Research Article

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A non-ideal hybridization issue for vertical TFET-based dielectric-modulated biosensor

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Abstract: This article evaluates SiGe/Si heterojunction vertical tunnel field-effect transistor (VTFET-hetero) biosensors, using SiGe in the source region to enhance sensitivity. It detects smaller analyte concentrations for biomedical applications. Non-ideal sensor behavior is explained by steric hindrance and irregular probe/receptor positions. Based on the simulation results, sensitivity is determined for four different cases in which partially filled nanogaps have decreasing, increasing, concave, and convex profiles. Simulation shows concave step profiles having the highest sensitivity. The VTFET-hetero structure exhibits higher sensitivity than horizontal biosensors, achieving a sensitivity of 8.64×10^7 for immobilized charged biomolecules.

Keywords: vertical TFET-based biosensor, steric hindrance, heterojunctions structure, drain current sensitivity, biomolecules

1 Introduction

A significant amount of attention has been paid to biosensors for identifying biological molecules, such as proteins and glucose, using label-free technology in various fields, such as medical, environmental, and agricultural fields, as well as criminal identification [1]. The accuracy of biosensors depends on the type of molecule being detected, its concentration, and the specificity of the sensor. In addition, biosensors require minimal sample preparation and are simple to operate. A comparison of different possible devices for bio-sensing functions shows that the field-effect transistor (FET) exhibits classic performance as a label-free bio-sensor because it is compatible with CMOS technology, has higher scaling capabilities, is more cost-effective, and is extremely sensitive [2]. A wide range of applications are available for biosensors, including in the food sector, the environment monitoring domain, and the medical field. FET-based biosensors are also suitable for real-time monitoring and rapid detection of pathogens, toxins, and other contaminants. Furthermore, they are capable of measuring several signals, such as electrical, optical, and chemical [2–4]. A biomolecule's neutral or charged charge can alter the oxide capacitance, altering the drain current or threshold voltage when it occupies the nanogaps. The charge of the biomolecule can affect the electric field in the nanogaps, which can affect the drain current or threshold voltage. This change in voltage can be used to detect the biomolecule. Aspartic acid (Asp), lysine (Lys), arginine (Arg), glutamic acid (Glu), and aspartic acid (Asp) have dielectric constants [5] ranging from 11 to 25.6, whereas gluten, keratin, and zenin have dielectric constants ranging from 5 to 10 [6–8]. These differences in dielectric constants can be used to distinguish between different types of biomolecules, allowing for more sensitive and accurate detection [9]. In addition, they can be used to optimize the design of nanogap-based biosensors. Dielectric-modulated biosensors can perform biosensing by etching a nanogap in the gate dielectric material, resulting in a change in the dielectric constant, which in turn changes the drain current [10–13]. Because of this, the analyte can be detected in a sample since the dielectric constant changes with the analyte's concentration. Biomolecules induce this change, which can be used to determine whether or not they are present in a sample. Nanogap-based biosensors can also be used to measure biomolecule concentrations. This inductive coupling, which is made possible by a nanogap between the gate electrode and the channel, is what drives the operation of dielectric-modulated FETs. This allows the conductance of the nanogap to be modulated, hence allowing control over the transistor's performance. The nanogap can detect various small particles in addition to molecules. Biomolecule concentrations can be determined by varying the electrical current flowing through the nanogap [14].

Tunnel field-effect transistors (TFETs) with source pockets perform better than ordinary TFETs in terms of subthreshold properties [15]. The suppression of short-channel

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effects in the source pocket area is the cause of this improved performance. As a result, it is possible to manage the sub-threshold current more precisely, which increases energy efficiency [16]. Low-band-gap materials like Ga and InAs are frequently employed in the source region of TFETs with silicon channels to decrease the tunneling width and boost the drain current. TFETs are perfect for low-power applications because of their increased energy efficiency, and they can occasionally take the place of MOSFETs due to their superior energy efficiency. OFF Current, however, exceeded its ideal value due to the tunneling breadth. To further enhance source pocket-engineered TFETs, the drain-to-source extension (DSE) was implemented. By decreasing IOFF, the DSE lowers the tunneling width while maintaining appropriate current flow, increasing TFET efficiency. At low voltages, energy consumption and performance are balanced in III–V materials by using staggered hetero-junctions at the source-channel junctions. This produces a highly efficient, low-power gadget that is perfect for low-power applications. In addition to offering increased on-current and improved performance at lower voltages, the DSE reduces tunneling current, which helps to reduce power consumption [17–21].

A vertical tunnel field-effect transistor (V-TFET) based on staggered heterojunctions for SiGe/Si heterojunctions is thus proposed in this study. V-TFETs consume less power than conventional MOSFETs and can be fabricated using existing semiconductor fabrication techniques. V-TFETs are promising candidates for energy-efficient integrated circuits in the future. With and without source pockets, SiGe/Si-staggered heterojunction V-TFETs were analyzed using the commercial SILVACO ATLAS TCAD simulation system [22]. The proposed V-TFET is fabrication-feasible since SiGe can be fabricated on clean Si substrates. The energy efficiency and switching speed of V-TFETs were improved. In addition, the SiGe/Si-staggered heterojunction design allows for an ultra-thin source channel, resulting in a lower leakage current [23].

The purpose of this study was to comprehend and explain the effects of partially filled cavities on the performance of potentiometric biosensors in a dry environment and their implications for practical applications.

2 Proposed device structure

According to Figure 1(a), two different cavities have been created in the gate oxide region to represent the real-life situation. In Figure 1(b)–(e), the steps within the cavity are nonuniformly concave, decremented, convex, and increased. This is done to simulate the effects of different voltages on the

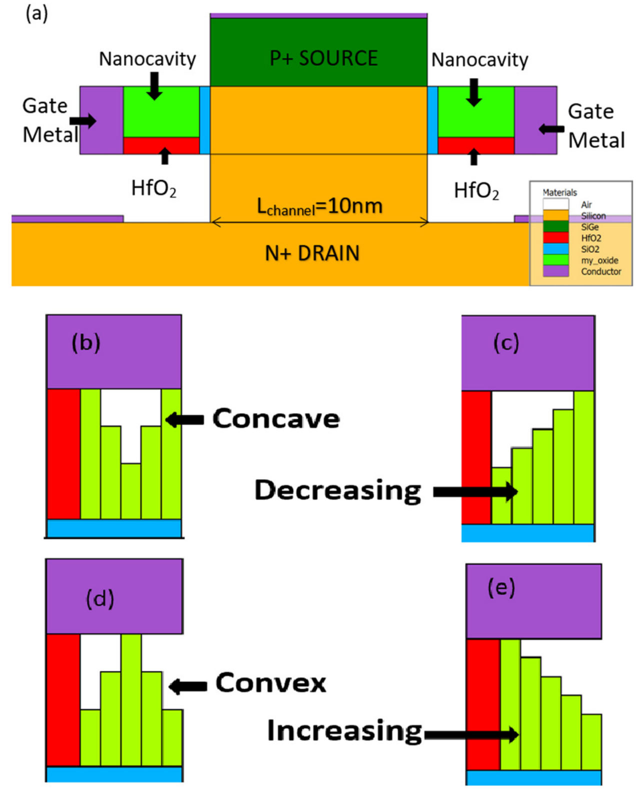

Figure 1: Schematic representation of SiGe/Si heterojunction vertical tunnel FET (VTFET-hetero structure) based label-free biosensors having (a) fully filled cavity, (b) concave step pattern, (c) decreasing step pattern, (d) convex step patterns, and (e) increasing step of bioanalytes.

gate oxide region and to observe how it affects the breakdown voltage of the transistor. By varying the shape of the step patterns, it is possible to study the effects of different voltages on the breakdown voltage.

A nanogap cavity is formed by etching a certain part of the gate oxide for heterojunction vertical tunnel FET (VTFET-hetero) structures. The nanogap cavity provides a path for electrons to travel through the transistor, allowing it to switch faster. This increased switching speed is important for modern electronic devices. In the source, channel, and drain regions, the uniform doping concentrations are 5×10^{20}, 1×10^{16}, and $5 \times 10^{18}/cm^{-3}$, respectively. The nanogap cavity is then filled with a dielectric material, and the gate electrode is fabricated. A high I_{ON} current, when source region with a low bandgap SiGe is projected in the proposed structure. The gate electrode controls the current flow, allowing control of the amount of charge stored in the nanogap cavity. The oxide layer is HfO_2, and the gate metal is aluminium (4.0 eV).

An implementation of a hetero-TFET [8] is preferred to enhance the I_{ON} and steepen the SS. Researchers have studied completely filled cavities [10,12,13]. Completely filled cavities can provide better electrostatic control and can also be used to reduce parasitic capacitance. They also allow for higher electric field strengths, which can help to enhance I_{ON} and steepen the SS. Finally, completely filled cavities can provide better isolation between the source and drain regions, which is important for device performance. The low-binding probability and the functionality of the surface of the cavity have led to the assumption that in the proposed architecture, the array of bioanalytes inside the cavity is uneven and composite due to the low-binding probability and functionality of the surface. Practicality would dictate this approach. Additionally, steric hindrances do not permit the cavity to be completely filled. Therefore, the array of bioanalytes in the cavity needs to be carefully optimized to achieve desired performance. Moreover, the bioanalytes should be chosen based on their binding properties to ensure efficient isolation between the source and drain regions.

ATLAS-TCAD simulations for the SiGe/Si-based VTFET-hetero structure biosensor with source pocket presented in this article are illustrated in Figure 1(a). Based on the simulation results of conventional vertical TFETs [24], Figure 2 shows their metrics. A non-local band-to-band tunneling (BTBT) accounts for local variations within the energy band to improve tunneling accuracy. When SiGe and Si have different lattices and thermal coefficients, defects can form in SiGe–Si heterojunctions [25]. These defects can degrade the device performance and reduce its lifetime. The BTBT helps to reduce the defects and improve TFET performance. This prompted us to include non-locally trap-assistive models, such as TAT.NLDEPTH, in our model. This model helps to capture the non-locality of the defects and accurately simulate the SiGe–Si heterojunctions. This helps to improve the performance of the device, increase its lifetime, and reduce its cost. These statements improved the relevance of the results. There is also a Shockley–Read–Hall generation–recombination architecture, a Fermi–Dirac statistical model, and a field-dependent mobility structure included [26–28]. To improve the drain current and fabrication compatibility of the proposed V-TFET device, a high-k HFO_2 material is used as a gate oxide in the proposed VTFET-hetero structure. In Table 1, you can find a summary of the different parameters used to simulate the device.

3 Results and discussion

The VTFET heterostructure biosensor is examined in this section for its performance in sensing neutral and charged biomolecules according to different metrics like energy band diagram and drain characteristics. The VTFET heterostructure biosensor showed good performance in sensing neutral and charged biomolecules. The drain characteristics also changed significantly in the presence of biomolecules, indicating that the biosensor could detect the biomolecules. A conventional vertical TFET simulation environment (models and dimensions) was used to validate the simulation. Nanocavities are built to recognize biomolecules in the proposed structure model, which has the same parameters as conventional models. A VTFET-hetero structure biosensor simulation was performed using the Silvaco Atlas system [22]. Using a dielectric constant (=1) value to represent air-filled cavities, the cavity is represented as being filled with air. There is no biomolecule in the cavity, which is fundamentally true. Similarly, the value of the dielectric constant increases as the dielectrics of the biomolecule increase

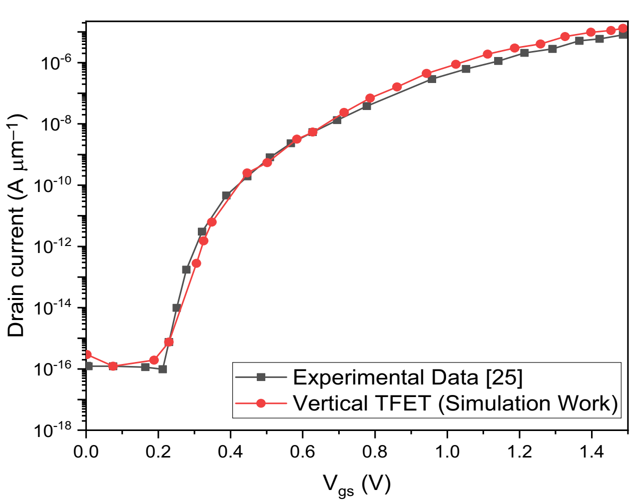

Figure 2: TFET output curves simulated for conventional vertical structures [24].

Table 1: The proposed VTFET-hetero structure: different values

Parameters	Values
Source region concentration	5×10^{20} cm^{-3}
Drain region concentration	5×10^{18} cm^{-3}
Channel concentration	1×10^{16} cm^{-3}
Source length	30 nm
Drain length	50 nm
Channel length	20 nm
Oxide width (SiO_2 and HfO_2)	0.5 and 3.5 nm
Shape of the cavity	Convex, Concave, Increasing and decreasing pattern
Gate metal work function	4.0 eV
Length of cavity	15 nm
Thickness of cavity	3.5 nm

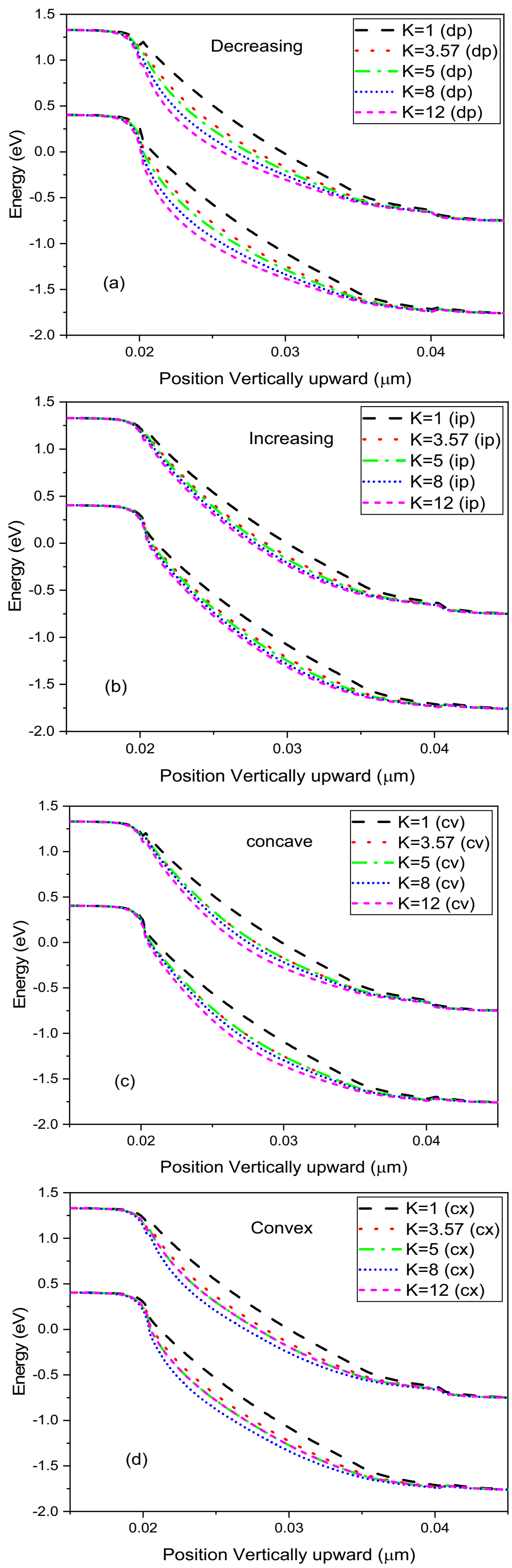

Figure 3: Energy band variation at different dielectric constants, κs of the proposed structure with a cavity length of 15 nm. Here, (a) decreasing, (b) increasing, (c) concave, and (d) convex patterns of biomolecules.

($\kappa > 1$). The increased dielectric constant changes the electrostatic field in the device, which affects the tunneling current and sensing performance of the device. Therefore, it is important to consider the dielectric constant when simulating VTFET heterostructure biosensors.

3.1 Assessing the performance of the proposed biosensor under partial filling of the cavity with neutral bioanalytes

A nanogap cavity region is formed by removing the gate oxide from the device, enabling proper surface functionalization of the target biomolecules. The nanogap cavity regions were filled with air without the target biomolecules. The nanogap cavity regions were then used as a platform for attaching biomolecules. The biomolecules can then be used for sensing, imaging, and drug delivery applications. In this scenario, target biomolecules (such as streptavidin and biotin) are present within a cavity with 0.8 V and N_f = 0 to capture the biotarget in the cavity. Figure 3 illustrates the variations in energy band intensity at different dielectric constants for different patterns of biomolecules demonstrated at 15-nm cavity length for (a) decreasing, (b) increasing, (c) concave, and (d) convex patterns. Biomolecule conjugation is also impacted by band bending that occurs under the cavity region because of the intrinsic material properties of the samples. The dielectric constant value for biomolecules inside the nanogaps increased, resulting in an increase in hole density in the source region. SiGe–Si layers generate a conduction band arrangement between the source and channel valence bands beneath the cavity for the source region. This band bending is beneficial for biomolecular conjugation because it creates a large electrostatic field inside the nanogap. This field can be used to effectively attract and bind biomolecules to the nanogap. The field can also be used to control the charge transport properties of the nanogap. Reduced tunneling barriers increase electron tunneling rates. The ON current of the device improves as tunneling increases.

A high capacitive effect results in significant band bends at the source/pocket interface in the proposed VTFET-hetero structure as k increases. This bend shifts the conduction band edge closer to the interface, resulting in higher current densities at the interface. As a result, a more efficient device can be realized with higher on-currents and improved gate control. Thus, V_{TH} is reduced and I_{ON} is increased in Figure 4 with a cavity length of 15 nm, the proposed structure has different I_{DS}–V_{GS} characteristics at different dielectric

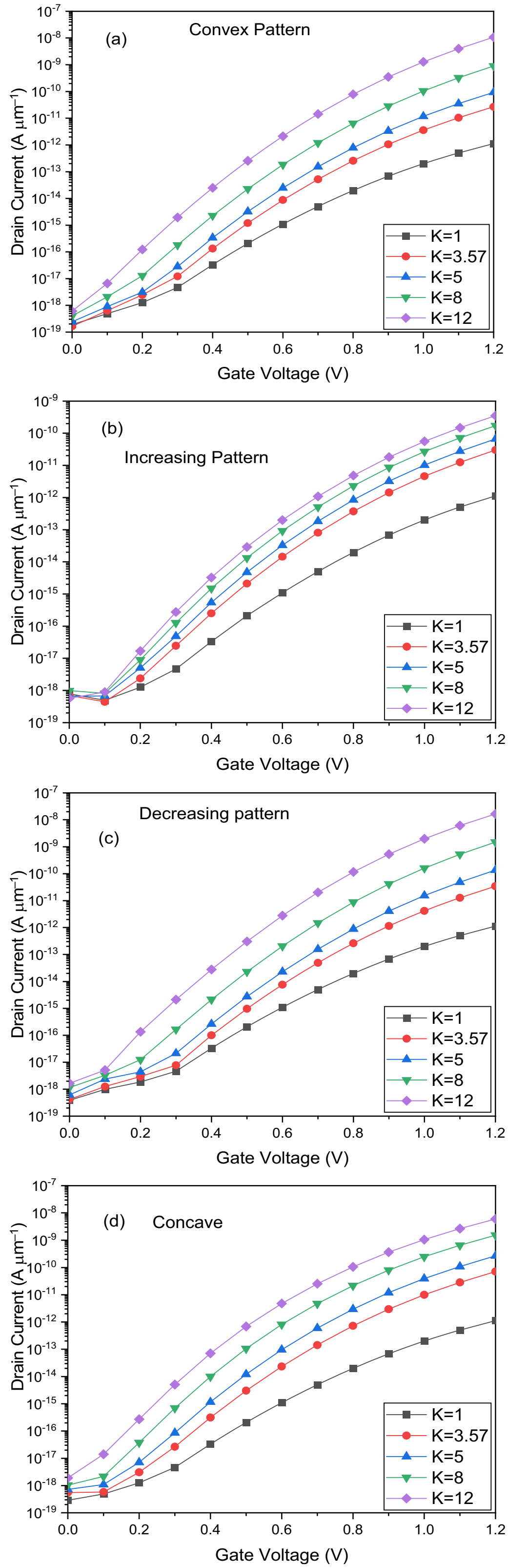

Figure 4: I_{DS}–V_{GS} characteristics at different dielectric constants, *κ*s of the proposed structure with a cavity length of 15 nm. Here, (a) convex, (b) increasing, (c) decreasing, and (d) concave patterns of biomolecules.

constants. Here, (a) convex, (b) increasing, (c) decreasing, and (d) concave patterns of biomolecules. The simulation results showed that the VTFET-hetero structure has an improved drain current and leakage current compared with the conventional structure. The VTFET-hetero structure has potential applications in low-power and energy-efficient electronic devices. Elevated steps near the tunneling interface are more electrostatically coupled to the gate as "*k*" of bioanalytes increases [29]. This increases the gate voltage sensitivity and reduces the threshold voltage of the VTFET-hetero structure. Furthermore, the VTFET-hetero structure is suitable for bio-sensing applications due to its high sensitivity to biomolecules.

3.2 Assessment of the sensitivity of a proposed biosensor considering the irregular arrangement of bioanalytes

Previous research assumed that biomolecules filled all nanogaps in nanostructures. This new research, however, suggests that biomolecules may not be the only molecules that can form these gaps. Ions and other materials can also be used to fill them. By understanding these properties, new nanomaterials with improved properties may be developed. Nevertheless, this assumption is not often made in practice. Partial hybridization of biomolecules can occur in four possible patterns, including decreasing, increasing, concave, and convex, as described in this article. By analyzing these patterns, scientists can gain a deeper understanding of nanomaterial interaction and gap formation. With this understanding, nanomaterials with desirable properties, such as electrical conductivity, optical transparency, and strength, can be created. This could lead to new applications in fields such as nanotechnology, medicine, and energy production. Additionally, this knowledge can be used to improve the performance of existing nanomaterials. Due to steric hindrance, biomolecules show nonuniform step patterns [18–20]. Using the formula below, you can estimate the sensitivity factor

$$S_{\text{Drain current}}(\%) = \left(\frac{I_D^{\text{bio}} - I_D^{\text{air}}}{I_D^{\text{air}}} \times 100\right). \tag{1}$$

It is considered a reference to have a cavity completely filled with air. At fully filled conditions, the sensitivity parameters increase as the percentage of the filling factor increases. With an increasing filling factor, the cavity becomes more sensitive to external forces. In certain applications, such as accelerometers based on MEMS, this sensitivity can be advantageous.

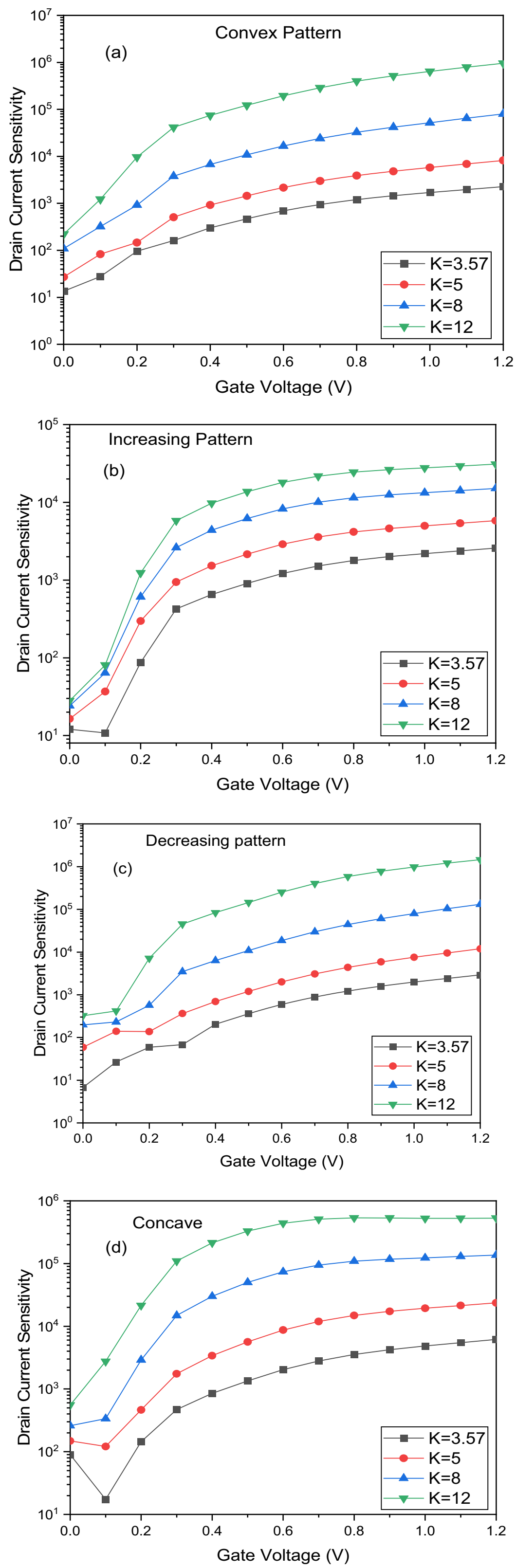

Figure 5: Assessment of VTFET-hetero structure biosensor drain current sensitivity in the presence of neutral bioanalytes (N_f = 0) at V_{ds} = 0.8 V. Here, (a) convex, (b) increasing, (c) decreasing, and (d) concave patterns of biomolecules.

3.2.1 Impact of neutral biomolecules on sensitivity for irregular arrangement of bioanalytes

Depending on the biological molecule, the dielectric constant of the target biomolecule (neutral) within the nanogap is changed from k = 1 to k = l to detect its reflective nature. By adjusting the distance between the electrodes, we can adjust the performance of the system. The current flow between the two electrodes can be used to measure the change in the dielectric constant. A biological sample is tested for the presence of various molecules using this technique. As a result of confined biological molecules with a high dielectric constant, ON current appears to increase. Biomolecular sensors can be designed using this increase in ON current. A solution sample can be measured for a specific molecule's concentration using the sensor and a specific molecule can also be detected using it. The gate bias' effective field forces the channel to become more capacitive across the nanogap as the dielectric constant of the nanogap increases. When the field effects increase, the barrier width between the source and channel decreases, resulting in an increase in drain current and band bending. This increase in drain current and band bending results in improved performance of the nanogap transistors. Additionally, the gate bias can be used to control the performance of nanogap transistors [20].

As shown in Figure 5(a)–(d), sensitivity is evaluated for different patterns. As neutral bioanalytes are immobilized inside the cavity, N_f = 0 when the different biomolecules are immobilized. Elevated steps nearer the tunneling interface exhibit enhanced electrostatic coupling with the increase of k of bioanalytes. As the elevated steps are positioned far from the source-to-channel tunneling interface, the sensitivity of the biosensor is superior in decreasing and convex step patterns. The sensitivity of the biosensor is maximized when the steps of the pattern are located at the interface between the tunneling interface and the bioanalytes.

A neutral biomolecule enters a nanogap and receives immobilization and hybridization from a receptor or probe. In this case, the hybridization process [29] may stop before the nanogaps have been fully filled, resulting in steric hindrance, which prevents more biomolecules from entering. A steric hindrance creates non-uniform step profiles inside nanogaps due to steric hindrance. The step profiles can then be used to detect biomolecules of interest. This technique can be used to detect and localize single molecules in nanogaps. An irregular hybridization profile along the nanogap length is shown in Figure 5 for the VTFET-hetero structure. The assessment of drain current sensitivity between nonuniform step patterns (at V_{ds} = 0.8 V, V_{gs} = 1.2 V) is illustrated by Figure 5(a)–(d), which shows the

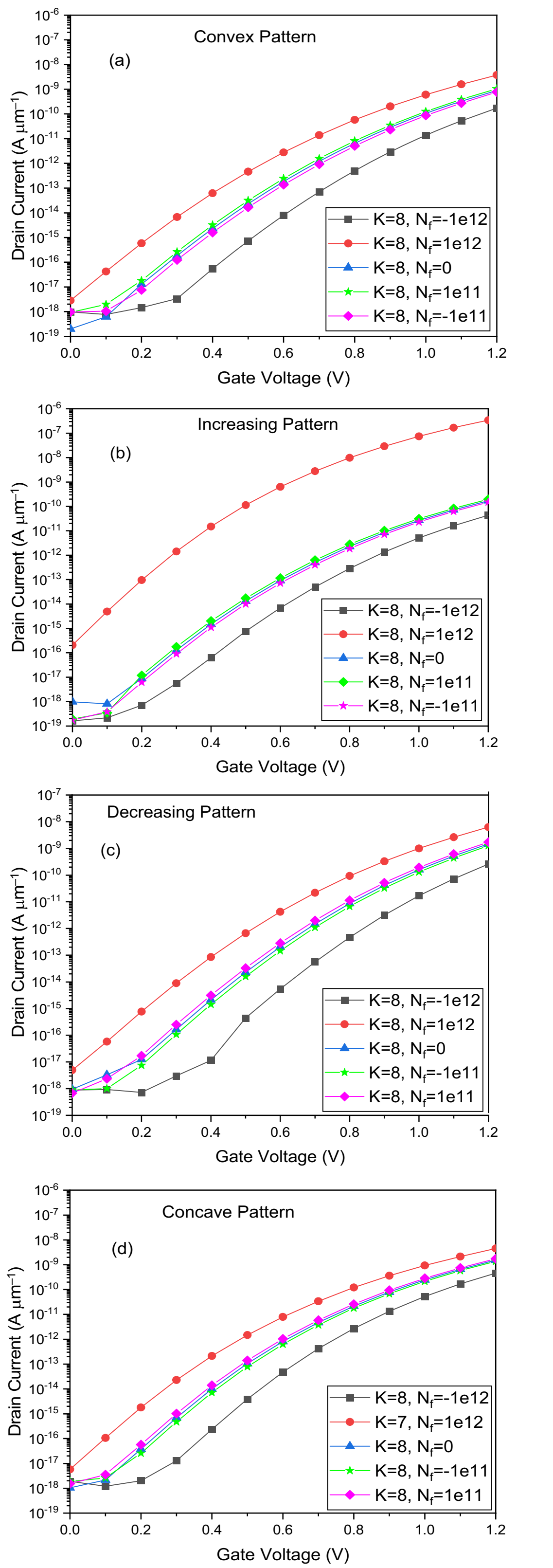

Figure 6: Assessment of VTFET-hetero structure biosensor in the presence of charged bioanalytes ($N_f = -1 \times 10^{12}$, 0, 1×10^{12}) at $V_{ds} = 0.8$ V. Here, (a) convex, (b) increasing, (c) decreasing, and (d) concave patterns of biomolecules.

linker immobilized in the cavity at an $N_f = 0$ charge density as a neutral bioanalyte. The results indicate that this method is able to detect and localize a single molecule in a nanogap. All the steps of nanogaps were compared for their sensitivities while maintaining the same fill factor for the VTFET heterostructure biosensor. Biomolecules have been considered in various nonuniform step patterns due to steric hindrance issues [29–31]. For the remainder of this paper, we will analyze the VTFET-hetero structure biosensor using the convex step pattern since this pattern produces the best results.

3.3 Proposed biosensor performance assessment considering the irregular arrangement of charged bioanalytes after partial filling

According to Figure 6(a)–(d), the drain current varies with respect to the V_{GS} for positively and negatively charged biomolecules having k = 8 for all four structures. With increasing positive (negative) charges on biomolecules, the drain current is observed to increase (decrease). Biomolecules that occupy the nanogaps affect the surface potential of the biosensor, which further impacts the drain current when the nanogaps are occupied by positive (negative) charged biomolecules. This indicates that the biosensor is sensitive to the charge density of the biomolecules. Furthermore, this suggests that the biosensor can be used for a wide range of applications, such as sensing the concentration of biomolecules in solution.

For partially filled nanogaps of the proposed VTFET-hetero structure biosensor, Figure 6(a)–(d) shows sensitivity plots versus magnitudes of negative charges. It can be seen that the sensitivity of the nanogap increases with the negative charge magnitude. Furthermore, the sensitivity also increases with the decreasing thickness of the nanogap. These results show that the proposed VTFET-hetero structure biosensor is highly sensitive and efficient. The graphs show that sensitivity decreases as negatively charged biomolecules are magnified. This indicates that the sensitivity of the nanogap is highly dependent on the size of the biomolecules. This indicates that the biosensor can be used to measure a variety of biomolecules of different magnitudes. Additionally, the nanogap can also be used to measure biomolecules of different thicknesses. Although concave pattern biosensors possess higher sensitivity than others due to their different pattern of cavity filling. A higher I_{ON} and therefore a higher sensitivity are

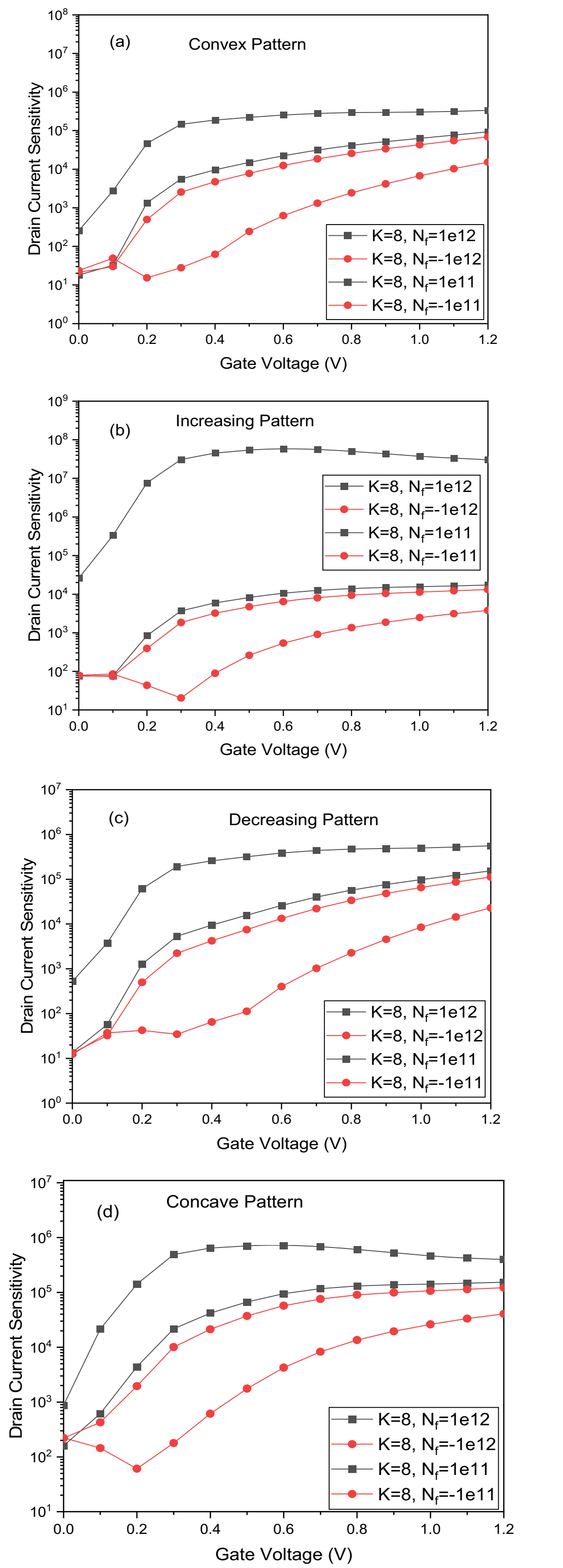

Figure 7: Assessment of VTFET-hetero structure biosensor sensitivity in the presence of charged bioanalytes ($N_f = -1 \times 10^{12}, 0, 1 \times 10^{12}$) at $V_{ds} = 0.8$ V. Here, (a) convex, (b) increasing, (c) decreasing, and (d) concave patterns of biomolecules.

achieved by increasing pattern assessment of proposed structures.

3.4 Impact of positively and negatively charged biomolecules on sensitivity:

In this section, we investigate whether biomolecules with positive or negative charges are more sensitive to drain currents. According to Figure 7, the steepest and concave step profiles are generally more sensitive than the steepest and convex profiles. In TFETs, the drain current results mainly from electron tunneling at source-channel junctions whose tunneling probability is influenced by gate oxide dielectric constants. Since the dielectric capacitance around the tunneling junction is increased by the increasing step profile, the sensitivity is increased as well. The dielectric constant increases with increasing gate-channel coupling, which increases sensitivity. The increased sensitivity allows for more accurate control of the drain current, allowing for better performance in TFETs. Furthermore, the gate-channel coupling allows for better control over device operation, resulting in better energy efficiency.

It can be seen in Figure 7 that the steps that decrease and have convex profiles exhibit low sensitivity, whereas the steps that increase and have concave profiles exhibit a greater response. This agrees with the principle that increasing the slope of the graph also increases the sensitivity of the system. This is reflected in the response of the steps, which have a greater response when the graph is concave than when it is convex. Tunneling electrons at the source-channel junction are mainly responsible for the TFET drain currents.

Thus, based on the variation in the fill-in factor and the position of biomolecules in the cavity region, we can draw the following conclusions: DG-VTFETs detect biomolecules more sensitively when a biomolecule has a higher fill-in factor. This is because the higher filling in the channel of the proposed device allows more electrons to pass through and be detected [30]. In addition, the smaller size and higher mobility of the electrons in the DG-VFETs allow them to be detected more easily.

An overview of the performance of the TFET-based biosensors can be found in Table 2. By comparing the sensitivities of recently proposed TFET-based biosensors, an approximate idea can be provided as to which sensor will perform better in a certain operating range. Vertical TFET-based biosensors have higher sensitivities than horizontal TFET-based biosensors, making them a better choice for most applications.

Table 2: Analysis of published TFET-based biosensor's performance

Sr. no.	Name of the biosensors	Paper reference	Sensitivity
1.	SiGe source DM PNPN TFET with 10% Ge	[24]	6×10^3
2.	DM JLTFET	[27]	1.9×10^4
3.	DM DG TFET	[28]	2.84×10^5
4.	DG TFET	[29]	1.05×10^2
5.	DM FET [31]	[31]	3×10^4
6.	VTFET-hetero structure	[Our work]	8.64×10^7

4 Conclusion

In this study, a heterojunction vertical tunnel FET (VTFET-hetero structure) based on SiGe/Si heterojunctions is proposed. With this model, the drain current sensitivity is maximized to increase the step pattern of the proposed biosensor when charged biomolecules are immobilized. The performance of the sensor has been studied in relation to negatively and positively charged biomolecules. Compared with the other profiles, the concave step profile has the highest sensitivity. The lack of sensitivity was caused by the slopes of the decreasing step profiles and the convex partially filled profiles. A comparison table of published work is shown at the end, revealing that the proposed VTFET heterostructure biosensor can act as an excellent low-power biosensor with high sensitivity. Because of an analysis of the electrical parameters and device immunity of SCEs, the proposed model proves to be an effective biosensor for the detection of charged/neutral biomolecules. The biosensor is suitable for biomedical applications that require high sensitivity and low power consumption. In addition, the biosensor is low cost and can be easily integrated into existing technologies.

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Conflict of interest: Authors state no conflict of interest.

Data availability statement: The data that support the findings of this study are available from the corresponding author upon reasonable request.

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