene at room temperature creates large potentials for the fabrication of electronic and spintronic devices [1,2]. Using zigzag graphene nanoribbon (ZGNR) on dielectric [3] or metallic [4] substrates, on one hand, leads to the appearance of localized states with energies close to the Fermi level, on the other hand, opens an energy gap in the zero-gap low-energy spectrum of the π-electrons of graphene [5]. Recent research has demonstrated [6] that h-BN(0001) used as the substrate facilitates high carrier mobility (125000 cm^2/V.s, at room temperature) in graphene. DFT study of electronic structure of graphene on h-BN(0001) substrate revealed the emergence of energy gap of 53 meV at the Dirac point along the bond length 0.324 nm between the graphene and the substrate[1]. The use of ZGNR width (N) of 8 carbon dimers (1.56 nm) in 8-ZGNR/h-BN(0001) heterostructure for the antiferromagnetic ordering, produces appearance of the energy gap about 380 meV for the bond length of 0.339 nm according to DFT calculation.

For creating HEMT (high electron mobility transistor) devices based on ZGNR it is extremely important to study charge carriers mobility. It is necessary to understand and to be able to control the transport properties of electronic devices. Thus, in this work, the effects of the edge and substrate on the band gap, magnetism and transport properties of the charge carriers in 8-ZGNR/h-BN(0001) heterostructure, as a component of spintronic devices, are studied by using the DFT.

Figure 1 demonstrates a fragment of the 8-ZGNR/h-BN(0001) slab. The surface and the 8-ZGNR/h-BN(0001) boundary was simulated as a slab consisting of three atomic layers of h-BN(0001) and a monolayer of ZGNR positioned at the distance d_1 of the bond. The basic supercell consisted of 90 atoms; each slab was isolated from others by 1.5nm vacuum space. In Fig. 1c, a fragment of the similar slab is shown, which can be used to create graphene field-effect transistors (FET). The slabs with various ribbons widths (N = 2, 4, 6, 8) were modeled similarly.

Band structure calculations were performed using the Quantum Espresso [7] software suite based on the DFT [8]. Nonlocal exchange correlation functional was used in Perdew-Burke-Ernzerhof (PBE, PBEsol) parametrization. The plane waves cutoff energy for self-consistent field (SCF) calculation was 410 eV. Self-consistent total cell energy convergence threshold was chosen of less than 10^{-4} Ry/cell. To integrate linear Brillouin zone (BZ), 18 points in reciprocal space were used. Spin-polarized calculations of electron density $\rho(r)$ for 8-ZGNR were made with ferromagnetic (FM) and antiferromagnetic (AF) orderings. In this work we have taken into account the dispersion interaction within DFT framework using an empirical potential of the form C_6R^{-6} added to the density functional energy (DFT-D2) as proposed by the author of [9]. Within DFT-D2 calculations we exploited the well-known GGA density functional of PBE in its original form. Evaluation of the carrier mobility tensor components will be performed in the relaxation time approximation similarly to [10]. The analysis of the data allows several conclusions: first, PBEsol and PBE-D2 calculations give comparable results of the effective masses and carrier mobility: for the 8-ZGNR/h-BN(0001) heterostructure the difference is only 10%; second, the electron mobility obtained by both evaluations are of the same order of magnitude as the data of previous works [11-14]; third, the hole mobility appears to be more than four times lower compared to the electron mobility.

For both carrier types in the N-ZGNR/h-BN(0001) heterostructures a common picture is observed: increasing carrier mobility with the decrease of the number of dimers in nanoribbon. For electrons, the mobility increases from 21.86×10^4 cm^2/V.s (N = 8) to 24.76×10^4 cm^2/V.s (N = 2). The obtained results on the carrier mobility at the GNR/h-BN(0001) interface correlate well with reported data [10]. It should also be noted that according to the PBEsol (PBE-D2) calculations the values of the carrier mobility in N-ZGNR/h-BN(0001) heterostructures appear to be 3.5% (7%) higher than in ZGNR without substrate.

Thus, the influence of substrate and nanoribbon width on the low-energy spectrum of π-electrons, local magnetic moments of interface atoms, and the mobilities of charge carriers in N-ZGNR/h-BN(0001) (N = 2, 4, 6, 8) heterostructures have been studied using ab-initio plane-wave pseudopotential method within the DFT framework. Using two different approximations for total energy functional (PBEsol, PBE-D2) we have ascertained the effect of increase of charge carriers mobility by reduction of dimers' number in nanoribbons. Our DFT study have shown that the mobilities of charge carriers in N-ZGNR/h-BN(0001) heterostructures were 5% higher than in suspended nanoribbons. Predicted high electron

mobility in the N-ZGNR/h-BN(0001) (N = 2, 4, 6, 8) heterostructures may serve as a good foundation for the fabrication of graphene-based electronic components.

References

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Figures

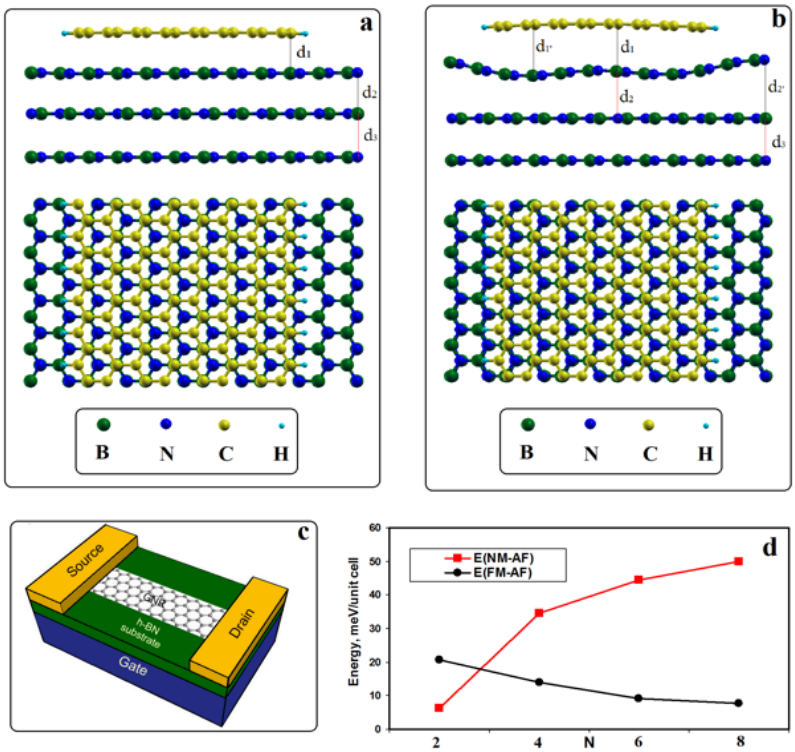

Figure 1. The relaxed atomic structure of 8-ZGNR/h-BN(0001) calculated within two different approximations: DFT-D2 (a) and GGA-PBEsol (b), where top – front view, bottom – top view. A model of GNR-FET (c) with Au contacts (Source and Drain, yellow) on substrate h-BN (blue); the total energy difference (d) between the non-magnetic (NM) and magnetic (FM, AF) states, depending on the number of C dimers in ZGNR.