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Device Performance Analysis of Graphene Nanoribbon Field-Effect Transistor with Rare-Earth Oxide (La_2O_3) Based High-k Gate Dielectric

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Abstract: ***Graphene nanoribbon field-effect transistors (GNRFETs) are promising devices for beyond-CMOS nano electronics in favor of logic applications because GNR offers high mobility for ballistic transport, high carrier velocity for fast switching, monolayer thin body for optimum electrostatic scaling, and excellent thermal conductivity. In this study, the device performance and limitations of GNRFETs are investigated by reducing the channel length below 10 nm. The double gate GNRFET structure is considered where the armchair GNR is sandwiched between two ultrathin La_2O_3 high-k gate dielectrics. The double gate geometry together with CMOS compatible La_2O_3 high-k dielectric offers large gate electrostatic control and consequently large insulator capacitance, which lead to the operation of GNRFET close to quantum capacitance limit. The simulation study was performed using self-consistent solution of the 3D Poisson equation and 1D Schrödinger equation within the non-equilibrium Green's function formalism.***

Keywords: Graphene Nanoribbon (GNR), Field effect Transistor (FET), High-k gate dielectric, La_2O_3, CMOS.

I. INTRODUCTION

The recent discovery of graphene in 2004, which is a single atomic sheet of graphite forming a dense honeycomb two-dimensional (2D) crystal structure, is considered as a promising materials for future non-classical devices and nano electronics circuits because of its exceptional electronic properties such as the large carrier mobility, the possibility tunable band gap and planer structure [1-5]. The high mobility and carrier velocity of graphene promises ballistic and high switching speed devices. Graphene also offers ultrathin body for optimum electrostatic scaling as well as excellent thermal conductivity. Moreover, the biggest advantage of graphene is the potential to produce wafer-scale graphene films with full planar processing which further guarantees high integration potential with conventional Si CMOS (complementary metal-oxide semiconductor) fabrication processes, that makes graphene a significant advantage over carbon nanotubes. Indeed, 2D graphene is a semi-metal without a band-gap. However, a band-gap can be obtained by using a narrow graphene nanoribbon (GNR). Unlike carbon nanotubes (CNTs), which are mixtures of metallic and semiconducting materials, a recent experiment demonstrated that all sub-10nm GNRs are semiconducting due to the edge effect, which make them more attractive for electronic device applications [6-8]. Recently, a silicon compatible, transfer-free, and in situ GNR FET-manufacturing technique has been demonstrated experimentally which further promises the possibility of integrating GNRFETs into existing silicon technology [9].

On the other hand, the gate dielectric is an essential component of a transistor, which can significantly impact the critical device parameters such as trans conductance, sub-threshold swing and frequency response. Therefore, exploring graphene for future electronics requires effective integration of high quality gate dielectrics, in particular the high-κ dielectrics. High-k dielectrics are being actively pursued by the semiconductor industry to replace traditional SiO_2 as the gate dielectric for future generations of CMOS transistors. The concept of using a high-k dielectric's larger physical thickness to achieve the same EOT (Equivalent oxide thickness) so as to reduce the tunneling leakage current, and the search for the best high-k gate dielectric has continued ever since. Among many high-k gate dielectrics investigated so far, rare-earth based high-k gate dielectrics particularly La_2O_3 has been demonstrated promising for next generation scaled MOSFETs below sub-nm EOT level [10-11].

In this report, the device performance of GNRFETs have been studied by reducing the channel length below 10 nm. In the proposed double gate GNRFET structure, the armchair GNR is considered as a sandwiched structure between two ultrathin La_2O_3 high-k gate dielectric. Indeed, the double gate geometry as well as chosen La_2O_3 high-k dielectric together leads to the operation of GNRFET close to quantum capacitance limit due to large insulator capacitance of La_2O_3. The device simulation studied here have been performed using self-consistent solution of the 3D Poisson equation and 1D Schrödinger equation within the non-equilibrium Green's function formalism.

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II. SIMULATION OF La_2O_3 GNRFET DEVICE

A. Graphene and GNR Properties

Graphene is basically a single atomic layer of graphite with honeycomb crystal lattice. Unfortunately, a 2D graphene sheet has zero band gap, which makes it metallic and unable to be turned on or off as shown in Fig. 1.

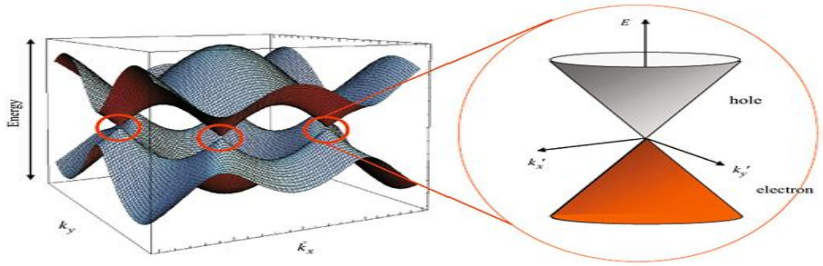


Fig. 1: The energy band structure of graphene. The valence band (lower band) and conduction band (upper band) touch at six points, (Dirac points) where the Fermi level is located.

However, in order to make graphene a good semiconductor, the energy band gap needs to be open. This is possible by patterning graphene into 1-D graphene nanoribbons (GNRs) with widths below 10 nm [10]. In fact, the band gap of a GNR varies inversely proportional to its width. Now, if the width of the GNR increases, the band structure of GNRs gradually returns to that of a 2-D graphene sheet. Meanwhile, based on the edge geometry, GNRs are categorized in two types: armchair-GNRs and zigzag-GNRs [12] as shown in Fig. 2.

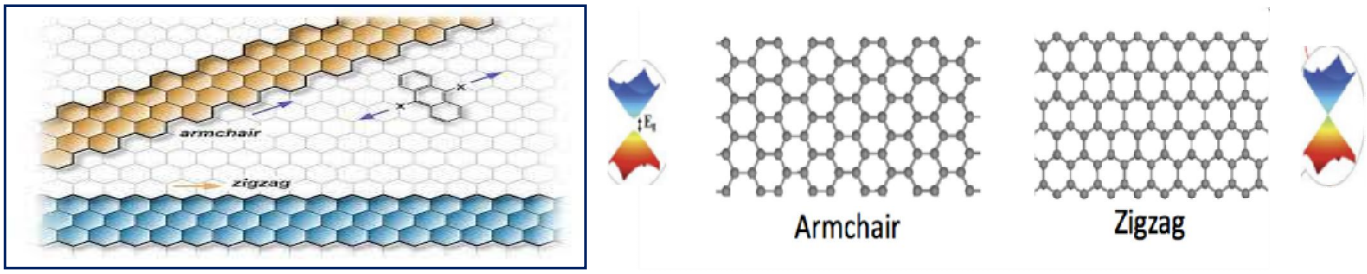


Fig. 2: Cuts along two directions of a 2-D graphene sheet will produce zigzag and armchair termination of the GNRs.

The armchair GNR can yield semiconducting properties having finite band gap depending on the number of atoms in transverse direction while the zigzag GNR mainly exhibits metallic characteristics. Therefore, in this study we have considered armchair-GNR to exploit its semiconducting properties for GNRFETs.

B. Proposed La_2O_3 GNRFET structure

The double gate GNRFET structure used in this study is shown in Fig. 3. In this structure the armchair GNR is sandwiched between two ultrathin La_2O_3 insulator layers with the relative dielectric permittivity, ε_r =24, and the oxide thickness 1 nm in a double metal gate topology. The armchair GNR (7,0) considered here has a ribbon index of 7 which is basically represented by the number of dimer lines in transverse direction. The double gate geometry with La_2O_3 offers large gate electrostatic control and resulting large insulator capacitance, which lead to the operation of GNRFET close to quantum capacitance limit. Now for source and drain ohmic contacts, the extensions of GNR on both sides of intrinsic channel are needed to be doped in order to tune the carrier injection from source to GNR channel. In this simulation, the source and drain sides are heavily doped by keeping doping concentration around $0.01n^{++}$ -type dopants per carbon atom.

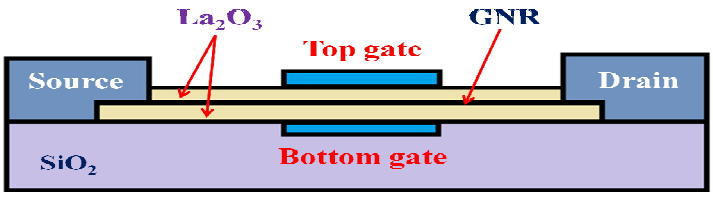


Fig. 3: 2D vertical cross-section of double gate La_2O_3 GNRFET.

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C. Simulation approach for La_2O_3 GNRFET structure

To evaluate the performance of GNRFETs, the quantum based transport simulation is used where non-equilibrium Green's function (NEGF) approach is implemented to solve the Schrodinger equation under non-equilibrium condition [13]. The NEGF method is capable of providing the atomistic description of channel materials as well as the effects of ohmic contacts on carrier transport in the GNR channel. Meanwhile, the charge density and potential profile has been evaluated by constructing a self-consistent calculation between electrostatic *i.e.* Poisson formulism and transport *i.e.* NEGF formulism. The effective masses of the GNR (7,0) sub-bands have been evaluated by tight-binding (TB) calculation for the selected unit block initially with zero potential so as to use the successive transport calculations in the self-consistent fashion. The unit block dimension considered in the simulation is of the length of $3a_{cc}$ and 14 atoms (where a_{cc} is carbon-carbon bond length). Next by considering the initial potential distribution, the corresponding conduction and valence band energies along with associated wave function have been evaluated by repeated tight-binding calculation at every unit block. Thereafter, the effective concentration of electron and holes are evaluated considering transport equations in NEGF formulism for 1D subbands. Now, considering profile of charge concentrations and the potentials at electrodes, The Poisson equation is solved with proper boundary conditions. Finally, the source to drain current, I_{ds} is calculated by determining the transmission function [14-15]. Figure 4 illustrates a flowchart for the detail of self-consistent algorithm used to simulate the device performance of La_2O_3 GNRFET using numerical software, Matlab.

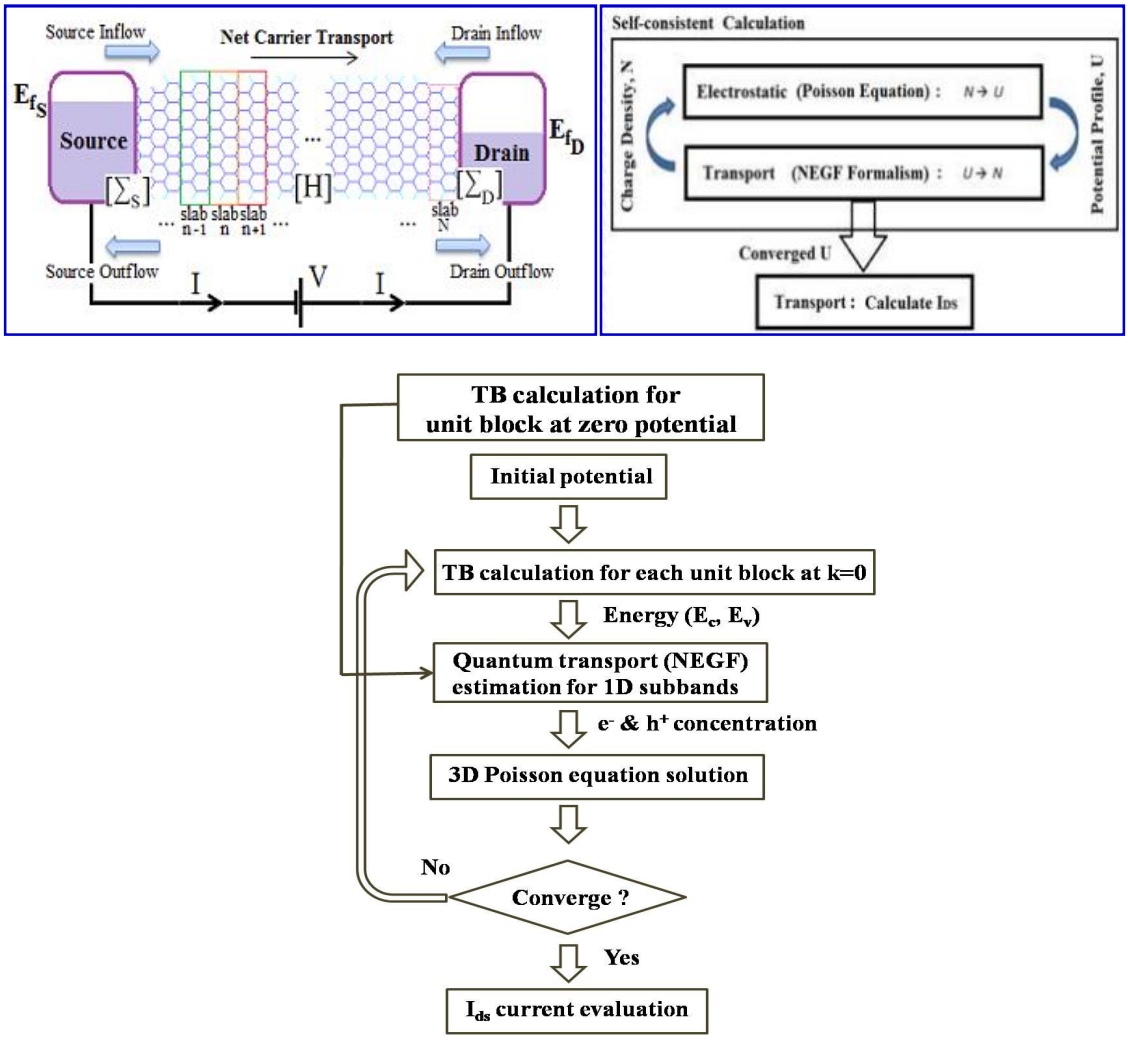


Fig. 4: The flowchart for the self-consistent algorithm used to simulate the device performance of La_2O_3 GNRFET.

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III. RESULTS AND DISCUSSION

Figure 5 shows the energy dispersion relation of considered GNR (7,0) structure which opens a bandgap over 1eV, thus confirms its semiconducting properties.

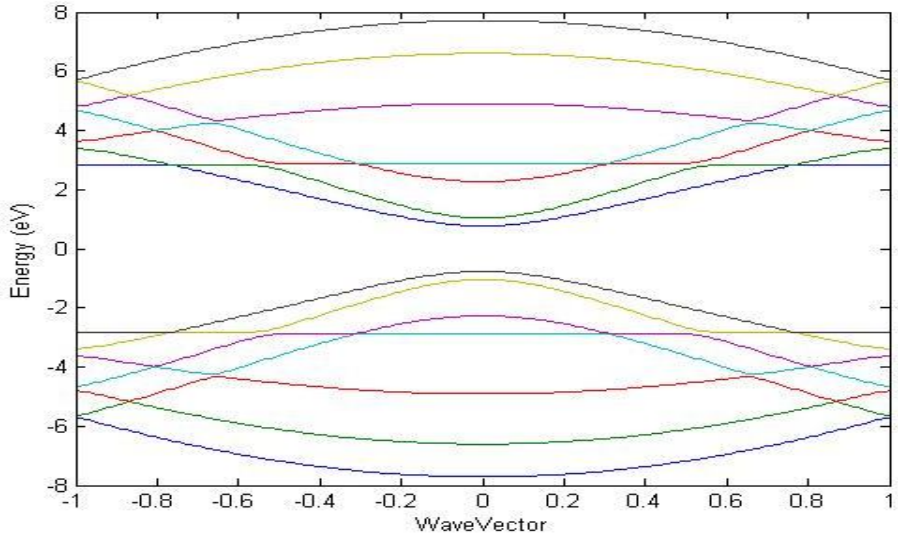


Fig. 5: The energy dispersion of GNR (7,0) having bandgap > 1 eV.

The output characteristics (I_{ds} *vs* V_{ds} for different values of V_{gs}) of La_2O_3 GNRFET is shown in Fig. 6. The presence of saturation region for the short channel length, L_g= 5nm, indicates good MOSFET type device behavior.

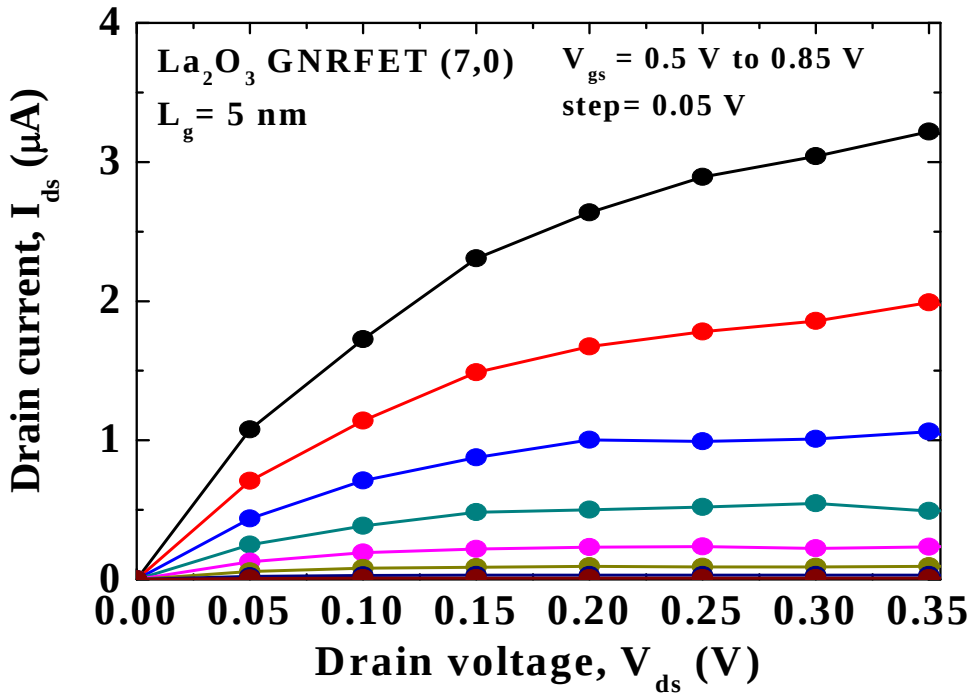


Fig. 6: The output characteristics (I_{ds}-V_{ds}) of La_2O_3 GNRFET (7,0) with gate length, L_g=5nm.

Indeed, the saturation slope in GNRFET mainly depends on GNR width. When V_{ds} increases, the wider GNR structure may increase the depletion of electrons in the valence band. This leads to the accumulation of positive changes in GNR channel and therefore saturation region does not vary with decreasing channel length. On the other hand, the transfer characteristics (I_{ds}-V_{gs} at different V_{ds}) of La_2O_3 GNRFET is shown in Fig. 7.

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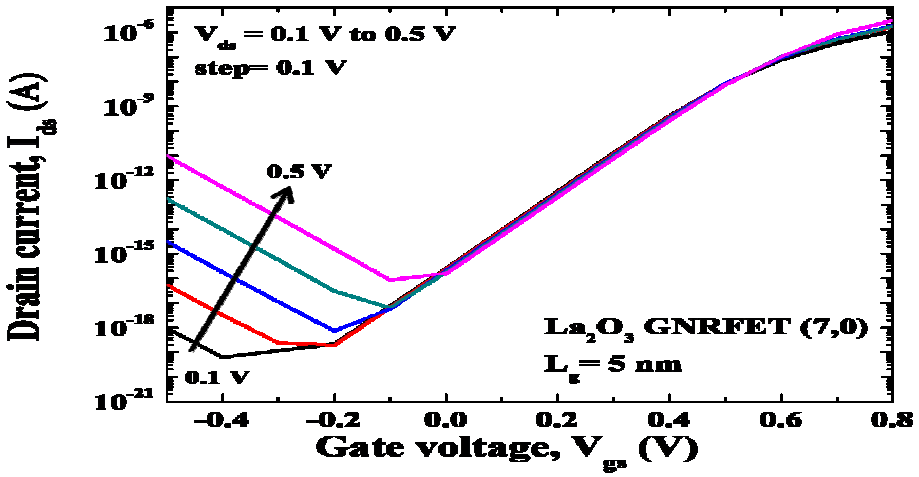


Fig. 7: The transfer characteristics (I_{ds}-V_{gs}) of La_2O_3 GNRFET (7,0) with gate length, L_g=5nm.

The drain current, I_{ds} shows a minimum current at a particular gate voltage, V_{gs}. This minimum current occurred at the charge neutrality point where the electron concentration is equal to the hole concentration. However, due to applied gate voltage the induced electrostatic potential changes the amount of charge carriers in GNR channel. Meanwhile, the minimum current is increased and shifted by increasing drain voltage as a result of accumulation of positive charges in GNR channel due to band-to-band tunneling from the source to GNR channel as well as with drain induced barrier lowering (DIBL) effect in short channel devices.

Figure 8 shows the 3D potential distribution of La_2O_3 GNRFET calculated by solving 3D Poisson equation.

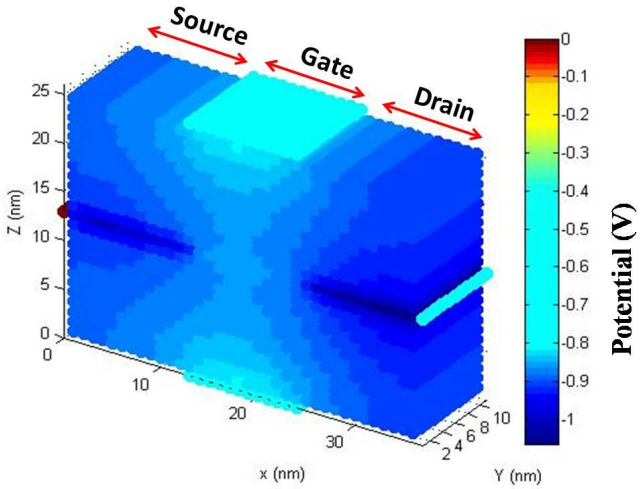


Fig. 8: The typical 3D potential distribution evaluated by solving 3D Poisson equation for La_2O_3 GNRFET (7,0) with gate length, L_g=5nm.

IV. CONCLUSION

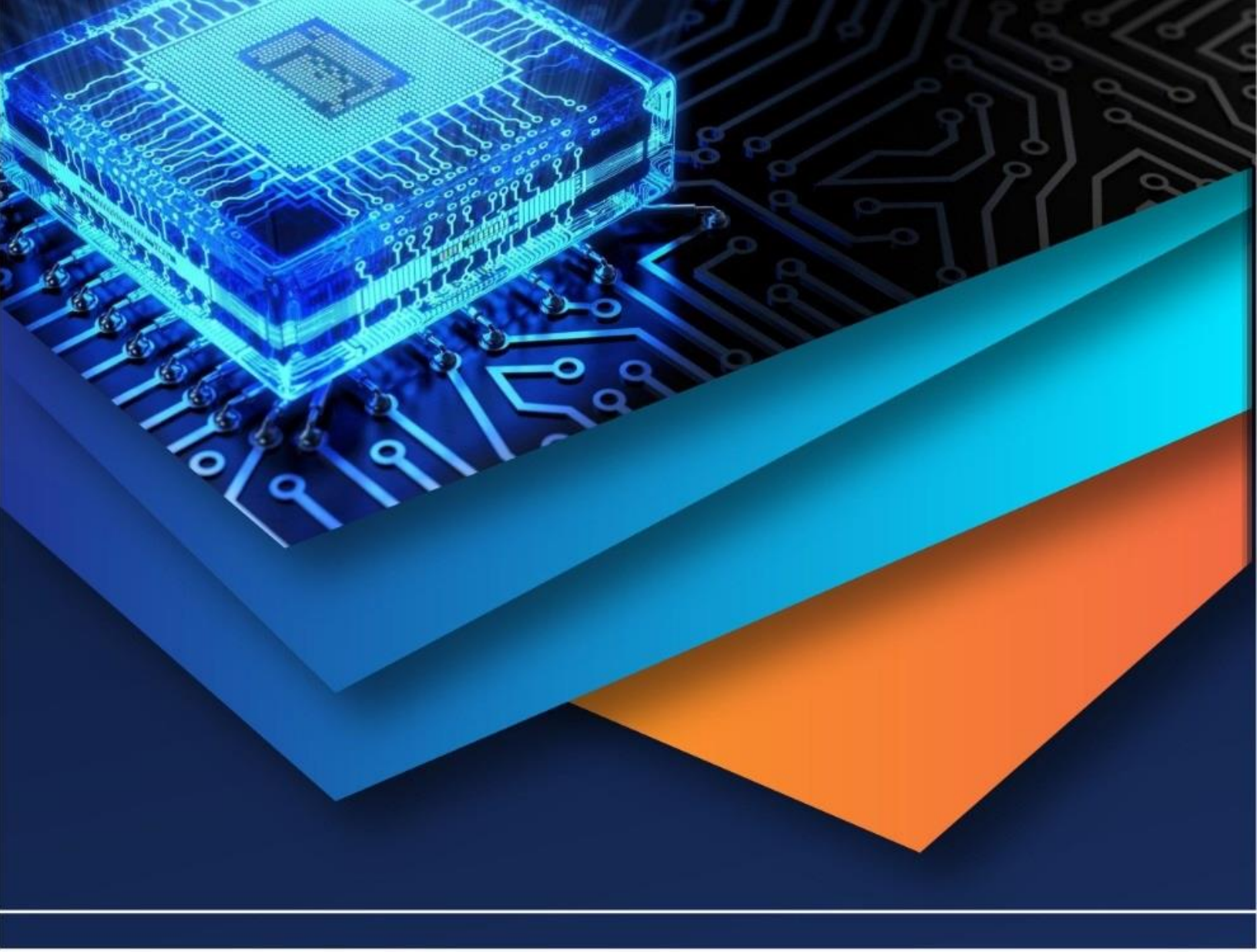
In conclusion, a promising alternative and good MOSFET type device behavior has been demonstrated for graphene nanoribbon field-effect transistors (GNRFETs) using CMOS compatible La_2O_3 high-k dielectric. The double gate GNRFET structure is considered where the armchair GNR is sandwiched between two ultrathin La_2O_3 high-k gate dielectrics. The double gate La_2O_3 GNRFET has been simulated by solving quantum transport equation with self-consistent electrostatics in mode space. The quantum transport simulation has been performed using non-equilibrium Green's function (NEGF) approach, where Schrödinger equation is solved under non-equilibrium condition. Because, NEGF model provides the atomistic description of channel material, a comprehensive understanding of tunneling effects, as well as the effects of metallic contacts on carriers transport in the GNR channel.

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