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Towards single-gate field effect transistor utilizing dual-doped bilayer graphene

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ABSTRACT

In this work, based on experimental possibilities, our first-principles calculations predict a sizeable bandgap opening in bilayer graphene (BLG) by n-doping from decamethylcobaltocene (DMC) and p-doping from functionalized amorphous SiO_2 (a-SiO_2) gate dielectric. With DMC monolayer on BLG and the maximum O_2^- on the surface of a-SiO_2 gate dielectric, the dual-doped BLG presents a bandgap of 390–394 meV and a Dirac level shift of −59 to −52 meV. The former is very close to the technical requirement of 400 meV, while the latter properly lies in the accessible range of the gate voltage of 300 meV. The high carrier mobility largely remains with the on/off current ratio satisfying the technical requirement of 10^4–10^7. The external electric field is not needed in this technique, which avoids a complex fabrication step for preparing a dual-gate structure and a substantial reduction in carrier mobility and on/off current ratio induced by adding an extra gate.

1. Introduction

Modern digital logic is based on Si complementary metal-oxide-semiconductor (CMOS) technology, where the logic gates consist of Si metal-oxide-semiconductor field effect transistors (MOSFETs). For decades, making MOSFETs smaller has been the key to improve the digital logic [1]. However, MOSFET scaling is approaching its limits due to the physical limitation of Si as well as the short-channel effects [2,3]. Thus, the CMOS-based technology has been forecasted to end by 2022 [4]. To continue the development in this field, a suitable substitute of Si is necessary as the channel material of field effect transistors (FETs). Graphene, a two-dimensional sheet of C atoms tightly packed into a honeycomb lattice, has attracted considerable attention since its discovery in 2004 [5]. According to the scaling theory, a FET with a thin barrier and a thin gate-controlled region will be robust against the short-channel effect down to very short gate lengths [6]. Therefore, the possibility of making channels at atomic layer thick is considered as the most attractive feature of graphene for use in FETs [7]. Moreover, graphene has an extremely high carrier mobility (μ) up to 2×10^5 cm^2 V^{-1} s^{-1} [8,9]. Both impressive properties make graphene a promising channel material for high-speed FETs. However, due to the absence of a bandgap, the pristine graphene-based FETs have a very low on/off current ratio (I_{on}/I_{off}) [10,11], leading to high static power dissipation [7].

As put forward by the International Technology Roadmap for Semiconductors, any successor to Si MOSFET used in CMOS-like logic must have excellent switching capabilities and an I_{on}/I_{off} between 10^4 and 10^7, which requires the semiconducting channel with a sizeable bandgap close to 400 meV or more [4,7]. Additionally, for graphene FETs, the shift of the Dirac level (E_D, the energy level in the middle of the bandgap opened in graphene) should be within the gate voltage accessible range, where the typical FETs exhibit 300 meV shifts at

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100 V gate voltage [12]. Although the sizeable bandgaps larger than 400 meV have been opened by lateral quantum confinement [13–16], heteroatom doping [17,18], and covalent functionalization of graphene [19,20], the conical bands of graphene disappear and μ value is drastically reduced due to the strong scattering from edges for lateral quantum confinement and from heteroatoms for heteroatom doping, and the removal of π electrons for covalent functionalization. To maintain high μ values, the structure of graphene should be intact, and the interface interaction between graphene and other materials should be weak. Up to now, two feasible schemes have been proposed to open bandgaps in graphene without degrading its high μ value. One is breaking the equivalence between the A and B sublattices of single-layer graphene (SLG), which has been achieved by the adsorption of aromatic molecules [21], depositing SLG on hydrogenated or fluorinated hexagonal BN [22], sandwiching SLG between hexagonal BN or partially hydrogenated SLG [23,24], and the epitaxial growth of SLG on SiC substrate [25]. Although the E_D shift is small, the opened bandgap is unfortunately lower than 270 meV without an external electric field [21–25]. Another is destroying the inversion symmetry of bilayer graphene (BLG), by applying an external electric field perpendicular to BLG [11,26–28] or by charge transfer doping from the single-side adsorption of organic molecules or metallic atoms [10,29–35]. In the former case, the largest bandgap opening is confined to 250 meV due to the limited strength of gate dielectric stacks [11,26–28]. Moreover, a dual-gate structure is required to apply an external electric field [11,28], which increases the complexity and the cost of FETs. Also, the addition of an extra gate results in a substantial reduction of μ and I_{on}/I_{off} values in graphene FETs [36]. In details, if this deduction is denoted as the ratio of single-gate/dual-gate, the corresponding ratios for μ values of graphene hole (μ_h) and electron (μ_e) are 6.75/1 and 9.02/1, respectively; while the corresponding ratios for I_{on}/I_{off} values are 3.04/1 and 1.81/1 under negative and positive gate voltage, respectively [36]. From a device design point of view, it is desirable to control a FETs electrical conductivity by a single gate. Fortunately, the charge transfer doping from organic molecules or metallic atoms can generate an interlayer electric field, leading to a significant bandgap opening for single-gate applications [10,29–35]. In general, the clustering of metallic atoms always happens on the graphene surface, which brings out charged impurities and leads to serious reduction of μ value [37]. On the contrary, this clustering can be avoided by molecular doping due to the intermolecular repulsion [29,30,32]. So far, the bandgap opening of BLG by single-side molecular doping is usually lower than 230 meV [29–32]. Although the bandgap can be further increased through enhancing doping, the E_D shift may exceed the accessible range of the gate voltage.

For molecular doping, the deposition of organic molecules is usually at single-side, limiting the bandgap opening of BLG. If an opposite doping is introduced into BLG at another side, two layers are needed to carry different types of charges, which can significantly increase the interlayer electric field and thus the opened bandgap. Moreover, the E_D shift can be reduced, which has been proven by a dual molecular doping of BLG [12,38,39]. Up to now, the reported bandgap opening by dual molecular doping is less than 310 meV [12,38–40]. In a conventional FET, one side of the channel always contacts with the gate dielectric. From a technical viewpoint, it is more meaningful to introduce an additional doping from a functionalized gate dielectric. Both experiments and theoretical calculations have revealed that O_2 can bind to the 3-fold-coordinated Si atoms at the widely used amorphous SiO_2 (a-SiO_2) surface to form O_2^-, which brings about a strong p-doping of BLG [10,40,41]. To realize the strongest p-doping of BLG, the O_2 adsorption sites at a-SiO_2 surface should be maximally created. Once the p-doping is identified, an n-type molecular dopant with adequately low ionization energy should be deposited on the other side of BLG. Note that decamethylcobaltocene (DMC) with a D_{5d} symmetry is a promising candidate. Under this symmetry, DMC has an electronic state of $^2E_{1g}$ and an electronic configuration of $(a_{1g})^2(a_{2u})^2(e_{1g})^4(e_{1u})^4(a_{1g})^2(e_{2g})^4(e_{1g})$ [42], where one electron fills the high-energy e_{1g} orbital. This leads to a remarkably low solid-state ionization energy for DMC (3.3 eV) [43], which is even smaller than that of Cs atom. In particular, DMC has been successfully used as an efficient n-dopant in organic electronic materials and devices [43].

In this contribution, we investigate the electronic properties of BLG by p-doping from functionalized a-SiO_2 gate dielectric and n-doping from DMC. First-principles density functional theory (DFT) calculations demonstrate a large bandgap opening of 390–394 meV in this dual-doped BLG with a proper Dirac level shift by −59 to −52 meV. Moreover, a single-gate FET based on this dual-doped BLG shows a high μ value and an I_{on}/I_{off} ratio within 10^4 and 10^7, facilitating its application in CMOS-like logic.

2. Experimental

It is well known that, as a widely used gate dielectric, a-SiO_2 can be obtained by thermal oxidation of Si wafer in a wet environment. The gotten a-SiO_2 layer is coated with hydroxyls [44–46]. The maximal concentration of hydroxyls can reach $(4.9 \pm 0.5)/nm^2$ (arithmetical mean), which includes isolated, geminal, and vicinal ones [45]. If O_2 is adsorbed on the vicinal 3-fold-coordinated Si atoms, the outside O atoms of two adjacent O_2^- may combine to form one O_2. The remaining O atoms will covalently interact with BLG [47], which seriously decreases the μ value. Namely, the vicinal adsorption sites are useless. Therefore, a vacuum pretreatment at 673 K is necessary. With this pretreatment, the vicinal hydroxyls disappear through a dehydration reaction by forming siloxane bridges [45]. Following this, the O_2 adsorption sites can be created by removing the residual hydroxyls with a multistep thermochemical method [48]. Here, the O_2 adsorption sites are composed of 3-fold-coordinated (93.2%) and 2-fold-coordinated (6.8%) Si atoms [45]. Note that O_2^- may also be built when O_2 is adsorbed on the 2-fold-coordinated Si atoms at a low concentration [47]. Finally, the a-SiO_2 gate dielectric with maximal O_2^- concentration [about $(2.34 \pm 0.5)/nm^2$] [45] could be produced by the adsorption of dry O_2. The cell parameters of the functionalized a-SiO_2 gate dielectric are chosen to match the 4×4 supercell of BLG. In the cell, there are two O_2^-, which corresponds to a concentration of 2.39/nm^2 and relates to the experimental possibilities discussed

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