Ultrahigh on/off-current ratio γ-graphyne-1 nanotube-based sub-10-nm TFET modeling and simulation

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Abstract
The use of γ-graphyne-1 nanotubes (GyNTs) in tunneling field effect transistors (TFETs) suppresses ambipolarity and enhances the subthreshold swing (SS) of TFETs, due to the large energy band gap and high electron effective mass of GyNTs. In this research, the analysis of the structural, electronic and thermoelectric properties of the γ-graphyne-1 family under the deformation potential (DP) approach reveals that the electron–phonon mean free path (MFP) of an armchair GyNT (3AGyNT) and zigzag GyNT (2ZGyNT) are 24 and 279 nm, respectively. Therefore, ballistic transport of sub-10-nm 3AGyNT-TFETs and 2ZGyNT-TFETs in different channel lengths is investigated utilizing the non-equilibrium Green's function (NEGF) formalism in the DFTB platform. An ultrahigh on/off-current ratio (OOCR) value of $1.6 \times 10^{10}$ at $V_{DD} = 0.2$ V and very low point SS of 5 mV/dec were demonstrated by the 3AGyNT-TFET with a channel length of 9.6 nm. 2ZGyNT-TFETs show higher on-state current and SS and lower OOCR than those of 3AGyNT-TFETs. A linear relationship was found between channel length and logarithmic off-state current that is consistent with the WKB approximation. The obtained results along with the ultralow power consumption of the proposed GyNT-TFETs make them candidates to replace digital silicon MOSFETs in next-generation nanoelectronic devices.

Keywords γ-Graphyne-1 · DFTB · TFET · I–V characteristic · Mean free path · Subthreshold swing

1 Introduction
Over the past several years, numerous theoretical and experimental efforts have been carried out to enhance the efficiency of metal–oxide–semiconductor field-effect transistors (MOSFETs) with sub-10-nm gate length [1–4]. Thermionic emission (TE), which is the basis for the operation of conventional MOSFETs, is the main obstacle to decreasing the threshold voltage ($V_{th}$) and power dissipation of transistors by imposing a lower limit on the subthreshold swing (SS) equal to 60 mV/dec at room temperature [5]. On the other hand, quantum mechanical tunneling current through the potential barrier of the channel is comparable to the $I_{off}$ within the sub-10-nm gate length. Therefore, MOSFETs suffer from a lower limit of SS and both TE and tunneling current simultaneously in the off-state.

Gate-all-around (GAA) MOSFETs have the ideal geometrical structure to efficiently control the channel current and short-channel effects (SCEs) to achieve SS levels as close to 60 mV/dec as possible. According to the International Technology Roadmap for Semiconductors (ITRS) and International Roadmap for Devices and Systems (IRDS) documentation, the lower limit of gate length in silicon nanowire-based GAA MOSFETs is 10 nm, and reduction of the technology node will only be achieved via monolithic 3D (M3D) integration by stacking several layers of devices after 2024 [6–8]. New structures and technologies together with the innovative materials have been widely investigated by the electronic industries and researchers to scale down channel length and/or SS of MOSFETs. Nano-electromechanical gate FETs (NEMFETs) [9], ferroelectric dielectric...
FETs [10], negative capacitance FETs (NCFETs) [11], and impact ionization FETs [12] have potentially lower SS than conventional MOSFETs. However, the common drawback in these transistors is an intrinsic delay in their switching mechanisms [13].

The transient mechanism of NEM-FETs is based on the mechanical forces via electrostatic forces with a high delay that limits their application in very high-frequency (VHF) and ultrahigh-frequency (UHF) bonds [9].

The structure of an impact ionization MOS (IMOS) is the same as a p-i-n TFET with an added gate underlapped portion in the channel. The IMOS needs positive feedback to break down material of the gate underlapped portion of the channel, and then the excess carriers will transfer to the drain via band-to-band tunneling (BTBT). Therefore, the delay of IMOS is the delay required for avalanche breakdown and the delay of its based TFET.

Ferroelectric FETs (FeFETs) and NCFETs have an added ferroelectric layer on the oxide layer of FinFETs. The polarization–electric field (PE) characteristic of the ferroelectric layer has two NC and hysteresis regions. Selecting the load line in the NC region of the PE curve causes an increase in the gate voltage and finally a decrease in the SS of FeFETs, while simultaneously increasing the delay of the FeFETs to several times the delay of their based FinFETs via the NC effect [14]. Only a sufficiently thick ferroelectric layer enhances the SS of FeFETs, but by increasing it beyond a certain thickness, the load line tends to enter the hysteresis region, which prevents a further increase in the gate voltage and simultaneously increases the delay in the FeFET because of the high intrinsic delay of the polarization change, which is normally avoided in digital applications. Thus, these transistors suffer from a trade-off between lowering of SS and an increase in delay.

The delay in TFETs is the same as in MOSFETs, which is based on the time required to charge $C_{gs}$ via the transistor current, without any added delay, the same as the aforementioned transistors. GyNT-TFETs have very low on-state and off-state current, but simultaneously have very low quantum capacitance in their channel; hence the delay remains constant. The delay of TFET is equal to the $\tau = \Delta Q/l_{on}$ in the channel from the off-state to the on-state. By the calculation of Mulliken charge utilizing the Atomistix ToolKit (ATK) package, the delay of 2ZGyNT-TFET in the current of $1 \times 10^{-8}$ A is $\tau = 0.15e/10^{-8} = 2.4$ ps.

TFETs are gated p-i-n junction devices which are biased in the reverse direction, with ultralow SS and high mobility at room temperature. Carbon nanotube (CNT)-based GAA TFETs (CNT-TFETs) are important homojunction transistors using semiconducting CNTs with $n \neq 3v$ in the source, channel, and drain regions [15, 16]. From a material point of view, since a graphene sheet has metallic properties, CNTs have the ability to convert the channel of the CNT-TFET from semiconductor to metal by changing its chiral vector to $n = 3v$, which can degrade the overall operation of a digital transistor. Hence, CNTs cannot provide reliable performance for use in the electronics industries, which tend to use semiconducting channels in nanoelectronic devices, particularly in high on/off-current ratio (OOCR) digital transistors [17].

Graphyne is another 2D allotrope of carbon that was first predicted by Baughman in 1987 [18]. Four types of high-symmetry nanostructures of the graphyne family are α, β, γ, and 6,6,12-graphynes. Among carbon allotropes consisting of all types of graphyne, only γ-graphyne-n are intrinsic 2D semiconductors which have n acetylenic linkages consisting of two sp hybridized carbon atoms between hexagonal rings of sp² hybridized carbon atoms of graphene.

Using cross-coupling reaction, γ-graphyne-2 (graphdiyne) multilayer sheets and graphdiyne multi-walled nanotube arrays were successfully fabricated by Guoxing Li et al. in 2010 and 2011, respectively [19, 20]. It was shown that the graphdiyne sheets have a semiconducting behavior. Qiaodan Li and teammates succeeded to synthesize monocrystalline single layer γ-graphyne-1 sheets through a mechanochemical reaction in 2018 [21]. The atomic and electronic structure of the synthesized samples were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), energy-dispersive X-ray spectroscopy (EDX), transmission electron microscopy (TEM), and ultraviolet (UV)–visible spectroscopy. They found that the band gap energy and lattice constant of γ-graphyne-1 sheets are 2.53 eV and 0.69 nm, respectively.

The electronic and transport properties of the graphyne sheet and its related GyNTs and GyNT-TFETs need to be calculated based on a single method, which in this paper is DFTB utilizing NEGF formalism. GW is a time-consuming method and used only for band gap calculation. The previously computed band gap of graphdiyne using the GW method is 1.1 eV [22]. Density functional theory (DFT) calculations reveal that the band gap of graphyne is nearly the same as that of graphdiyne [23]. The previously calculated band gap energy of γ-graphyne-1 sheets using different DFT, HSE06, DFTB, and B3LYP methods shows diverse values of 0.45 eV [17, 24, 25], 0.98 eV [24, 26], 1.28 eV [24, 27], and 2.23 eV [28], respectively. The single aforementioned experimental result shows an overestimated band gap value of 2.53 eV because of the presence of oxygen in the synthesized γ-graphyne-1 sheet [21]. The calculated band gap in DFT methods are usually underestimated, particularly in large band gap materials like γ-graphyne-1 [28, 29]. In this research, the band gap energy calculated with the DFTB method is 1.34 eV, which agrees with the previous calculations and is between the comparably precise HSE06 method and the single experimental results [30, 31]. Hence, DFTB is a reliable method and is utilized in all calculations in this
paper. The band gap of graphene calculated with different methods shows their convergence to the results of the DFTB method with respect to their complexity, from the DFT, HSE06, and GW methods with calculated band gap values of 0.45 eV, 0.98 eV, and nearly 1.1 eV, respectively, to the DFTB method with computed band gap of 1.34 eV.

The electronic and structural properties of γ-graphyne nanotubes have been investigated and it is shown that the lower limit band gap energy of high diameter GyNTs is the band gap of γ-graphyne-1 sheet [30]. In 2016, Desai successfully synthesized a homojunction MOSFET with 3.9 nm effective channel length. In this transistor gate was a metallic CNT with 1 nm diameter and the source-channel-drain material was a two layer MoS$_2$ that was electrostatically doped to $n^+$ in the source and drain regions via a bottom gate at 5 V bias [4].

In this paper, two GAA homojunction p-i-n TFETs as steep subthreshold slope transistors are constructed in virtual NanoLab (VNL) and investigated via the ATK package using 2ZGyNT and 3AGyNT. For the first time, the relaxation time, mobility, and mean free path (MFP) of the γ-graphyne-1 family are calculated. It is shown that the electron MFP of 2ZGyNT and 3AGyNT is 279 and 24 nm, respectively. Ballistic transport calculations show that the $I_{on}$ of the 2ZGyNT-TFETs is nearly $10^3$ times that of the 3AGyNT-TFETs. An ultrahigh OOCR value of $8.9 \times 10^{15}$ at $V_{th} - V_{gs} = 0.5$ V and ultralow point SS value of 5 mV/dec at $V_{gs} = V_{th}$ are achieved, where $V_{th}$ is the threshold voltage. At the bias conditions of $V_{th} - V_{gs} = V_{ds} = 0.2$ V, the calculated $I$–$V$ characteristic of the 3AGyNT-TFET with a channel length of 9.6 nm shows OOCR and SS values of $1.6 \times 10^{10}$ and 19 mV/dec, respectively. The average SS and OOCR of the 3AGyNT-TFET with $L_{ch} = 3.6$ nm are 59 mV/dec and $2.4 \times 10^3$, respectively. The impact of channel length on the performance of the TFETs is considered via the $I$–$V$ characteristic of the GyNT-TFETs in the subthreshold region, which is compatible with the WKB (Wentzel–Kramers–Brillouin) approximation.

2 Computational methods

γ-Graphyne-1 nanotubes and transistors are constructed using the VNL software. Atomistic calculations of GyNTs and GyNT-TFETs are carried out via the ATK package. In the geometrical relaxation of GyNTs, the atomic force tolerance is set to 0.01 eV/Å. The convergence criterion of Hamiltonian energy is $10^{-2}$ in DFTB- and DFT-based calculations. A basis set of mio is used in the DFTB method. In the DFT method, the core-valance interactions are calculated by the PseudoDojo pseudopotential, which is a norm-conserving Troullier–Martins pseudopotential. The basis set is set to the medium. The electron–electron interactions are taken into account by the exchange–correlation functional of the Perdew–Burke–Ernzerhof (PBE) approach of generalized gradient approximation (GGA) [32]. The vacuum space is more than 17 Å in the simulations. A Monkhorst–Pack grid of k-points is used in the reciprocal lattice sampling in the k-space and is set to $1 \times 1 \times 70$ for 1D GyNTs. The real space grid is based on the mesh cutoff energy of 50 Ry. Bulk nanomaterials and devices are investigated at room temperature (300 K) in all simulations. The current of the TFETs is calculated utilizing the Landauer–Büttiker formula in the non-equilibrium Green’s function (NEGF) approach [33]:

$$I(V_h) = G_0 \int_{-\infty}^{+\infty} dE/e[f_L(E - \mu_L) - f_R(E - \mu_R)]T(E,V_{ds})$$

where $G_0 = 2e^2/h = 77.4 \mu S$ is the conductance of one level channel, $e$ is the electron charge, $T(E,V_{ds})$ is the transmission coefficient in the $V_{ds}$, $f_L$ and $f_R$ are the Fermi–Dirac distribution functions, and $\mu_L$ and $\mu_R$ are the electrochemical potentials of the left and right electrodes, respectively.

3 Results and Discussion

The unit cell of γ-graphyne-1 contains of a basis of 12 carbon atoms. As depicted in Fig. 1a, the 2D γ-graphyne-1 sheet has a chiral vector of $C_\parallel = n_1 a_1 - n_2 a_2$, where $a_1 = a_{1x} \text{ and } a_2 = a_{1y}$ are unit vectors. Zigzag and armchair γ-graphyne-1 nanotubes are formed via rolling the γ-graphyne-1 sheet along its zigzag and armchair chiral vectors, respectively. The 2ZGyNT unit ring (UR) is constructed by rolling up a supercell consisting of two unit cells in the zigzag direction (2,2), and the UR of 3AGyNT is constructed via the (3,0) chiral vector, as shown in Fig. 1b and c.

As acetylenic linkages in the γ-graphyne-1 sheet break up bonding between the hexagonal rings of graphene, a gap grows in the band structure of the γ-graphyne family, turning them into intrinsic semiconductors. Therefore, GyNT-TFETs are reliable devices and appear promising as an alternative to silicon nanowire GAA MOSFETs, whereas CNT-TFETs are not reliable devices.

To scale down the size of TFETs, GyNTs with small diameter and high chemical stability are utilized. The 2AGyNT and 2ZGyNT are the smallest nanotubes, but 2AGyNT has relatively lower chemical stability due to its lower cohesive energy $E_{coh} = -8.13 \text{ eV}$, whereas 3AGyNT and 2ZGyNT, with nearly equal $E_{coh} = -8.30 \text{ eV}$, have chemically higher stability. Additionally, the diameter of 2AGyNT is 4.4 Å, with high in-plane strain which causes the length of its UR to shrink up to 2% [30]. As a result, in this work, two
GAA homojunction p–i–n TFETs are constructed and investigated using 2ZGyNT and 3AGyNT with diameter values of 7.6 Å and $7.6\sqrt{3}/2 = 6.6$ Å, respectively.

The GyNT has heavy p$^+$ and n$^+$ doping in the source and drain regions, respectively. The only difference between n-i-n conventional MOSFETs and p-i-n TFETs is the doping of their sources from n$^+$ to p$^+$. Therefore, TE in the source is not able to excite enough electrons from the valence band (VB) to the conduction band (CB), specifically in high-energy band gap nanomaterials such as GyNTs. Thus, the current of TFETs is due to the transmission of electrons via BTBT in the on-state and direct tunneling in the off-state.

The concentration of dopants in the source and drain regions are set to as high as values to align the Fermi level energies to their valence band maximum (VBM) and conduction band minimum (CBM), respectively.

The GyNTs are defect- and dislocation-free, and channel regions of TFETs are intrinsic without ionized impurity atoms and unavoidable cross sections, so scattering of electrons in the channel is elastic at low temperatures. At room temperature, transport of electrons is ballistic provided that their MFP is greater than the channel length. Electron-longitudinal acoustic (LA) phonon MFP ($\lambda_{ph}$) of GyNT is much greater than its LA phonon–phonon MFP [34] with a value of $\lambda_{ph} = 15nm$ [35]. $\lambda_e$ of a $\gamma$-graphyne-1 sheet and GyNTs is calculated via $\lambda_e = v_g\tau_{els}$ formula where $v_g$ and $\tau_{els}$ are group velocity and relaxation time of carriers, respectively. $\tau_{els}$ for electrons and holes is calculated via deformation potential (DP) theory. The dispersion relation expression utilizing parabolic approximation of band structure at the lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) of graphyne is $E(k) = h^2k^2/2m^*$, where $h$ is the reduced Planck’s constant and $m^*$ is the effective mass of carriers achieved by $m^* = h^2/\partial^2E(k)/\partial k^2$. By taking into account electron-LA phonon scattering, Bardeen and Shockley in 1950 proposed an analytical formula under the effective mass approximation in the framework of DP theory to
calculate relaxation time $\tau_{rel}$ and mobility $\mu$ of carriers in 2D nanomaterials (Eq. (2)) \[36–38\]. Equation (3) is the amended formula for 1D nanomaterials \[39, 40\]:

$$\tau_{rel} = \frac{2hC}{3k_BTm^*DP^2}$$  \hspace{1cm} (2)

$$\tau_{rel} = \frac{h^2C}{(2\pi k_BT)^{1/2}m^{1/2}DP^2}$$  \hspace{1cm} (3)

where $T$ is temperature, $C$ is the elastic constant, and $DP$ is the deformation potential constant. By investigating the structural and electronic properties of the $\gamma$-graphyne-1 sheet, 2ZGyNT, and 3AGyNT under uniform strain in the range of $-2\% < \Delta a/a_0 < 2\%$, $C = 2\Delta E_{tot}/(S(\Delta a/a_0)^2)$ for 2D and $C = a_0\Delta E/\Delta a^2$ for 1D nanomaterials and $DP = \Delta E_{edge}/(\Delta a/a_0)$ are calculated, and $m^*$ is achieved using the ATK package \[39\]. $\Delta E_{tot}$ is the average increase in the total energy of the $\gamma$-graphyne-1 sheet and nanotubes, and $\Delta E_{edge}$ is the energy shift at the edge of CBM and VBM for electrons and holes, respectively.

As depicted in Table 1, the relaxation time $\tau_{rel}$ and mobility $\mu = e\tau_{rel}/m^*$ of a $\gamma$-graphyne-1 sheet for holes are 0.52 ps and $3.18 \times 10^{13} \text{cm}^2\text{V}^{-1}\text{s}^{-1}$, respectively, agree with the previous calculations and for electrons are 1.05 ps and $7.39 \times 10^{13} \text{cm}^2\text{V}^{-1}\text{s}^{-1}$, respectively, lower than those of previous calculations, which is due to the lower calculated value of $m^*$ in the DFT method relative to the DFTB method \[38, 41\].

The relaxation time and mobility of 2ZGyNT are nearly one order of magnitude higher than those of 3AGyNT, as illustrated in Table 1. This is because of both simultaneously higher $m^*$ and DP of 3AGyNT in comparison with 2ZGyNT. The higher DP constant reveals higher electron–phonon coupling of 3AGyNT relative to 2ZGyNT. The MFPs of electrons and holes of 2ZGyNT and 3AGyNT in this work are greater than the maximum channel length of 10 nm, which thus cannot severely constrain the transmission of carriers through the channel. As a result, the scattering of carriers in sub-10-nm 2ZGyNT-TFETs and 3AGyNT-TFETs is elastic and the transistors work in the ballistic regime.

Two TFETs are constructed in VNL utilizing URs of 2ZGyNT and 3AGyNT. Each UR of 2ZGyNT and 3AGyNT has 48 and 72 carbon atoms with length values of 6.893 Å and 12.061 Å and diameters of 7.6 Å and 6.6 Å, respectively. Table 1 shows the 2ZGyNT-TFET with gate length of 5.5 nm comprising 8 URs. The 2ZGyNT-TFETs and 3AGyNT-TFETs have 4 and 3 URs with doping concentration of 0.003 and 0.008e/atom in the source and drain regions, respectively.  The upper channel length of both the zigzag and armchair sub-10-nm TFETs is 9.65 nm with 14 and 8 URs under the gate, respectively.

Based on the WKB approximation, the transmission coefficient of a square potential barrier is:

$$T = \exp \left(-2L\sqrt{2m^*E_{bar}/\hbar}\right)$$  \hspace{1cm} (4)

where $L$ and $E_{bar}$ are the length and height of the potential barrier, $m^*$ is the effective mass of the material, and $\hbar$ is the reduced Planck's constant. Hence, to maintain the performance of the TFETs in the off-state it is essential to avoid OOCR pinning via leakage current of the insulator utilizing an oxide layer with a sufficiently high effective mass band gap product ($m^*E_{ins}$) (Eq. 4) with simultaneously high dielectric constant (K). SiO$_2$ is an excellent insulator, with $m^*E_{ins} = 0.42 \times 8.9 = 3.7$ but with a low K value of 3.9 \[42\]. HfO$_2$ with better K = 25 has weak insulator properties, with $m^*E_{ins} = 0.17 \times 5.7 = 0.97$ \[43\]. TiO$_2$ in brookite phase has higher $m^*E_{ins} = 1.46 \times 3.5 = 5.1$ than SiO$_2$ and higher K = 80 than HfO$_2$, and so it has relatively lower leakage current and higher performance than the other insulators \[44\]. Hence it is used as gate insulator material in this work and in previous investigation of TFETs \[45\].

In this paper, the graphene sheet and nanotubes are perfect and defect-free, and so there are no trap states associated with any atoms other than carbon. In atomistic quantum calculations, the electronic and transport properties of GyNTs are determined only after relaxation of the sheet and GyNTs. However, in the transport calculation using the ATK

| Table 1 | Calculated electron and hole relaxation time, mobility, and MFP of a $\gamma$-graphyne-1 sheet, 2ZgyNT, and 3AGyNT |
|---------|----------------------------------------------------------|
| $m^*/m_0$ | Electron | Hole | Electron | Hole | Electron | Hole |
| $\gamma$-Graphyne-1 sheet | 0.25 | 0.29 | 0.23 | 0.28 | 0.43 | 0.52 |
| 2ZGyNT | | | | | | |
| 3AGyNT | | | | | | |
| $C [\text{Jm}^{-2}]$ | 762 | | 5.44 | | 1.68 |
| $C [10^9 \text{eVcm}^{-1}]$ | | | | | | |
| $D P [\text{eV}]$ | 4.9 | 6.45 | 1.44 | 2.56 | 1.85 | 3.35 |
| $\tau_{rel} \text{[ps]}$ | 1.05 | 0.52 | 2.49 | 0.71 | 0.34 | 0.10 |
| $\mu [10^4 \text{cm}^2\text{V}^{-1}\text{s}^{-1}]$ | 7.39 | 3.18 | 19.04 | 4.48 | 1.40 | 0.37 |
| $\text{MFP} [\text{nm}]$ | 177 | 81 | 279 | 72 | 24 | 11 |
package utilizing NEGF formalism, all subbands in the VB, CB, and trap states, if any, following relaxation are taken into account, and so with or without trap states, the results of electronic and transport calculations are accurate and correct in this paper.

The $I$–$V$ characteristic of the 2ZGyNT-TFET with 8 URs in its channel (Fig. 2) on bias conditions of $V_{ds} = 0.2$V and $-2V < V_{gs} < 0$ is extracted and depicted in Fig. 3. The same curve of TFET is reproduced for Si and InAs nanowire TFETs utilizing the WKB approximation [46]. It is obvious that two unipolar transistors consisting of n-TFET and p-TFET are constructed with threshold voltage at $V_{th}^n = -0.3V$ and $V_{th}^p = -1.8V$, respectively. Contrary to the higher OOCR and lower SS of the p-TFET relative to the n-TFET, because of the higher work function of the metal gate in the n-type TFET than the p-type TFET, as well as the higher mobility and MFP of electrons than those of holes, this paper is focused on the n-TFETs.

As shown in Fig. 3, the $I$–$V$ characteristic of TFET has two regions. At $V_{gs}^n < V_{th}^n$ and $V_{gs}^p < V_{th}^p$, the TFET is in the saturation region. At $V_{th}^n < V_{gs}^n$, the electrons can tunnel via BTBT from the VB of the source, through a triangular potential barrier, to the CB of the channel, and at $V_{gs} < V_{th}^p$, holes can tunnel from the CB of the drain to the VB of the channel. Between two BTBTs, the gate voltage is in the range of $V_{th}^p < V_{gs} < V_{th}^n$ and TFET is in the subthreshold region in which $I_{ds}$ is characterized by $I_{on}$ and transmission coefficient of the channel.

Unlike conventional MOSFETs, whose SS has a lower limit of 60$mV/dec$, in the TFETs the SS is not constant and has no lower limit, but instead is an increasing function of $|V_{gs} - V_{th}|/m^2$ with the lowest value at $V_{gs} = V_{th}$ (Fig. 3).

By increasing the negative voltage on the metal gate in the subthreshold region, $Log(I_{ds})$ decreases on a nearly parabolic curve versus $V_{gs}$, and SS gradually increases, so the best point as the on-state in a digital TFET is just near the $V_{th}$ with the lowest value of SS. However, in a digital TFET, the average SS is desired, not the point SS, which is the slope of the tangent line of the $I$–$V$ curve. The OOCR and average SS values of the TFET in Fig. 3 are $6.8 \times 10^2$ and 52$mV/dec$ for the n-type TFET, and $1.8 \times 10^3$ and 38$mV/dec$ for the p-type TFET, respectively. Because of higher effective mass, the p-type TFET has higher OOCR and lower SS than the n-type TFET.

TFETs are ambipolar devices whose total current is the sum of the electron and hole current in each $V_{gs}$. In the subthreshold region, electron current is due to the direct tunneling of electrons from the VB of the source to the CB of the drain, and hole current is due to the direct tunneling of holes in the opposite direction in the transmission window of $eV_{gs}$. Hence, by increasing the negative voltage of $V_{gs}$, the electron current decreases while the hole current increases, so ambipolarity causes the $I$–$V$ characteristic of TFETs to gradually deviate from the curve of pure electron or hole current, and finally at $V_{gss} = -1.1V$, the two curves of the electron and hole current contact each other with equal values and opposite slopes, so the slope of the $I$–$V$ curve is zero and the current value is two times that of the individual electron or hole current. However, the profile of potential barrier in the source-channel-drain is not constant and gradually changes with $V_{gs}$ as it helps to increase the current and finally at $V_{gss}$ it increases more than 2 times of pure carrier currents. As a result, to prevent degradation of operation of a digital TFET by ambipolarity, a nanomaterial with a sufficiently high energy band gap of $E_{g}/2 \gg eV_{DD}$ must be selected.

By constructing 2ZGyNT-TFETs in different channel lengths $L_{ch} = nL_{UR}$ with $n$ in the range of $7 \leq n \leq 14$, the impact of $L_{ch}$ in the range of $4.8 \text{nm} < L_{ch} < 9.6 \text{nm}$ on the performance of TFETs is investigated. The $I$–$V$ characteristics of the TFETs are calculated and depicted in Fig. 4. For n-type and p-type TFETs, the $V_{gs}^n \approx -0.3V$ and $V_{gs}^p \approx -1.8V$, respectively.

Under the bias condition of $V_{th} - V_{gs} = 200$mV and $V_{ds} = 200$mV, the OOCR and SS of the TFETs are calculated and demonstrated in Fig. 5. It is obvious that $Log(\text{OOCR})$ is linear with respect to $L_{ch} = nL_{UR} = n \times 0.69 \text{nm}$. The SS of the n-type TFET with 7 URs in the channel is 60.9$mV/dec$, nearly equal to the minimum SS of MOSFETs. The n-type TFETs with channel length of 8 and 7 URs need $V_{th} - V_{gs} = 208$mV and $V_{th} - V_{gs} = 244$mV to obtain an OOCR value of $1 \times 10^7$, nearly equal to the minimum requirement for the OOCR according to the ITRS [6].
In the subthreshold region of the n-type, where, using the WKB approximation [Eq. (4)], and so the calculated approximation formula of the n-type TFET in the subthreshold region of the n-type TFET is $I_{\text{off}} \approx I_{\text{on}} \exp(-6.5L_{\text{ch}} \sqrt{m^*(V_{\text{th}} - V_{\text{gs}})})$ [46, 47]. For a precise model, the imaginary band dispersion of GyNTs must be taken into account in the WKB formula [46].

By increasing the work function of the metal gate by $eV_{\text{eff}} = -0.5eV$, the $I-V$ characteristic of the TFETs shifts to the right so that the origin of the coordinates corresponds to the off-state and a transfer curve of TFETs as digital transistors is created. The TFETs are able to switch from the off-state to the on-state via $V_{\text{gs}} = 0.2V$.

γ-Graphyne-1 armchair nanotubes have higher effective mass and lower mobility than zigzag nanotubes. Therefore, 3AGyNT-TFETs have potentially lower $I_{\text{on}}$ and power consumption and higher OCR than 2ZGyNT-TFETs. Figure 7 shows a 3AGyNT-TFET with a gate length of 6nm, which comprises 5 URs.

On the bias condition of $V_{ds} = 0.2V$ and $-2.8V < V_{gs} < 0$, the $I-V$ characteristics of sub-10-nm 3AGyNT-TFETs with $L_{\text{ch}} = nL_{\text{UR}}$ when $n$ is in the range of $3 \leq n \leq 8$ are calculated and depicted in Fig. 8, and the impact of channel length $3.6nm < L_{\text{ch}} < 9.6nm$ on the performance of TFETs is investigated. As shown in Fig. 8, the threshold voltage values of n-type TFETs and p-type TFETs are $V_{\text{th}}^n \approx -0.5V$ and $V_{\text{th}}^p \approx -2.5V$, respectively. The red and blue shaded regions are two parts of the subthreshold region of the 3AGyNT-TFETs in which two digital n-type TFETs and p-type TFETs are constructed.

As shown in Fig. 9, Log(OCR) and SS are linear and reciprocal functions of $n$, respectively. The minimum SS and maximum OCR are found for the longest TFET with 8 URs in its channel where its OCR at $V_{gs} = V_{\text{gmin}} = -1.1V$ is $5.7 \times 10^{19}$ and its point and average SS at $V_{gs} = V_{\text{gs}}^p = -0.5V$ and $V_{\text{gs}}^n - V_{gs} = 0.2V$ are $5mV/\text{dec}$ and $19mV/\text{dec}$, respectively. The n-type TFET with $L_{\text{ch}} = 3L_{\text{UR}} = 3.6nm$ has an SS value of $59mV/\text{dec}$. At $V_{\text{gs}}^n - V_{gs} = 0.24V$, its OCR value reaches $10^4$.

The application of GyNT-TFETs as digital transistors is in the future design of microprocessor units (MPUs) in which all transistors are TFETs with simultaneously very low on- and off- and leakage current. Any possible trap near the VBM of the source via transfer charges between the $p^+$ and $n^+$ regions can cause trap-assisted BTBT whose effects on current are calculated in the NEGF formalism.

Leakage current in GAA transistors is mainly related to the insulator layer tunneling current that has to be lower than the off-state current of the transistor. The tunneling direction of electrons in the insulator from the metallic gate to the channel is perpendicular to the transport direction of the channel, so electrons have to scatter with a nanotube structure to diffuse to the drain region, which causes resistance to the leakage current. On the other hand, the transmission coefficients of off-state tunneling current and leakage tunneling current are comparable to each other, $T_{\text{ins}} = T_{\text{ch}}$, where, using the WKB conditions for tunneling current in the insulator and channel, respectively.
approximation \[ b_{\text{ins}} \approx \frac{b_{\text{ch}}}{2} \left( \frac{V_{\text{th}} - V_{\text{gs}}}{} \right) \]

where \( L_{cr} \) is the critical length, and for 2ZGyNT-TFETs with brookite as insulator, \( m^*_{\text{ins}}E_g = 5.1 \), \( t_{\text{ins}} = 1 \) nm, \( b_{\text{ins}} = 2 \), \( m^*_{\text{ch}} = 0.21 \), \( (V_{\text{th}} - V_{\text{gs}}) = 0.2V \), and \( b_{\text{ch}} = 1.6 \).
which because of tunneling of electrons in the transmission window is lower than 2 for square tunneling barriers. Finally, the critical length of the channel is \( L_{cr} = 9.71 \) nm, which is higher than the channel length of the zigzag TFETs in this paper, and so the leakage current is lower than the off-state current in all zigzag transistors. For 3AGyNT-TFETs \( m_{ch}^{*} = 0.43 \), and \( b_{ch} = 1.5 \) and \( L_{cr} = 7.33 \) nm, which is lower than the channel length of armchair transistors with 7 and 8 URs, where using \( V_{DD} = 0.1 \) V the critical length will increase to \( L_{cr} = 10.33 \) nm. Therefore, scattering of leaky carriers with nanotube structure and shorter channel length than the critical length of the channel causes the leakage current of the insulator to be less than the off-state current.

By increasing the work function of the metal gate by \( eV_{off} = -0.7 \) eV, the \( I-V \) characteristic of the TFETs shifts to the right so that the n-type TFETs are able to switch between the off-state and on-state via \( V_{gs} = 0.2 \) V.

4 Conclusion

Band gap engineering in \( \gamma \)-graphyne-1 suggests possible applications in nanoelectronic device technology, especially in the FET platform. GyNT-TFETs, due to their novel structure, material and technology, with potential application as high-performance digital transistors in nanoelectronic devices, require in-depth investigation from a physical point of view. In this study, the calculated electron MFP of GyNTs in the effective mass approximation and DP theory are sufficiently high to provide reliable ballistic transport properties of sub-10-nm GyNT-TFETs. The \( I-V \) characteristics are obtained for armchair and zigzag TFETs in different channel lengths. At a channel length of 9.6 nm, the 2ZGyNT-TFET and 3AGyNT-TFET show ultrahigh average OOCR values of 1.2 x 10\(^2\) and 1.6 x 10\(^6\), respectively. 3AGyNT-TFET with channel length of 3.6 nm has an SS value of 59 mV/dec, which is nearly equal to the minimum SS of conventional MOSFETs. A model of \( I_{off} \) based on the WKB approximation and linear relationship between \( Log(I_{off}) \) and \( L_{ch} \) is proposed. Future studies will explore optimizing the doping concentration and electric field in the source and drain regions at shorter channel lengths.

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References

1. Ni, Z., Ye, M., Ma, J., Wang, Y., Quhe, R., Zheng, J., Dai, L., Yu, D., Shi, J., Yang, J., Watanabe, S., Lu, J.: Performance upper limit of sub-10 nm monolayer MoS2 transistors. Adv. Electron. Mater. (2016). https://doi.org/10.1002/aelm.201600191
2. Zhou, W., Zhang, S., Guo, S., Wang, Y., Lu, J., Ming, X., Li, Z., Qu, H., Zeng, H.: Designing sub-10-nm metal-oxide-semiconductor field-effect transistors via ballistic transport and disparate effective mass: the case of two-dimensional BiN. Phys. Rev. Appl. 13, 1–9 (2020). https://doi.org/10.1103/PhysRevApplied.13.044066
3. Yang, J., Quhe, R., Li, Q., Liu, S., Xu, L., Pan, Y., Zhang, H., Zhang, X., Li, J., Yan, J., Shi, B., Pang, H., Xu, L., Zhang, Z., Lu, J., Yang, J.: Sub 10 nm bilayer Bi2O2Se transistors. Adv. Electron. Mater. 5, 1–10 (2019). https://doi.org/10.1002/aelm.201800720
4. Desai, S.B., Madhuvathy, S.K., Sachid, A.B., Llinas, J.P., Wang, Q., Ahn, G.H., Piner, G., Kim, M.J., Bokor, J., Hu, C., Wong, H.-S.P., Javey, A.: MoS2 transistors with 1-nanometer gate lengths. Science 354(6308), 99–102 (2016). https://doi.org/10.1126/science.aab4698
5. Ionescu, A.M., Riel, H.: Tunnel field-effect transistors as energy-efficient electronic switches. Nature 479, 329–337 (2011). https://doi.org/10.1038/nature10679
6. International Technology Roadmap for Semiconductors (ITRS), (2015). www.itrs.net
7. International Roadmap for Devices and Systems (IRDS), (2016). https://irds.ieee.org/reports
8. International Roadmap for Devices and Systems (IRDS), (2020). https://irds.ieee.org/reports
9. Kim, J.-H., Chen, Z.C.Y., Kwon, S., Xiang, J.: Three-terminal nanoelectromechanical field effect transistor with abrupt sub-threshold slope. Nano Lett. 14(3), 1687–1691 (2014). https://doi.org/10.1021/nl5006355
10. Cristoloveanu, S., Wan, J., Zaslavsky, A.: A review of sharp-switching devices for ultra-low power applications. IEEE J. Electron. Devices Soc. 4(5), 215–226 (2016). https://doi.org/10.1109/JEDS.2016.2545978
11. Tian, H., Li, Y.-X., Li, L., Wang, X., Liang, R., Yang, Y., Ren, T.-L.: Negative capacitance black phosphorus transistors with low SS. IEEE Trans. Electron. Devices 66(3), 1579–1583 (2019). https://doi.org/10.1109/TED.2018.2890576
12. Musalgaonkar, G., Sahay, S., Saxena, R.S., Kumar, M.J.: An impact ionization MOSFET with reduced breakdown voltage based on back-gate misalignment. IEEE Trans. Electron. Devices 66(2), 868–875 (2018). https://doi.org/10.1109/TED.2018.2887168
13. Seabaugh, A.C., Zhang, Q.: Low-voltage tunnel transistors for beyond CMOS logic. Proc. IEEE 98(11), 2095–2110 (2010). https://doi.org/10.1109/JPROC.2010.2070470
14. George, S., Aziz, A., Li, X., Kim, M.S., Datta, S., Sampson, J., Gupta, S., Narayanan, V.: Device circuit design of FEFET based logic for low voltage processors. In: Paper presented at the 2016 IEEE computer society annual symposium on VLSI (ISVLSI), Pittsburgh, PA, USA Jul. https://doi.org/10.1109/ISVLSI.2016.116
15. Tamesis, K.: Sub-10 nm junctionless carbon nanotube field-effect transistors with improved performance. Int. J. Electron. Commun. 124, 10 (2020). https://doi.org/10.1016/j.ijelec.2020.153354
16. Shirazi, S.G., Karimi, G.R., Mirzakuchaki, S.: GAA CNT TFETs: structural engineering: a higher ON current, lower ambipolarity. IEEE Trans. Electron. Devices 66(6), 2822 (2019). https://doi.org/10.1109/TED.2019.2912990
17. Wu, S., Yuan, Y., Cho, D., Lee, J.Y., Kang, B.: Chiral \( \gamma \)-graphyne nanotubes with almost equivalent bandgaps. J. Chem. Phys. 150, 1–6 (2019). https://doi.org/10.1063/1.5065558
18. Baughman, R.H., Eckhardt, H., Kertesz, M.: Structure-property predictions for new planar forms of carbon: layered phases containing sp2 and sp atoms. J. Chem. Phys. 87, 6687–6699 (1987). https://doi.org/10.1063/1.453405
19. Li, G., Li, Y., Qian, X., Liu, H., Lin, H., Chen, N., Li, Y.: Construction of tubular molecule aggregations of graphdiyne for highly efficient field emission. J. Phys. Chem. C 115, 2611–2615 (2011). https://doi.org/10.1021/jp107996f
20. Li, G., Li, Y., Liu, H., Guo, Y., Lia, Y., Zhu, D.: Architecture of graphdiyne nanoscale films. Chem. Commun. 46, 3256–3258 (2010). https://doi.org/10.1039/b922733d
21. Li, Q., Li, Y., Chen, Y., Wu, L., Yang, C., Cui, X.: Synthesis of γ-graphyne by mechanochemistry and its electronic structure. Carbon 136(248–254) (2018). https://doi.org/10.1016/j.carbon.2018.04.081
22. Luo, G., Qian, X., Liu, H., Qin, R., Zhou, J., Li, L., Gao, Z., Wang, E., Mei, W.-N., Lu, J., Li, Y., Nagase, Q.: Quasiparticle energies and excitonic effects of the two-dimensional carbon allotrope graphdiyne: theory and experiment. Phys. Rev. B 84, 075439 (2011). https://doi.org/10.1103/PhysRevB.84.075439
23. Zhou, J., Lv, K., Wang, Q., Chen, X.S., Sun, Q., Jena, P.: Electronic structures and bonding of graphyne sheet and its BN analog. J. Chem. Phys. 134, 174701–174706 (2011). https://doi.org/10.1063/1.3583476
24. Wu, W., Guo, W., Zeng, X.C.: Intrinsic electronic and transport properties of graphyne sheets and nanoribbons. Nanoscale 5, 9264–9276 (2013). https://doi.org/10.1039/c3nr03167e
25. Hou, X., Xie, Z., Li, C., Li, G., Chen, Z.: Study of Electronic Structure, thermal conductivity, elastic and optical properties of α, β, γ-Graphyne. Materials 11(2), 1–14 (2018). https://doi.org/10.3390/ma11020188
26. Kang, J., Li, J., Wu, F., Li, S.S., Xia, J.B.: Elastic, electronic, and optical properties of two-dimensional graphyne sheet. J. Phys. Chem. C 115, 20466–20470 (2011). https://doi.org/10.1021/jp206751m
27. Wang, X.-M., Lu, S.-s.: Thermoelectric transport in graphyne nanotubes. J. Phys. Chem. C 117(38), 19740–19745 (2013). https://doi.org/10.1021/jp406536e
28. Srinivasu, K., Ghosh, S.K.: Graphyne and graphdiyne: promising materials for nanoelectronics and energy storage applications. J. Phys. Chem. C 116, 5951–5956 (2012). https://doi.org/10.1021/jp212181h
29. Puigdollers, A.R., Alonso, G., Gamallo, P.: First-principles study of structural, elastic and electronic properties of α-β- and γ-graphyne. Carbon 96, 879–887 (2016). https://doi.org/10.1016/j.carbon.2015.10.043
30. Rouzkhash, B., Salehi, A., Ahmadi, M.T.: Bandgap modulation of low-dimensional γ-graphyne-1 under uniform strain. J. Comput. Electron. 19, 947–956 (2020). https://doi.org/10.1007/s10825-020-01521-6
31. Rouzkhash, B., Salehi, A., Ahmadi, M.T.: γ-Graphyne-1 band structure modeling and simulation. Solid State Commun. 325, 114164 (2020). https://doi.org/10.1016/j.ssc.2020.114164
32. Perdew, J.P., Burke, K., Ernzerhof, M.: Generalized gradient approximation made simple. Phys. Rev. Lett. 77(18), 3865–3868 (1996). https://doi.org/10.1103/PhysRevLett.77.3865
33. Buttiker, M., Imry, Y., Landauer, R., Pinhas, S.: Generalized many-channel conductance formula with application to small rings. Phys. Rev. B 31(10), 6207–6215 (1985). https://doi.org/10.1103/physrevb.31.6207
34. Reihani, A., Soleimani, A., Kargar, S., Sundararaghavan, V., Ramazani, A.: Graphyne nanotubes: materials with ultralow phonon mean free path and strong optical phonon scattering for thermoelectric applications. J. Phys. Chem. C 122(39), 22688–22698 (2018). https://doi.org/10.1021/acs.jpcc.8b05898
35. Ramazani, A., Reihani2, A., Soleimani, A., Larson, R., Sundararaghavan, V.: Molecular dynamics study of phonon transport in graphyne nanotubes. Carbon 123, 635–644 (2017). https://doi.org/10.1016/j.carbon.2017.07.093
36. Bardeen, J., Shockly, W.: Deformation potentials and mobilities in non-polar crystals. Phys. Rev. 80(1), 72–81 (1950). https://doi.org/10.1103/PhysRev.80.72
37. Price, P.J.: Two-dimensional electron transport in semiconductor layers. I. Phonon scattering. Ann. Phys. 133(2), 217–239 (1981). https://doi.org/10.1016/0003-4916(81)90250-5
38. Tan, X., Shao, H., Hu, T., Liu, G., Jiang, J., Jiang, H.: High thermoelectric performance in two-dimensional graphyne sheets predicted by first-principles calculations. Phys. Chem. Chem. Phys. 17(35), 22872–22881 (2015). https://doi.org/10.1039/C5CP03466C
39. Long, M., Tang, L., Wang, D., Li, Y., Shuai, Z.: Electronic structure and carrier mobility in graphyne sheet and nanoribbons. ACS Nano 5, 2593–2600 (2011). https://doi.org/10.1021/nn10472s
40. Beleznay, F.B., Bogar, F., Ladik, J.: Charge carrier mobility in quasi-one-dimensional systems: application to a guanine stack. J. Chem. Phys. 119(11), 5690–5695 (2003). https://doi.org/10.1063/1.1595634
41. Xi, J., Wang, D., Yi, Y., Shuai, Z.: Electron-phonon couplings and carrier mobility in graphyne sheets calculated using the Wannier-interpolation approach. J. Chem. Phys. 141, 1–11 (2014). https://doi.org/10.1063/1.4887538
42. Chanana, R.K.: Determination of hole effective mass in SiO2 and SiC conduction band offset using Fowler-Nordheim tunneling characteristics across metal-oxide–semiconductor structures after applying oxide field corrections. J. Appl. Phys. 109, 1–6 (2011). https://doi.org/10.1063/1.3587185
43. Liu, Q.-J., Liu, Z.-T., Feng, L.-P.: Electronic structure, effective masses and optical properties of monoclinic HfO2 from first-principles calculations. Adv. Mater. Res. 216, 341–344 (2011). https://doi.org/10.4028/www.scientific.net/AMR.216.341
44. Landmann, M., Rauls, E., Schmidt, W.G.: The electronic structure and optical response of rutile, anatase and brookite TiO2. J. Phys. Condens. Matter 24, 1–6 (2012). https://doi.org/10.1088/0953-8984/24/19/195503
45. Ajay, Narang, R., Saxena, M., Gupta, M.: Two-dimensional (2D) analytical investigation of an n-type junctionless gate-all-around tunnel field-effect transistor (JL GAA TFET). J. Comput. Electron. 17, 713–723 (2018). https://doi.org/10.1007/s10825-018-1151-7
46. Luisiera, M., Klimeck, G.: Simulation of nanowire tunneling transistors: From the Wentzel–Kramers–Brillouin approximation to full-band phonon-assisted tunneling. J. Appl. Phys. 107, 1–6 (2010). https://doi.org/10.1063/1.3386521
47. Sze, S.M., Ng, K.K.: Physics of Semiconductor Devices, 3rd ed. Wiley, New Jersey (2006). https://doi.org/10.1002/0470068329

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