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Synopsis Of

Numerical and Analytical Modeling of B or N Substitution Doped Single Layer Graphene FET: RF and Synaptic Applications

A Thesis

To be submitted by

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For the award of the degree

Of

DOCTOR OF PHILOSOPHY

1 Abstract

The uniqueness and excellent electronic properties of graphene (Neto *et al.*, 2009) are accelerating the interest of research in emerging nanoelectronic devices. Therefore, in this work, boron (B) or nitrogen (N) substitution doped graphene field effect transistor (GFET) is explored extensively. The memoryless non-linearity performance of B-doped GFET have investigated by proposing an accurate electrical equivalent circuit model for B-doped GFET. A phenomenological self-consistent drain current model for B/N substitution doped bottom gated GFET is developed. The effects of substitution doping such as: (i) shift in Dirac points; (ii) induced non-zero bandgaps; are explicitly captured in this model. The self-consistent drain current model is predicting an excellent agreement with experimental data. A simplified region-wise potential-based analytical model is established for B or N substitution doped GFET. The closed-form direct analytical relation between graphene channel potential and applied bias condition is developed by imposing the effective approximation for Fermi-Dirac integral function in various regions of operation. In addition to that, the drift and diffusion current components for B and N substitution doped GFETs have been modeled individually and their influence on total current is discussed. The proposed region-potential-based analytical model has shown good agreement with numerically solved self-consistent model. The synaptic devices based on B/N doped GFET have analytically modeled to manifest dynamic mimicking of synaptic plasticity. The hysteresis conduction behaviour due to interface traps is utilized to accomplish the synaptic plasticity. The metal-insulator-graphene equivalent model is proposed to capture the physical insights of interface traps, which pave a route to establish the trap state time-dependent drain current model.

2 Objectives

The objectives of this thesis are outlined as follows:

(a) To investigate memoryless linearity and non-linearity performance of B-doped GFET and to compare with undoped GFET and conventional MOSFET.

(b) To develop a self-consistent drain current model for B/N substitution doped GFETs by incorporating the essential impacts of doping in single layer graphene such as: (i) shifting of Dirac points; (ii) induced non-zero bandgaps.

(c) To develop a computationally efficient region-wise potential-based extremely closed-form analytical model for B/N substitution doped GFETs.

(d) To model a B/N substitution doped synaptic GFET by utilizing the interface traps and to establish the dynamic emulation of synaptic plasticity.

3 Existing Gaps Which Were Bridged

In this thesis, based on the literature, the following research gaps are traced and bridged.

(a) The presence of nonlinearities in RF system will cause unfavourable effects such as distortions and gain compression. Therefore, it is indispensable to analyse the nonlinearity effects of the device at transistor level rather at system level. Though the nonlinearity effects of GFETs have been reported in literature (Rodriguez *et al.*, 2014; Alam *et al.*, 2015; Gao *et al.*, 2017), however these reports are on zero bandgap graphene. Therefore, B-doped graphene with non-zero bandgap is proposed to mitigate the nonlinearities in GFETs caused by zero bandgap.

(b) Diverse number of drain current models have been developed to analyse the large signal characteristics of GFETs (Fregonese *et al.*, 2013; Pasadas and Jiménez, 2016; Feijoo *et al.*, 2016). In (Fregonese *et al.*, 2013), the doping concentration is intentionally included, which do not capture the bandgap induced by dopant. However, substitution doping in graphene shifts Dirac point with significant non-zero bandgap and it affects density of states and carrier statistics. To address these issues, a phenomenal drain current model for B/N doped GFET is proposed, which solves self-consistently by capturing all physical significance of doping.

(c) The crucial limitations of the self-consistent drain current model are enumerated as: (i) The channel potential and drain current are having only numerical solutions; (ii) Dependency on the precise initial assumption of channel potential; (iii) Computationally exhaustive. Consequently, these hindrances make the self-consistent model inconvenient in compact modeling application, where the device behaviour has been mimicked in deigning of circuits. Therefore, a computationally efficient region-wise potential-based extremely closed-form analytical model is proposed for B/N substitution doped GFET.

(d) It is emphasized that the biologically plausible artificial synapses and neuromorphic systems with self-learning attributes, make it highly conquest the classical von Neumann bottleneck (Taherkhani *et al.*, 2020). The undoped GFETs based synapse exhibits relatively small synaptic weight change $\approx 10\%$ (Oshio and Souma, 2022) while comparing with biological synapse, which discloses more than 100%. Consequently, the undoped synaptic GFETs diminish to provide the synaptic plasticity. Hence, to overcome these issues, an analytical model for B/N doped GFET with interface traps is proposed to establish the synaptic plasticity.

4 Most Important Contributions

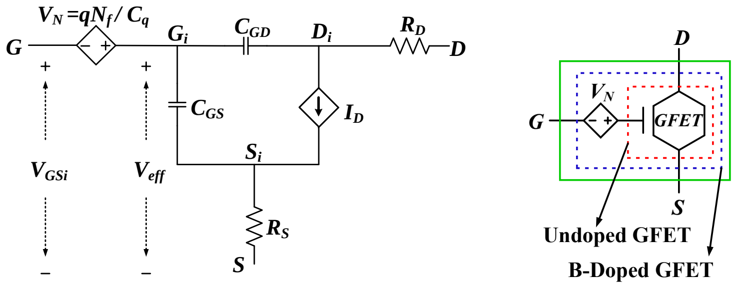
4.1 Linearity and Nonlinearity Investigation of Doped Graphene FET

The major contribution of this chapter is summarized as follows:

(a) To perform memoryless nonlinearity analysis by developing an electrical equivalent circuit model for undoped and B-doped GFET as shown in Fig. 1, which are the devices under nonlinearity investigation.

(b) The nonlinearity performance metrics have been evaluated in a comparative manner with undoped GFET to prove the enhanced linearity of B-doped GFET as mentioned in Table 1.

The simulation is also performed for undoped GFET and compared with the simulation results of (Rodriguez *et al.*, 2014) to prove the accuracy as listed in Table 1.



(a) (b)

Figure 1: (a) Electrical equivalent circuit for B-doped GFET. (b) Symbol for the proposed electrical equivalent circuit model.

Table 1: Calculated and Simulated Memoryless Linearity and Nonlinearity Effects for 12% B-Doped and Undoped GFETs

Name	**This work**				**From [8]**	
	Doped GFET		**Undoped GFET**		**Undoped GFET**	**CMOS**
FOMs	**Model**	**Spectre**	**Model**	**Spectre**	**Spectre**	**Spectre**
HD_2 **(dB)**	-57.33	-56.60	-55.66	-55.75	-57	-45.70
HD_3 **(dB)**	-108.41	-107.06	-105.03	-105.35	-108	-96.70
IM_2 **(dB)**	-51.31	-50.58	-49.64	-49.72	-51	-39.70
IM_3 **(dB)**	-98.87	-97.52	-95.49	-95.81	-96.10	-87.20
A_{IIP2} **(dBV)**	17.33	16.59	15.66	15.75	17	5.70
A_{IIP3} **(dBV)**	15.45	14.78	13.76	13.90	14	9.60
$A_{\mathrm{in,1dB}}$ **(dBV)**	5.82	5.48	4.13	4.53	-	-

4.2 Self-Consistent Drain Current Modeling of B/N Substitution Doped GFET

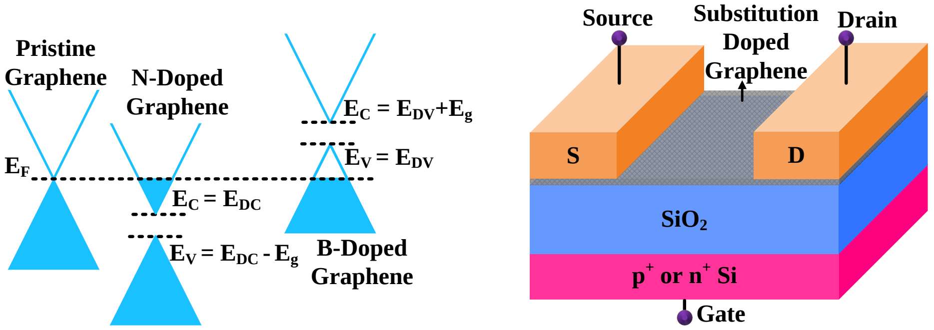
The principal contribution of this chapter can be outlined as follows:

(a) Modified energy-momentum ($E - k$) relation with shift in Dirac point and non-zero bandgap based on doping concentration has been considered as depicted in Fig. 2(a) to derive the electrostatics from DOS, total sheet charge density, quantum capacitance to complete drain current model.

(b) The total Sheet charge density (Q_{sh}) and change in channel potential (V_{ch}) are self-consistently solved through first order Newton-Raphson numerical method to evaluate appropriate V_{ch} and Q_{sh} and subsequently to obtain quantum capacitance (C_q) and mobility with respect to channel potential.

(c) The proposed model is validated with experimentally measure data, which is manifested in Fig. 3 and the model is compatible for all region undoped, n-type doped (N-doping), p-type doped (B-doping) bottom gated GFETs.

The Q_{sh} and C_q for B-doped graphene is modeled as in (1) and (2), respectively, which captures the key effects of substitution doping such as: (i) shifting of Dirac point; (ii)



(a) (b)

Figure 2: (a) $E-k$ relation of pristine and substitution doped (N and B) graphene. (b) Proposed schematic structure of B/N substitution doped bottom gated GFET.

induced bandgap. Similarly, Q_{sh} and C_q for N-doped graphene can also be derived.

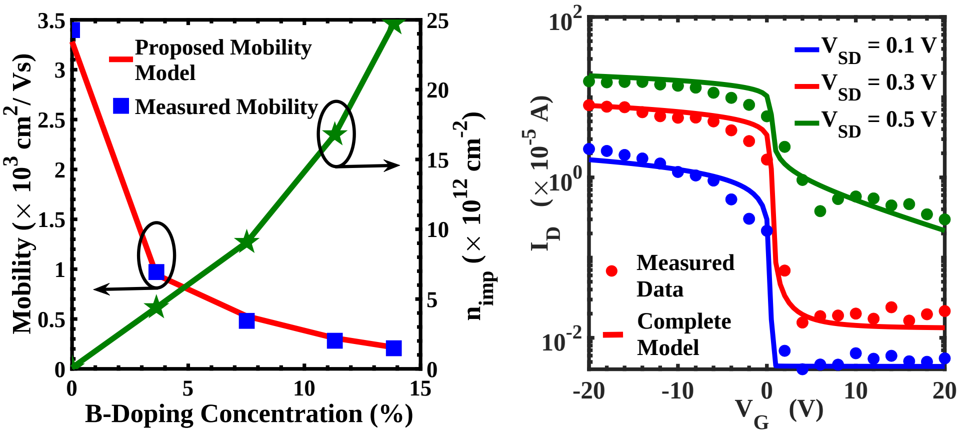
$$Q_{sh} = \frac{2q(k_BT)^2}{(\hbar v_f)^2}\left[\Im_1\left(\frac{-qV_{ch}}{k_BT}\right) - \Im_1\left(\frac{qV_{ch}-E_g}{k_BT}\right)\right] \tag{1}$$

$$C_q = \frac{2q^2k_BT}{(\hbar v_f)^2}\ln\left[\left(1+e^{\frac{-qV_{ch}}{k_BT}}\right)\left(1+e^{\frac{qV_{ch}-E_g}{k_BT}}\right)\right] \tag{2}$$

The relation between V_{ch} and Q_{sh} can be obtained for B/N doped GFET as shown in Fig. 2(b), which is represented as:

$$V_{ch} = V_G - V_{G0} - V(x) + (Q_{sh}/C_{ox}) \tag{3}$$

The expressions in (1) and (3) are in the form of transcendental. Hence, (1) and (3) should be solved self-consistently through numerical method. For a particular input bias condition, the V_{ch} and Q_{sh} are resulted from the self-consistent solution. Eventually, the



(a) (b)

Figure 3: (a) Validation of the proposed (a) mobility model and (b) complete self-consistent drain current model with experimental data (Tang *et al.*, 2012).

proposed self-consistent drain current model for B/N doped GFET is derived as:

$$|I_D| = \frac{W \int_{V_s}^{V_d} Q_{sh}\left(1 + \frac{C_q}{C_{ox}}\right) \mathrm{d}V_{ch}}{\left(L^{\gamma} + \left(\int_{V_s}^{V_d} \frac{\mu}{v_{sat}}\left(1 + \frac{C_q}{C_{ox}}\right) \mathrm{d}V_{ch}\right)^{\gamma}\right)^{\frac{1}{\gamma}}} \tag{4}$$

4.3 Region-wise Potential-based Closed-form Analytical Modeling of B/N Substitution Doped GFET

This chapter establishes a computationally efficient region-wise potential-based extremely closed-form analytical model for B/N substitution doped GFET and the key contributions are outlined as:

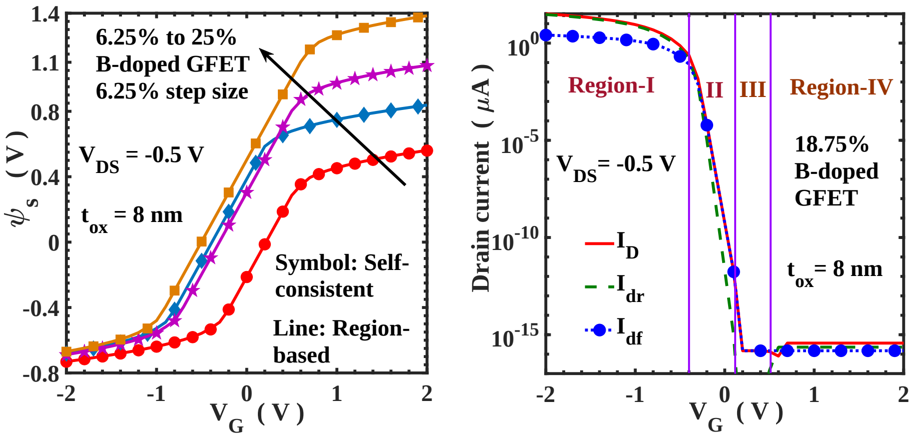
(a) The closed-form direct analytical relation between graphene channel potential and applied bias condition is developed by imposing the effective approximation for Fermi-Dirac integral function in various regions of operation, which is depicted in Fig. 4(a).

(b) In addition to that, the drift component, diffusion coefficient and its corresponding diffusion current component for B and N doped GFETs have been modeled individually and its influence on total current is discussed as shown in Fig. 4(b).

(c) The proposed region-potential-based analytical model has been shown good agreement with numerically solved self-consistent model as shown in Fig. 5.

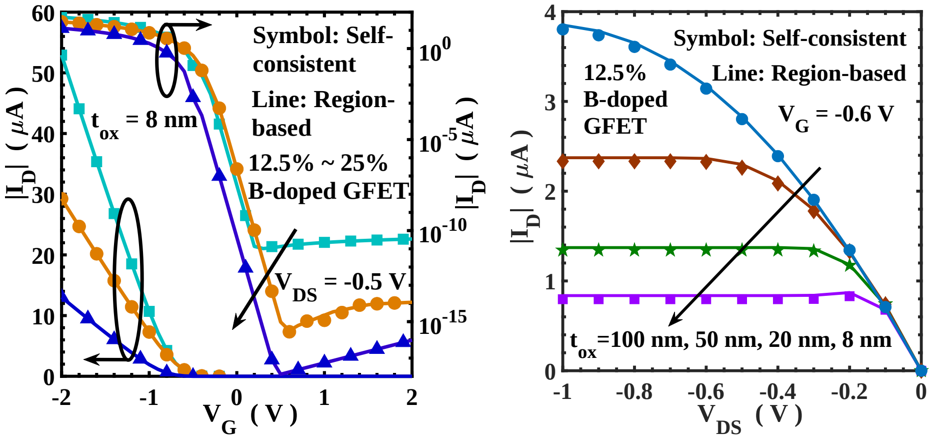
Under the different bias conditions, the four distinct operating regimes such as: region-I, region-II, region-III, and region-IV have been considered and its corresponding $_s$ for B-doped GFET is modeled in closed-form and presented as:

$$_s \approx V + \frac{1}{2} - \frac{1}{\sqrt{\;}} \sqrt{(V + V_{fb} - \;) - V_G + \frac{1}{4}} \tag{5}$$



(a) (b)

Figure 4: (a) Validation of the proposed region-based potential model (lines) against self-consistent model (symbols). (b) Interpreting the influence of individual drift (I_{dr}) and diffusion (I_{df}) current components on total drain current (I_D).



(a) (b)

Figure 5: Validation of the region-wise drain current model (lines) against self-consistent model (symbols): (a) Transfer and (b) Output characteristics.

$$_s \approx \ _tW_l \ \overline{\ _t}e^{\frac{V+V_{fb}\ +\alpha-V_G}{\phi_t}} \ - (V_{fb} + \ \ - V_G) \tag{6}$$

$$_s \approx V_G - V_{fb} - \ \ + \ e^{\frac{V-\phi_g}{\phi_t}} - \ _tW_l \ \overline{\ _t}e^{\frac{V_G-V_{fb}\ -\alpha-\phi_g+\beta e^{\frac{V-\phi_g}{\phi_t}}}{\phi_t}} \tag{7}$$

$$_s \approx \ _g - \frac{1}{2} + \frac{1}{\sqrt{\ }} \mathrm{q}\ \overline{V_G - V_{fb} - 2 \ \ - \ _g + \ e^{\frac{V-\phi_g}{\phi_t}}} \tag{8}$$

The drain current model of B-doped GFET for region-I and region-II is modeled as in (9) while for region-III and region-IV is modeled as in (10).

$$I_D = -\frac{W}{L} C_{ox} \ \mathrm{h}\ (V_G - V_{TB1})(\ _{sL} - \ _{s0}) - \frac{2 -}{2} (\ _{sL} - \ _{s0})^2 \ \mathrm{i} \tag{9}$$

$$I_D = -\frac{W}{L} C_{ox} \ (V_G - V_{TB2})(\ _{sL} - \ _{s0}) - \frac{1}{2}(\ _{sL} - \ _{s0})^2 \tag{10}$$

4.4 Application of B/N Doped GFET Model for Dynamic Mimicking of Synaptic Plasticity

In this chapter, the synaptic devices based on B/N substitution doped GFET with non-zero band gap has been analytically modeled and the major contributions are encapsulated as follows:

(a) The synaptic plasticity has been accomplished by utilizing the hysteresis conduction behaviour manifested through channel and gate-insulator interface traps.

(b) The physical significance of interface traps have been modeled explicitly through metal-insulator-graphene (MIG) equivalent circuit as shown in Fig. 6, which pave a route to establish the trap state time-dependent drain current model.

(c) The spike time dependent plasticity (denoted as STDP, which is a fundamental mechanism of learning and memory) for B/N doped synaptic GFETs have been

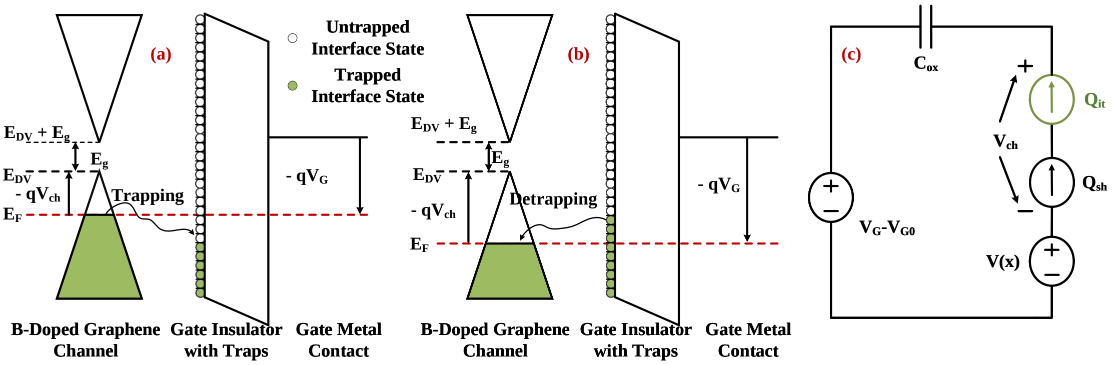


Figure 6: Interpretation of (a) trapping when $E_F > E_{it}$ and (b) de-trapping when $E_F < E_{it}$. (c) MIG equivalent model including the interface trap charges (Q_{it}).

enriched significantly by 20 times than the synapse made by undoped GFETs, which can be evident from Fig. 7.

The complete model for B/N substitution doped GFET including interface traps is represented in (11) to (13).

$$|I_D^{(i)}| = \frac{qW \int_{V_{cs}}^{V_{cd}} Q_{sh} \left(1 + \frac{C_q + C_{it}^{(i)}}{C_{ox}}\right) \mathrm{d}V_{ch}}{L + \int_{V_{cs}}^{V_{cd}} \frac{\mu}{v_{sat}} \left(1 + \frac{C_q + C_{it}^{(i)}}{C_{ox}}\right) \mathrm{d}V_{ch}} \tag{11}$$

$$C_{it}^{(i)} = \frac{\mathrm{d}Q_{it}^{(i-1)}}{\mathrm{d}V_{ch}} - qD_{it}(E)\left(q - \frac{\mathrm{d}E_{it}^{(i-1)}}{\mathrm{d}V_{ch}}\right)\left(1 - e^{-\frac{\Delta t}{\tau_{trap}}}\right) \tag{12}$$

$$\frac{\mathrm{d}E_{it}^{(i)}}{\mathrm{d}V_{ch}} = \left(q - \frac{\mathrm{d}E_{it}^{(i-1)}}{\mathrm{d}V_{ch}}\right)\left(1 - e^{-\frac{\Delta t}{\tau_{trap}}}\right) + \frac{\mathrm{d}E_{it}^{(i-1)}}{\mathrm{d}V_{ch}} \tag{13}$$

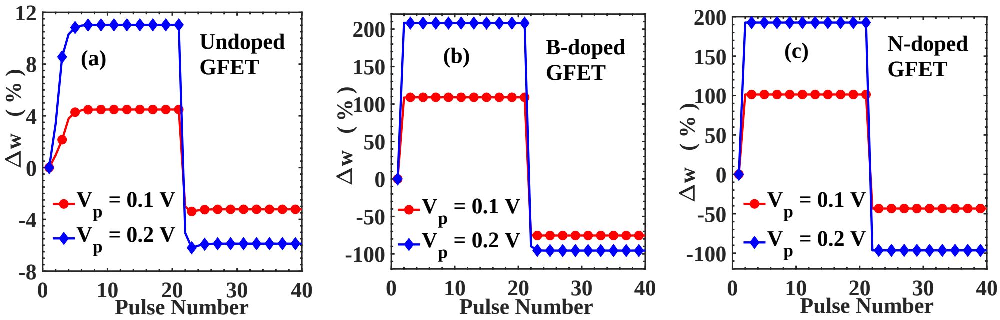


Figure 7: STDP characteristics of (a) Undoped (b) B-doped (c) N-doped GFET.

5 Conclusions

The key summary of this thesis in a brief manner is outlined as follows:

(a) The memoryless linearity and nonlinearity effects due to the drain current of B substitution doped GFET have been extensively modeled and various linearity and nonlinearity FOMs have been explored and compared with simulation results of undoped GFET.

(b) B or N substitution doped bottom gated GFETs completely suppress the bipolar gating effect as compared with undoped pristine GFET, which is disclosed from the transfer characteristics.

(c) The ON/OFF ratio for undoped GFET is ≈ 1, whereas for B and N substitution doped GFET, it has been extremely enhanced as $\approx 8\times10^4$ and $\approx 7.7\times10^4$ for 25% B-doped and N-doped GFET, respectively.

(d) A simplified computationally efficient region-wise potential-based analytical model has been developed for B/N doped GFETs and the closed-form relation between the graphene channel potential and applied bias condition has been established.

(e) The B/N substitution doped GFETs with interface traps have been analytically modeled to emulate biologically inspired synapses.

(f) The B/N doped GFETs based synapses exhibits substantial synaptic weight change Δw than the undoped GFETs. The vital attributes of STDP such as long-term potentiation and depression for B/N doped synaptic GFETs have been enhanced approximately by 20 times than the synapses made of undoped GFETs.

6 Organization of the Thesis

The proposed outline of the thesis is as follows:

(a) Chapter 1: Introduction

(b) Chapter 2: Literature Survey

(c) Chapter 3: Linearity and Nonlinearity Investigation of Doped Graphene FET

(d) Chapter 4: Self-Consistent Drain Current Modeling of B/N Doped GFET

(e) Chapter 5: Region-wise Potential-based Closed-form Analytical Modeling of B/N Substitution Doped GFET

(f) Chapter 6: Application of B/N Doped GFET Model for Dynamic Mimicking of Synaptic Plasticity

(g) Chapter 7: Conclusion and Future Scope

7 List of Publications

I. Refereed Journals Based on the Thesis

1. **L. Chandrasekar** and K. P. Pradhan,“Computationally Efficient Region-Wise Potential Based Extremely Closed-Form Analytical Modeling of B/N Substitution Doped GFETs," *IEEE Transactions on Electron Devices*, June 2022. (In Press), `https://doi.org/10.1109/TED.2022.3185950`.

2. L. Chandrasekar and K. P. Pradhan, “Self-Consistent Modeling of B or N Substitution Doped Bottom Gated Graphene FET With Nonzero Bandgap," in IEEE Transactions on Electron Devices, vol. 68, no. 7, pp. 3658-3664, July 2021, https://doi.org/10.1109/TED.2021.3080224 .

3. L. Chandrasekar and K. P. Pradhan, “Memoryless linearity in undoped and B-doped graphene FETs: A relative investigation to report improved reliability," in Microelectronics Reliability, Elsevier, vol. 125, no. 114363, October 2021, https://doi.org/10.1016/j.microrel.2021.114363 .

4. L. Chandrasekar and K. P. Pradhan, “Memoryless non-linearity in B-Substitution doped and undoped graphene FETs: A comparative investigation," in IET Circuits, Devices & Systems, vol. 15, no. 7, pp. 641-648, March 2021, https://doi.org/10.1049/cds2.12059 .

II. Communicated

1. L. Chandrasekar, R. R. Shaik and K. P. Pradhan, “An Analytical Model for B/N Substitution Doped GFET with Interface Traps: A Route towards Dynamic Mimicking of Synaptic Plasticity," IEEE Transactions on Nanotechnology, 2022 (Under Review).

III. Refereed Journals (Others)

1. A. Sariki, K. V. Rao, L. Chandrasekar, R. R. Shaik and K. P. Pradhan, “Is accumulation or inversion mode dielectric modulated FET better for label-free biosensing?: A comparative investigation," AEU-International Journal of Electronics and Communications, Elsevier, vol. 137, pp. 153791, July 2021, https://doi.org/10.1016/j.aeue.2021.153791 .

2. R. Priyanka, L. Chandrasekar, R. R. Shaik and K. P. Pradhan, “Label Free DNA Detection Techniques Using Dielectric Modulated FET: Inversion or Tunneling?," IEEE Sensors Journal, vol. 21, no. 2, pp. 2316-2323, August 2020, https://doi.org/10.1109/JSEN.2020.3019103 .

3. R. R. Shaik, G. Arun, L. Chandrasekar and K. P. Pradhan, “A study of Work-function variation in pocket doped FD-SOI technology towards temperature analysis," Springer Silicon, vol. 12, no. 12, pp. 3047-3056, March 2020, https://doi.org/10.1007/s12633-020-00399-0 .

IV. Publications in Conferences Based on the Thesis

1. L. Chandrasekar and K. P. Pradhan, “Modeling and Investigation of Electronic Transport Properties of B or N Substitution Doped Single Layer Graphene," 2021 16th IEEE Nanotechnology Materials & Devices Conference (NMDC), 2021, pp. 1-4, https://doi.org/10.1109/NMDC50713.2021.9677497 .

2. L. Chandrasekar and K. P. Pradhan, “Modeling the Electrostatics of 2-Terminal Boron or Nitrogen Substitution Doped Metal-Insulator-Graphene (MIG) Structure," 2020 5th IEEE International Conference on Emerging Electronics (ICEE), pp. 1-4, https://doi.org/10.1109/ICEE50728.2020.9776824 .