RESEARCH ARTICLE

A Feasibility Study of Vertical Dual Channel Extended Source Schottky Barrier MOSFET as a Highly Sensitive Biosensor

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ABSTRACT

In this research, we demonstrate an ultra-sensitive dielectric-modulated biosensor based on a vertical dual-channel extended-source Schottky barrier MOSFET. The proposed structure contains a nano-gap in which biomolecules are accumulated. The immobilization of biomolecules with different dielectric permittivity in the nano-gap modulates the effective gate capacitance and eventually results in a drain current deviation in comparison with the air-filled nanogap condition. By definition, on-state and off-state current variation before and after biomolecule absorption are considered two different measures for assessing the responsivity and sensitivity of the biosensor. Basically, the main focus of this paper is designing a low power device, in which the change in the electrical characteristics of the device under biomolecule absorption can be detected even in the absence of the gate bias. The high sensitivity of the proposed biosensor is mainly attributed to the extended source region, which provides a wider current transport area at the interface of the source and channel regions. We optimize the biosensor's properties by exploring the impact of critical physical and structural design parameters on the sensitivity and selectivity of the biosensor. In addition, statistical analysis is conducted to calculate the coefficient of variation (CV) measure for evaluating the change in the sensitivity of the biosensor based on the variation of fundamental design measures. The results pave the way for designing a low-power CMOS-compatible biosensor that has fast response with high distinguishing selectivity and can be scaled down to the nanoscale.

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INTRODUCTION

Recently, due to the pandemic situation, biosensors have gained significant attention for the detection and monitoring of a wide range of viral diseases. Basically, biosensors have been extensively employed in cancer diagnosis, blood glucose measurement, environmental monitoring, food analysis, toxicity detection, etc. [1-5]. Biosensors based on metal oxide semiconductor field effect transistor (MOSFET) have risen in popularity due to their intrinsic advantages of low power operation, scalability, and label-free detection. The device is fully compatible with the CMOS fabrication process, and the electrical conductance of the channel can be significantly modulated upon biomolecule absorption [6-8]. In principle, variations in the corresponding device characteristics can be used as markers for the detection and quantitation of targeted biomolecules.

Dielectric-Modulated (DM) FET-based biosensors are extensively used biosensor to detect neutral and charged biomolecules. In this type of biosensor, a nanocavity is embedded in the gate oxide region via thin-film deposition and wet-etching techniques for the immobilization of biomolecules. The effective capacitance of the gate oxide changes with the charge density and dielectric constant of the biomolecules that are accumulated in the cavity. It is evident that modulation of the gate oxide capacitance induces an effective capacitance coupling between the gate and channel region, and as a consequence, makes a significant shift in the threshold voltage and channel conductance compared to the air-filled cavity. Therefore, these electrical markers can be considered for assessing the sensitivity of the biosensor. Different configurations of dielectric-modulated biosensors, such as conventional MOSFET [9], junctionless MOSFET [10-12], tunnel FET [13-15], impact ionization MOSFET [16-18], and nanowire [19], have been reported in the literature. However, to further increase the sensitivity of biosensors, the considerable variability of their electrical characteristics before and after the absorption of biomolecules remains a significant obstacle to their efficient practical application. In addition, as the dimensions of conventional FET structures with doped source and drain regions are miniaturized, challenging fabrication processes of thin film heavily doped regions emerged, which can fundamentally degrade the biosensor efficiency in the nanoscale regime. By definition, Schottky barrier FET employs metal/silicide regions in the source and drain regions and is introduced as a potential candidate of conventional MOSFET for nanoscale regimes. This device has a low-temperature simple fabrication process and is fully compatible with the CMOS fabrication process [20-21].

In this paper, the feasibility of a dielectric-modulated vertical dual channel Schottky barrier field effect transistor with an extended source region (VDC-SBFET) as an efficient biosensor is thoroughly investigated. One distinguished feature of the proposed device is that the tunneling junction at the source-channel interface is extended vertically and two parallel channels are created at the source sidewalls, which considerably improves the device performance and provides high sensitivity of device electrical characteristics upon biomolecule absorption. When sufficient gate bias is applied, a high electric field distributes along the tunneling junction at the interface of the source and channel regions, and as a consequence, tunneling paths with a short barrier width are available in the on-state, effectively boosting the drive current of the device. Consequently, the electrical characteristics of the device, such as off-state and on-state current, are effectively changed as per the absorption of targeted biomolecules in the cavity, and

a higher sensitivity of the biosensor can be achieved. The role of various physical and structural parameters that influence the sensitivity of biosensors is taken into consideration. These proposed simulation results confirm that critical design parameters play a fundamental role in determining the sensitivity of biosensors. It is thus possible to manipulate the sensing properties to design an efficient biosensor. In addition, statistical analysis is carried out to assess the susceptibility of biosensor performance with respect to the variation of essential design parameters. The coefficient of variation (CV) of biosensor sensitivity is calculated for different biosensor measures. By definition, a CV is a statistical measure that determines how data points in a data set are distributed around the mean value. The lower the value of CV, the lesser the dispersion, and the more consistent will be the biosensor's sensitivity. However, on the other hand, a higher value of CV for a specific design parameter denotes the vulnerability of the biosensor's response with respect to the variation of that parameter, and it concludes that the optimum value should be determined for it.

The paper is organized as follows: the device structure of the VDSBFET along with different models that are employed for device simulation, followed by the operation principle of the biosensor are presented in Section 2. Next, the impact of the main design parameters on the sensitivity of the biosensor, is comprehensively discussed in Section 3. Finally, the paper is outlined in Section 4.

Simulation Setup and Biosensor Operation Principle

The schematic of the proposed dielectric modulated by the VDC-SBFET is illustrated in Fig.1 (a). The source and drain regions are ytterbium silicide, and silicon is considered the channel material. To boost the performance of VDC-SBFET, the source region is extended vertically, and two parallel channels are created at the source sidewalls that can fundamentally improve the on-state current. The main difference between a dielectric-modulated transistor and a conventional VDC-SBFET involves the embedded nano-gap in the gate dielectric at which certain biomolecules are immobilized. In order to sense different molecules, a portion of the gate oxide layer is etched to form a nanocavity in which proper bioreceptors are functionalized to enable the binding of targeted biomolecules.

Basically, each biomolecule has its own specific dielectric constant. In the case of the absorption of biomolecules in the nano-gap, the dielectric constant of the cavity increases from air ($k = 1$) to the related value of each specific biomolecule, resulting in a variation of gate capacitance. Therefore, modulation of the gate capacitance leads to a productive capacitive coupling between the gate and the channel, and as a result, a considerable increase in the drain current occurs in comparison with the air-filled nano-gap case. It is to be mentioned that for simulating the accumulation of an individual biomolecule in the nano-gap, the dielectric constant of the cavity is changed with respect to the accumulated biomolecules. The biomolecules that are considered are streptavidin ($k_{bio} = 2.1$), 3-aminoppropyltriethoxysilane (APTES) ($k_{bio} = 3.57$), and protein ($k_{bio} = 8$) [22].

The size of biomolecules that are taken into account is reported to be within deca nanometers for proteins and nearly 5 nm for streptavidin [23]. Accordingly, a vertical thickness of 10 nm for the cavity seems sufficient. Moreover, the trapping of streptavidin within the 10 nm cavity has been reported experimentally [24]. The preliminary design parameters are summarized in Table 1. The numerical simulations are conducted in the Silvaco device simulator [25], and the following models are activated for evaluating the device performance:

(1) Thermionic emission model, which accounts for the emission of thermally exited charge carriers from the surface of a metal. It is evident that, as a result of thermionic emission, carriers with energy higher than the Schottky barrier height can pass over the barrier and produce the thermionic emission current. This effect is more pronounced at elevated temperatures and low Schottky barrier heights.

(2) Direct tunneling of carriers. This tunneling current can be remarkably greater than the thermionic emission current, mainly at high gate voltage values where the tunneling barrier width at the metal-semiconductor interface is reduced. The lateral tunneling direction along the two parallel channels is demonstrated in Fig. 1 (a).

(3) Drift-diffusion models are set for calculating the carrier transport equations in the semiconductor channel.

(4) Auger and Shockley-Read-Hall (SRH) recombination models are set to describe the effect of recombination and generation of carries on carrier transport in the presence of defects and traps.

(5) Basically, carrier mobility plays a fundamental role in carrier drift velocity. The effect of horizontal and vertical applied electric fields on carrier mobility is considered, and related models are activated in the simulation. Moreover, dopants as impurities have a detrimental consequence on carrier mobility and may degrade velocity due to the scattering. The mobility models, considering the effect of dopants, are also set.

Figure 1(b) illustrates a simplified capacitance model for the dielectric-modulated VDC-SBFET for clarifying the bio-sensing action. The gate oxide capacitance (C_{ox}) consists of a combination of capacitances including the air-filled part of the nano-gap (C_{air}), the capacitance of the nano-gap that is accumulated by the biomolecules (C_{bio}), and the remnant gate oxide capacitance (C_{rox}).

$$\frac{1}{C_{ox}} = \frac{2}{C_{rox}} + \left(\frac{1}{C_{air+C_{bio}}}\right) \quad (1)$$

$$C_{bio} = k_{bio}\varepsilon_0 \frac{A}{T_{bio}} \quad (2)$$

Where k_{bio}, is the dielectric constant of the biomolecule, T_{bio} denotes the thickness of the nano-gap that is filled by the biomolecules, ε_0 is the vacuum permittivity and A is the nanogap area. It is evident that the accumulation of the whole volume of the nano-gap by molecules with different dielectric constant modifies the gate oxide capacitance, and as a consequence, a fundamental modulation in the channel charge density is expected. The device's main electrical characteristics highly depend on the capacitive coupled gate and the channel charge density, which can be considered efficient measures for assessing the biosensor's responsiveness. The fabrication method of VDC-SBFET is highly compatible with the CMOS fabrication process. In the first step, through a mask, exposure, ion implantation, and annealing on a silicon substrate, the entire channel of the device is grown. The doping concentration of the formed drain region is 10^{17} cm^{-3}, and the dopant ion is considered arsenic. Then the native SiO_2 region is grown on top of the silicon through masking, exposure, and oxidation. Next, in the source and drain regions, silicide is formed through sputtering and annealing. The side wall gate insulators can be fabricated via the atomic layer deposition (ALD) technique, which provides a uniform dielectric layer. Following that, the cavities are carved in HfO_2 on both sides of the gate via wet etching to obtain the few nanometer gaps in the proposed structure. Finally, metallization through the sputtering technique is carried out to pattern the electrodes.

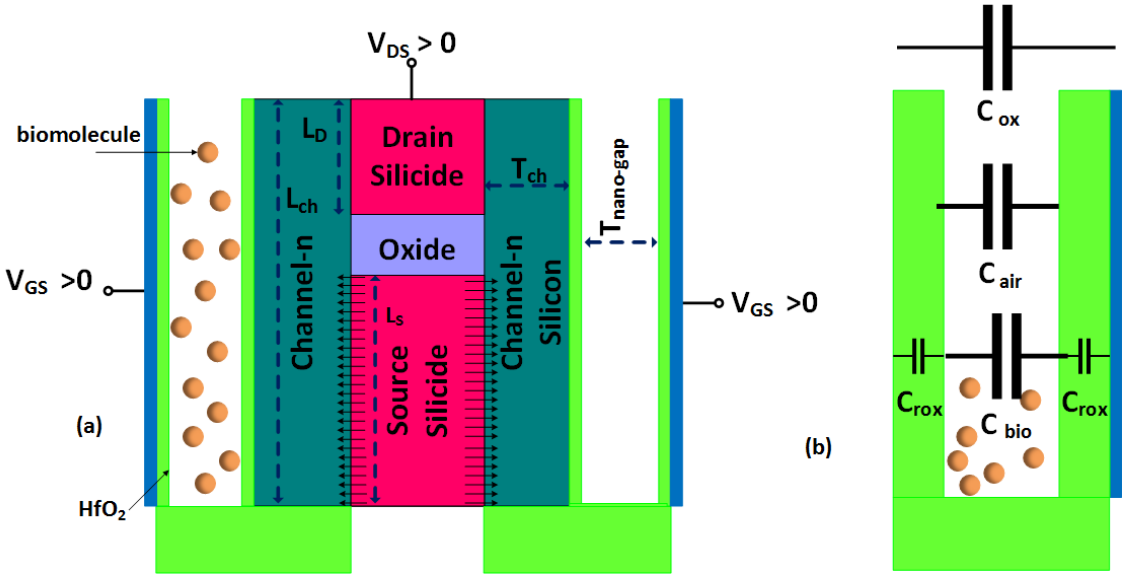

Fig. 1. (a) Schematic of a vertical dual-channel dielectric-modulated Schottky MOSFET as a dielectric-modulated biosensor. The source extended region and the tunneling direction at the interface of the source and channel regions are also demonstrated, (b) a simplified capacitance model for the dielectric-modulated VDC-SBFET.

Table 1. Initial physical and structural design parameters of VDC-SBFET

Parameter	Value
Gate Workfunction	4.5 eV
Lateral Channel Thickness (T_{ch})	5 nm
Gate Oxide Thickness (HfO_2)	1nm
Nano-gap Thickness ($T_{nano-gap}$)	10nm
Source Length (L_s)	130nm
Drain Length (L_D)	50
Channel length (L_{ch})	190 nm
Chanel Doping Density (n-type)	10^{17} cm^{-3}
Schottky Barrier Height	0.3eV
Drain Bias	0.05 V

RESULTS AND DISCUSSIONS

Fig. 2 illustrates the transfer characteristics of VDC-SBFET for different biomolecules that are accumulated in the nanogap. It is observed that the on-state (I_{on}) current increases as the molecules with high dielectric constants are immobilized in the nanogap. Basically, the principal current conduction mechanism in VDC-SBFET is tunneling through the Schottky barrier. In the off-state (V_{GS}=0 V, V_{DS}=0.05 V), the tunneling probability is very low due to the wide depletion region width at the interface of the source-channel junction. In the on-state (V_{GS}=1 V, V_{DS}=0.05 V), the tunneling barrier thickness becomes small enough that it allows the charge carriers to tunnel across the source-channel junction. The charge density in the channel is modulated by the gate oxide capacitance, and it has a direct relationship with the capacitance value. In the case of an air-filled cavity, the gate oxide capacitance is not high enough to accumulate an adequate concentration of charge

density in the channel for the onset of the tunnel. However, upon the absorption of biomolecules, the overall gate capacitance increases, which, as a consequence, enhances the channel charge density. In this situation, an increase in the on-state tunneling current is expected.

Moreover, it is evident that due to the excellent gate influence over the channel upon molecule absorption, the off-state current (I_{off}) considerably reduces. By definition, the variation of the on-state current and off-state current upon molecule accumulation in the nanogap with respect to the reference value can be considered two measures to assess the sensitivity of the biosensor. The reference value of VDC-SBFET is considered when the nanogap is devoid of molecules and hence, is assumed to be air-filled with a dielectric constant of $k = 1$.

The sensitivity of biosensors can be defined based on two measures:

$$S_1 = \frac{I_{off}\ K=1}{I_{off}\ K>1} \quad (3)$$

$$S_2 = \frac{I_{on}\ K>1}{I_{on}\ K=1} \quad (4)$$

Basically, by the variation of critical design parameters, it is evident that the proposed device shows variations in biosensor sensitivity. Thus, the impact of critical design parameters on the performance of the biosensor is thoroughly investigated. First, the impact of channel doping variation on the sensitivity of the biosensor is assessed, as depicted in Fig. 3. The results demonstrate that for the intrinsic channel and also when the doping concentration is still in an adequately low range not to influence the carrier mobility, the sensitivity of the biosensor in terms of both S_1 and S_2 measures is nearly unvarying. The sensitivity and responsivity of the biosensor highly depend on the modulation of channel charge density by the absorption of high-k biomolecules. However, in the case of heavily doped silicon substrates, a remarkable reduction in the sensitivity of biosensors is observed. Basically, the direct tunneling enhancement is due to a competition between two phenomena, including gate-induced electric fields and the effect of channel doping.

In principle, tunneling probability through the Schottky contact can be increased by increasing the channel doping. This effect is mainly attributed to the energy barrier width reduction related to the advantageous energy band bending induced by the n-type dopants. It is evident that the relative contribution of off-state and on-state current variation with respect to gate capacitance modulation gets smaller and that the rate of biosensor sensitivity declines.

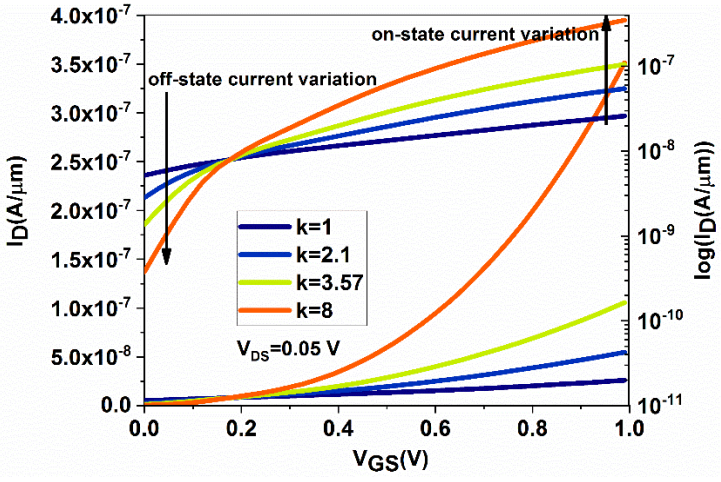

Fig. 2. Transfer characteristics of the VDC-SBFET before and after the absorption of the biomolecule.

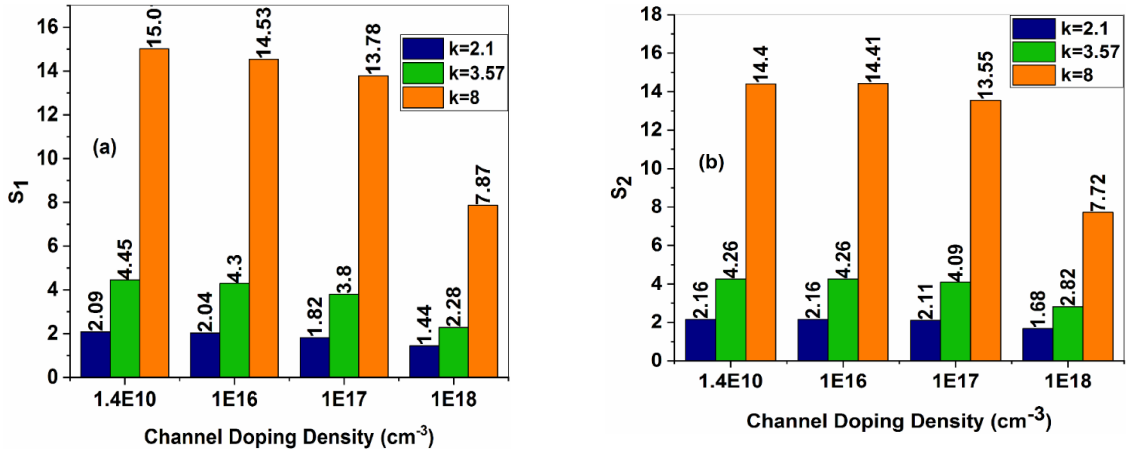

Fig. 3. Biosensor sensitivity in terms of (a) S_1 and (b) S_2 measures as the channel doping density are parametrized.

The effect of temperature on the sensitivity of biosensors is also comprehensively explored. The results depicted in Fig. 4 reveal a high dependency of biosensor performance upon temperature variation. It is evident that the rise in temperature degrades sensor responsiveness in terms of both S_1 and S_2 measures. In principle, the temperature increases, carriers have enough energy to surmount the Schottky barrier height, and the carrier transport is governed by the thermionic emission. This concludes that the accumulation of molecules in the nanogap cannot efficiently modify the tunneling current, and as a consequence, the device has less sensitivity. It is essential to analyze the sensitivity of dielectric-modulated VDC-SBFET based on the percentage of cavity volume filled by the biomolecules. Fig. 5 illustrates S_1 and S_2 measures versus the percentage of nano-gap that is filled by the molecules. It is observed that the sensitivity and selectivity of the biosensor are considerably improved as the whole volume of the nanogap is accumulated. In principle, as a greater fraction of the sensing volume is filled by the molecules, improved relative gate electrostatic controllability over the channel is achieved. Thus, the immobilized high-k dielectric molecules in the embedded nanogap can effectively reduce the off-state current and enhance the on-state drive current.

Next, the effect of lateral distance between the source extension and the gate insulator (channel thickness) on the sensitivity measures is investigated, and the results are shown in Fig. 6. It is observed that reducing the lateral channel thickness yields a higher sensitivity of the biosensor. Basically, decreasing the silicon lateral thickness leads to tighter gate control over the channel upon molecule absorption and thus sets about a strong reduction of the tunneling barrier width at the interface of the source and channel regions. It is expected that, due to the enhanced gate control of the drain current, improved electrical characteristics in terms of both off-state and on-state current can be achieved. The channel charge density (and consequently the off-state and on-state current) is modulated by the work function difference between the gate material and channel. Basically, for efficient performance of the biosensor, the channel charge density is strongly required to depend upon the dielectric constant of the biosensor, not the gate workfunction of the device. It is expected that for low values of the gate workfunction, the electron density increases, and as a consequence, the tunneling probability rapidly enhances. In this case, it is evident that the leakage current is unrelated to the biomolecule absorption. Therefore, it is essential to optimize the gate workfunction value.

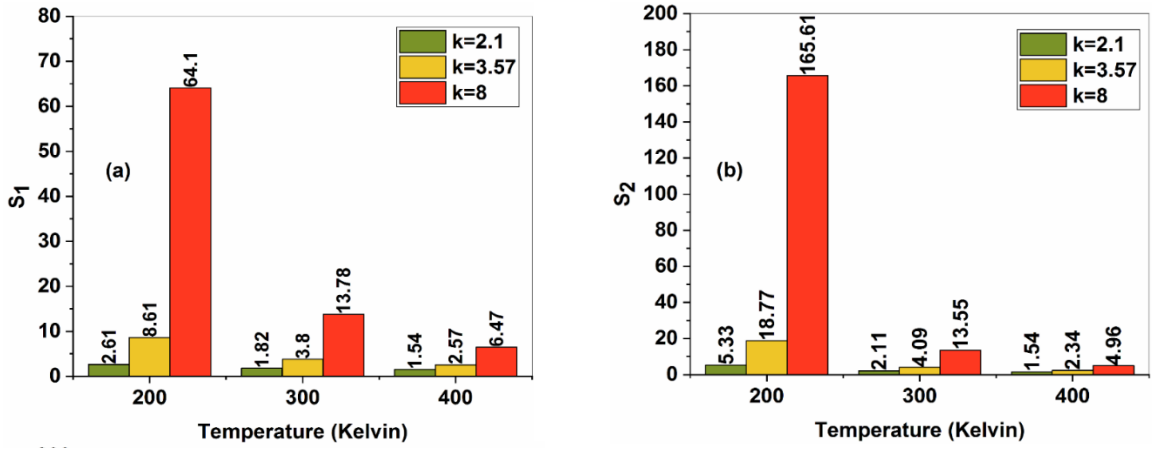

Fig. 4. Biosensor sensitivity in terms of (a) $S_1$and (b) S_2 measures as the ambient temperature is parametrized.

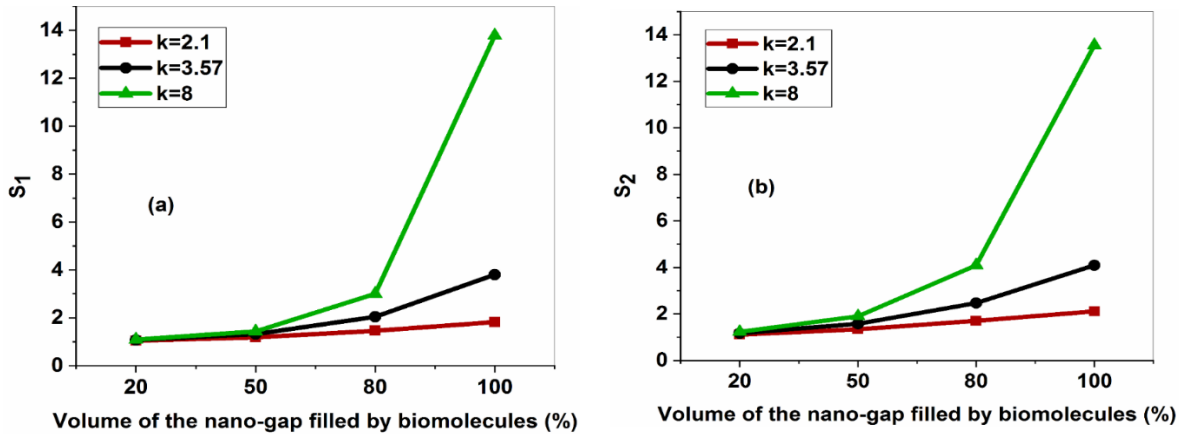

Fig. 5. Biosensor sensitivity in terms of (a) S_1 and (b) S_2 measures versus the nano-gap volume that is filled by the molecules (in percentile).

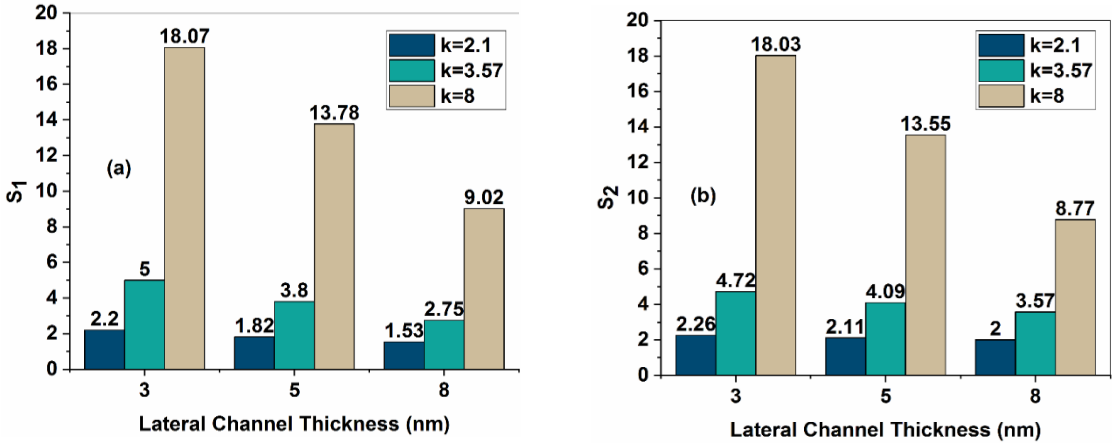

Fig. 6. Biosensor sensitivity in terms of (a) S_1 and (b) S_2 measures versus the lateral channel thickness.

It is important to assess the effect of the surface charge of biomolecules on the sensitivity of biosensors. The charge of biomolecules can be connected with the pH of the solution, the molar density of the biomolecules, and their related isoelectric point. The isoelectric or isoionic point is

defined as the particular pH at which the molecules carry no net electrical charge and, as a consequence, can be regarded as neutral. The difference between the pH and the isoelectric point can influence the charge of biomolecules. In principle, if the pH value is below their isoelectric point, molecules carry a net positive charge, while if the pH is higher than the related isoelectric point, they carry a net negative charge. Due to the importance of a biomolecule's charge on the sensitivity of the biosensor, the impact of the absorption of negative, positive and negative surface charge biomolecules on S_1 and S_2 measures is investigated, and the results are presented in Table 2. The accumulation of positive charge molecules at the interface of the gate insulator effectively modulates the channel charge density and induces excessive electrons in the channel. That being the case, the tunneling barrier becomes thinner, and the direct tunneling current is believed to dictate the carrier transport process independent of the dielectric constant of the absorbed biomolecules. The results demonstrate that the positive interfacial charge plays a crucial role in biosensor efficiency, and it is observed that in terms of S_1 measure, both the sensitivity and selectivity of the device are degraded. However, the thinner the overall barrier, the higher the tunneling probability and a higher variation of on-state current is expected after the absorption of biomolecules. Therefore, the sensitivity of the biosensor is improved in terms of S_2 measure.

It is observed that in terms of the absorption of negative molecules in the cavity, the opposite variation of S_1 and S_2 measures occurs compared with the absorption of positively charged atoms. The accumulation of negatively charged molecules reduces the electron density in the channel and creates a wider space charge region at the interface of the source and channel. It is evident that the off-state current of the device will be dramatically reduced, and a higher S_1 value will be expected. On the contrary, the S_2 measure considerably reduces as the surface density of the negative charge increases. Basically, the direct tunneling current is proportional to the channel electron density, bias voltage, and the Schottky barrier transmission coefficient. By definition, when the barrier width becomes wider, the electron wave cannot effectively penetrate the Schottky barrier, and it is continuously attenuated on its way to the channel region. It is evident that the transmission coefficient reduces, and a higher on-state current is expected. Basically, gate workfunction is a critical design parameter that can effectively modulate the channel charge density. It can be considered a fundamental design parameter that competes with the biomolecule dielectric constant to modify the drain current. The effect of gate workfunction on the sensitivity of the biosensor for S_1 and S_2 measures is illustrated in Fig. 7. The results demonstrate that the sensitivity of the biosensor increases in terms of the S_1 measure upon the increment of the gate workfunction. It is evident that in the off-state mode, the high value of the gate workfunction assists the biomolecules in reducing the off-state current in comparison with the air-filled cavity situation. In contrast, the increase in gate workfunction reduces the biosensor sensitivity in terms of the S_2 measure. Basically, a high value of the gate workfunction reduces the charge density in the channel and diminishes the role of the absorption of biomolecules. It is evident that for efficient performance of the biosensor, the optimum value should be determined for the gate workfunction. It is very important to estimate the susceptibility of the biosensor performance with respect to the variation of critical physical and structural design parameters. By definition, the coefficient of variation (CV) is a statistical parameter that shows a measure of relative variability. It is defined as the ratio of the standard deviation to the mean (average) value in percentiles and shows the relative dispersion of data points in a data series around the average value.

$$\mathrm{CV} = \frac{\sigma}{\mu} \times 100\% \qquad (5)$$

Where σ is the standard deviation and μ is the average value. By definition, the smaller the CV, the higher the consistency of the biosensor sensitivity. To calculate CV, all design parameters are adjusted based on their initial values. Next, one specific design parameter is varied, and the sensitivity of the biosensor for different molecules based on S_1 and S_2 measures is calculated. Following that, the standard deviation and mean value for S_1 and S_2 for each individual molecule are calculated, and their ratios are computed in percentiles.

The results demonstrated in Fig. 8 (a) show that in terms of the S_1 measure, gate workfunction is a fundamental factor that may modify the sensor's responsiveness. It is evident that the workfunction difference between the gate material and the underlying channel modulates the carrier density in the channel. In such a case, the off-state current variation highly depends on the metal gate workfunction rather than the absorbed molecule. That being the case, the optimum value of the gate workfunction plays a fundamental role. Moreover, Schottky barrier height is an important design parameter that effectively modifies the response consistency of the biosensor. In principle, thermionic emission is the main current mechanism for low Schottky barrier heights. In this case, the device's electrical characteristics have an exceedingly weak dependence on molecule absorption, and as a consequence, the responsivity of the sensor degrades. Similarly, high Schottky barrier heights provide a wider tunneling barrier width that cannot be effectively modulated by gate capacitance variation. It concludes that sufficient appropriate values should be considered for the Schottky barrier height to achieve a biosensor with high sensitivity and selectivity. Moreover, as depicted in Fig. 8(b), in terms of S_2 measure, temperature and Schottky barrier height are among the important design parameters that can modulate the drain current from a thermionic emission-dominated regime to a direct barrier tunneling-dominated regime. In addition, the nanogap volume is another fundamental design parameter that can substantially modulate the gate capacitance and the tunneling barrier width.

Table 2. The sensitivity of the biosensor in terms of (a) S_1 and (b) S_2 measures as the charge of the biomolecule is parametrized.

Positively Charged Biomolecule	**S1**			**S2**		
	k=2.1	k=3.57	k=8	k=2.1	k=3.57	k=8
Neutral	1.82	3.80	13.78	2.11	4.09	13.55
$+1\times10^{10}$	1.68	3.51	13.02	2.14	4.13	13.66
$+1\times10^{11}$	0.95	1.83	7.92	2.43	4.55	14.47
Negatively Charged Biomolecule	**S1**			**S2**		
	k=2.1	k=3.57	k=8	k=2.1	k=3.57	k=8
Neutral	1.82	3.80	13.78	2.11	4.09	13.55
-1×10^{10}	1.98	4.10	14.56	2.08	4.05	13.47
-1×10^{11}	4.49	8.54	24.15	1.81	3.65	12.70

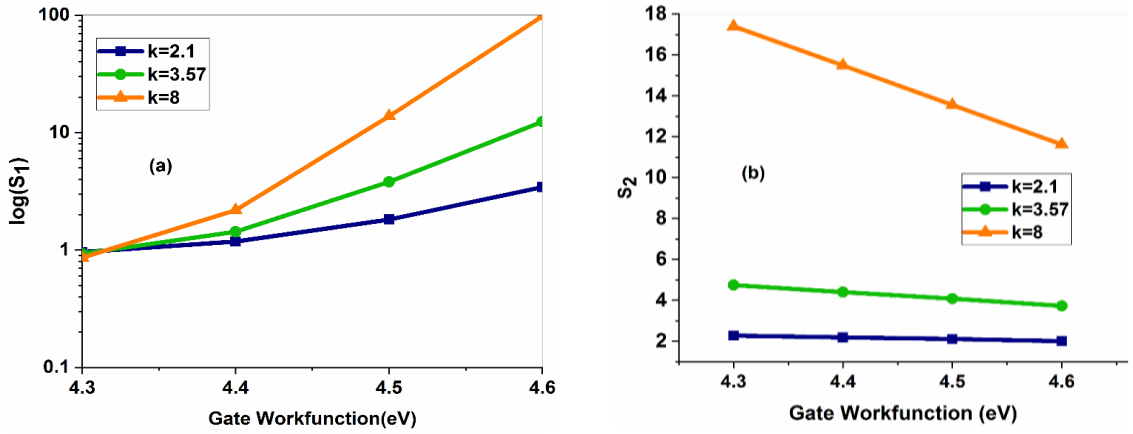

Fig. 7. Biosensor sensitivity in terms of (a) $\log(S_1)$ and (b) S_2 measures versus the gate workfunction.

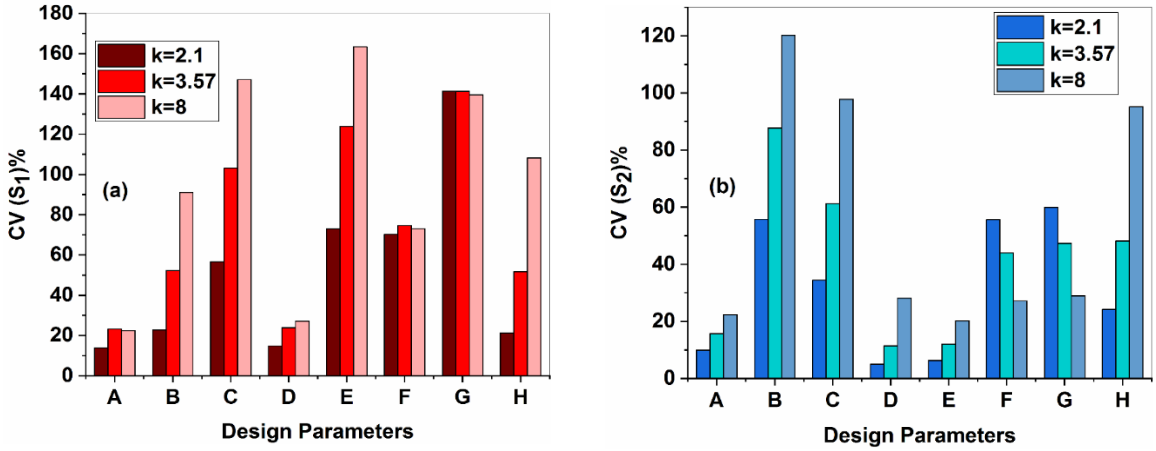

Fig. 8. Coefficient of variation (CV) for (a) S_1 and (b) S_2 measures as a function of different physical and structural design parameters. A: channel doping density; B: Temperature; C: Schottky barrier height; D: Lateral channel thickness; E: Gate workfunction value; F: Molecule with positive electric charge; G: Molecule with negative electric charge; and H: Volume of the nanogap that is filled by the biomolecules.

CONCLUSION

In this paper, the feasibility of a dielectric-modulated Schottky barrier MOSFET as a label-free biosensor is comprehensively investigated. The biosensor's response is measured employing two sensitivity measures: on-state and off-state current variations before and after the absorption of biomolecules. The biosensor performance evaluation is carried out upon variation of critical physical and structural design parameters. The results demonstrate that gate workfunction, channel thickness, and Schottky barrier height can compete with the capacitance of the nano-gap for modulating the channel charge density. Overall, in terms of the S_1 measure, the gate workfunction with a sensitivity value of about 163% is in the top rank, which indicates the importance of this design factor. Moreover, in terms of the S_2 measure, temperature is the most prominent physical parameter, with a sensitivity of nearly 120%. Consequently, these design parameters are found to be fully effective in modifying the sensitivity of the biosensor. That being the case, it is essential to find optimum values for these parameters. The demonstrated results pave the way for the future of integrating biodetection capabilities into existing low-power semiconductor technology.

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