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Proposal for tunnel-field-effect-transistor as ultra-sensitive and label-free biosensors

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Tunnel field-effect-transistor (TFET) based biosensor is proposed, and it is shown that they can surpass by several orders, the performance of those based on conventional FET (CFET) and hence, can potentially revolutionize the biosensing applications. Analytical formula is derived for the sensitivity and response time to provide physical insights in terms of material bandgap and operation regime of the TFET biosensor for achieving optimal results. At the same time, rigorous numerical simulations have been performed in order to obtain accurate values of sensitivity for both biomolecule and pH sensing operations. The time dependent response of the biosensors has also been discussed through analytical and numerical solutions. It is shown that while the CFET biosensors suffer from fundamental limitations on the maximum sensitivity and minimum detection time achievable, TFET biosensors, with their fundamentally different current injection mechanism in the form of band-to-band tunneling, can overcome such limitations and lead to over four orders of magnitude higher sensitivity and over an order of magnitude lower response time. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.3698093]

Biosensors based on field-effect-transistors (FETs)\textsuperscript{1–6} have attracted a lot of attention in recent times, due to their advantages of label-free electrical detection, small size and weight, low-cost mass production, and possibility of on-chip integration of both sensor and measurement systems. The principle behind electrical detection using FET biosensor is based on the \textit{gating effect} of the charged biomolecules on the semiconductor, which can be monitored directly by the change in electrical properties such as current, conductance, etc. For sensing purpose, the dielectric/oxide layer on the semiconductor is functionalized with specific receptors for capturing the desired target biomolecules. Sensitivity is a critical parameter for gauging the performance of the biosensors. Improved sensitivity is desired for detection of biomolecules at low concentration and reduction of detection time. However, the conventional FET (CFET) based biosensors suffer from theoretical limitations on the maximum achievable sensitivity and minimum detection time. We propose and show that the tunnel field-effect-transistors (TFETs)\textsuperscript{7–11} employing a fundamentally different current injection mechanism from the source to the channel in the form of band-to-band tunneling\textsuperscript{12} can overcome these limitations and lead to substantially higher sensitivity while retaining all other advantages of CFET sensors. The schematic diagram of a nanowire based TFET biosensor and its working principle is shown in Fig. 1. Before the attachment of biomolecules to the sensor surface, the tunneling barrier between source and channel is high (Fig. 2(a)), and hence, the current in TFET is low. After biomolecule-receptor conjugation, due to the charges present in the biomolecules (positive charge is assumed here), the bands in the channel bend down, leading to a decrease in the tunneling barrier (Fig. 2(b)) and, hence, increase in the tunneling current. Thus, the biomolecules can be detected by monitoring the change in current through the TFET biosensor device.

In the following discussion, we establish the supremacy of TFET biosensor compared to that based on CFETs. We present extensive numerical simulations based on non-equilibrium Green’s function formalism for accurate results as well as analytical solutions with the aim of providing easy physical insights. The modeling scheme can be divided into two major parts. First part deals with the kinetics of biomolecules within the electrolyte, their capture by the receptors, and thereby the development of surface potential (\(\phi_{\text{bio}}\)) on the oxide in the presence of electrostatic screening by the ions present in the electrolyte.\textsuperscript{5} Second part deals with the

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the electric field decreases. For deriving the length of channel region of TFET, we develop an analytical model for the potential profile in the device and thereby the band-to-band tunneling current \( I_{BTBT} \) in response to a particular oxide surface potential \( \phi \). The modified Poisson equation for 1D nanowires can be written as
\[
\frac{d^2\psi_j(x)}{dx^2} - \frac{\psi_j(x) + \phi}{\lambda^2} = 0,
\]
where \( \psi_j \) is the potential at the semiconductor-oxide interface, \( x \) is the direction along the channel as shown in Fig. 2(b), and \( \lambda \) is defined as the natural length scale.\(^{13} \) The right hand side of the above equation is set to zero since for TFETs the channel is intrinsic or very lightly doped. For the boundary condition at the left side, the potential at the source-channel junction is set to the potential of the source, and hence, \( \psi_j(0) = 0 \). To set this assumption is valid when the depletion region and the potential drop in the source are negligible, which is usually valid due to high doping of the source. Note that \( \psi_j(x) \) is defined as the potential energy profile of the valence band. The potential at channel-drain junction is taken as \( U_d \) so that \( \psi_j(L_{ch}) = U_d \), where \( L_{ch} \) is the length of channel region of TFET. Using the above boundary conditions, \( \psi_j \) can be derived as
\[
\psi_j = \frac{e^x(-U_d - \phi + \phi e^{-\lambda x}) - e^{-x}(-U_d - \phi + \phi e^{\lambda x})}{e^{\lambda x} - e^{-\lambda x}} - \phi.
\]
(1)

For \( L_{ch} \gg \lambda \) and considering only the potential profile near the source-channel junction \( (\psi_{BC}) \), we can simplify the above equation as \( \psi_{BC} = \phi(e^{-x/\lambda} - 1) \). This formula is valid when the effect of drain voltage on the potential profile at source-channel junction is negligible. The electric field/force is given by \( F = \phi e^{-x/\lambda} / \lambda \). For obtaining analytical expression for band-to-band-tunneling (BTBT) probability, the maximum value of electric field \( F_{mid-max} \) in the middle of the bandgap (since the region near the middle of the bandgap has maximum contribution to the tunneling probability\(^{14} \)) is required to be derived. The effective \( F_{mid-max} \) occurs at energy \( E = 0 \) as shown in Fig. 2(b), since above \( E = 0 \), the current is cut off by the bandgap of the semiconductor and as we go below \( E = 0 \) the electric field decreases. For deriving \( F_{mid-max} \) at \( E = 0 \), we first find the value of \( x_{mid} \), which is the point at which the intrinsic potential, i.e., the midgap potential falls to \( E = 0 \). \( x_{mid} \) can be found by solving the equation \( \phi e^{-x_{mid}/\lambda} - \phi + E_G/2 = 0 \). Hence, we derive the \( x_{mid} \) as
\[
-\phi + E_G/2 = 0.
\]
Substituting this value of \( x_{mid} \) in the equation for electric field given, \( F_{mid-max} \) can be derived as
\[
F_{mid-max} = (2\phi - E_G)/(2\lambda),
\]
where \( E_G \) is the bandgap of the semiconductor material in the units of electron volt (eV). Now, using the WKB approximation and the two-band approximation,\(^{12,15} \) the tunneling probability can be written as
\[
T = \exp \left( -\pi \sqrt{qm^* E_G^3 / 2} \lambda / \left( \sqrt{2} h (2\phi - E_G) \right) \right),
\]
(2)
where \( m^* \) is the carrier effective mass, \( q \) is the elementary charge of an electron, and \( h = h/2\pi \), where \( h \) is the Planck’s constant. Next, we derive the energy window \( \Delta E \) through which the effective tunneling occurs. As is clear from Fig. 2(b), \( \Delta E \) is defined from the valence band of the source to the point at which the conduction band in the channel becomes flat. By putting the double derivative of the conduction band potential profile with respect to \( x \) to zero and assuming \( L_{ch} \gg \lambda \), \( \Delta E \) can be derived as \( (\phi - E_G) \). Note that here \( \Delta E \) is derived for relatively small gate voltages such that \( \Delta E < U_d \), in which we are interested (as discussed in the paper). For larger gate voltages, \( \Delta E \) will be given by the difference in energy between the valence band of the source and conduction band of the drain. Finally, using the Landerer’s formula, the tunneling current can be written as
\[
I_{BTBT}(\phi) = 2q^2 \exp \left( -\pi \sqrt{qm^* E_G^3 / 2} \lambda / \left( \sqrt{2} h (2\phi - E_G) \right) \right) / \hbar \times Fnc(\phi - E_G),
\]
(3)
where the function \( Fnc(\phi - E_G) \) is given by
\[
\int_0^{\phi-E_G} \left( f_S(E - E_G) - f_D(E - E_G) \right) dE.
\]
Here, \( f_S, f_D \) are the Fermi functions and \( E_S, E_D \) are the Fermi levels at source and drain, respectively. In the energy window \( \Delta E \), the source has plenty of available electrons, and hence, \( f_S \) can be set to 1, while the drain is devoid of electrons and hence \( f_D \) can be set to 0. Thus, further simplification can be achieved, and \( Fnc(\phi - E_G) \) reduces to \( (\phi - E_G) \).

In this paper, we define the sensitivity of a biosensor as
\[
S_n = (I_{BTBT}(\phi_0 + \phi_{bio}) - I_{BTBT}(\phi_0)) / I_{BTBT}(\phi_0),
\]
where \( \phi_0 \) denotes the initial surface potential on the oxide before the attachment of biomolecules. In the above equation, it is implicit that \( \phi_0 \) is tuned such that the current is dominated by the source-channel BTBT and the energy window \( \Delta E \geq 0 \). The TFETs exhibit ambipolarity, and for \( \Delta E < 0 \), the current is mainly dominated by channel-drain tunneling.
is required to tune \( \phi_0 \) such that the operational mode of the biosensor always remains in the regime where source-channel current dominates. Using (3), the analytical formula for sensitivity can be derived as

\[
S_n = \exp \left( -\frac{\pi \sqrt{2} q m^{*1/2} E_G^{3/2} \lambda \phi_{\text{bio}}}{\hbar (2 \phi_0 - E_G)(2 \phi_0 + 2 \phi_{\text{bio}} - E_G)} \right) \times \left( 1 + \frac{\phi_{\text{bio}}}{\phi_0 - E_G} \right) - 1. \tag{4}
\]

The above analytical formula provides important insights regarding the dependence of sensitivity on the initial surface potential \( \phi_0 \). It can be observed that the sensitivity increases as \( \phi_0 \) is decreased (keeping \( \Delta E \geq 0 \)). This is because, for TFETs, the rate of increase in current with gate voltage is higher for smaller values of \( \phi_0 \) giving rise to increased sensitivity at lower values of \( \phi_0 \). Note that small value of \( \Delta E \) indicates TFET operation in the subthreshold regime. Thus, Eq. (4) indicates that in order to achieve high sensitivity, the TFET biosensor should be operated in the subthreshold regime. Equation (4) also provides direct physical insights regarding the dependence of the sensitivity on the bandgap of the material. As is evident from the equation, sensitivity increases with increase in bandgap. This is because of the decrease in the current before the capture of biomolecules, i.e., \( I_{\text{IBTBT}}(\phi_0) \) with increase in bandgap. For TFETs with relatively large bandgap materials or employing asymmetric design techniques at source and drain to reduce ambipolarity, \( \phi_0 \) may be tuned so that the current is mainly dominated by the relatively smaller reverse biased P-I-N junction current \( (I_{\text{rev}}) \) and the sensitivity will be given by \( S_n = (I_{\text{IBTBT}}(\phi_0 + \phi_{\text{bio}}) - I_{\text{rev}}(\phi_0))/I_{\text{rev}}(\phi_0) \). In this case, the sensitivity will increase with decreasing bandgap at the source-channel junction due to the exponential increase in \( I_{\text{IBTBT}}(\phi_0 + \phi_{\text{bio}}) \).

The subthreshold regime forms the optimal sensing domain not only for TFET biosensors as discussed above but also for the conventional FET biosensors. CFETs suffer from a fundamental limitation on the minimum achievable subthreshold swing (\( SS \)) of \([K_B q \ln(10)]\) due to the Boltzmann tyranny effect, where \( K_B \) is the Boltzmann constant and \( T \) is the temperature. However, the TFETs overcome this limitation due to the Fermi-tail cutting by the bandgap of the semiconductor. The charged biomolecules essentially produce gating effect on the semiconductor channel. Hence, the change in current in TFET biosensors, because of their smaller \( SS \), is substantially higher than that for CFET biosensors in the subthreshold region for the same surface potential developed due to attachment of biomolecules \( (\phi_{\text{bio}}) \) as illustrated in Fig. 3(a).

FIG. 3. (a) Current as a function of surface potential developed due to biomolecule conjugation \( (\phi_{\text{bio}}) \) at a drain voltage \( (V_D) \) of 0.3 V. Due to the smaller subthreshold swing in TFETs, they can lead to higher change in current compared to CFETs for the same change in surface potential. (b) Current as a function of drain voltage before and after biomolecule conjugation for \( \phi_{\text{bio}} = 0.1 \) eV. (c) Sensitivity for sensing of biomolecules as a function of biomolecule concentration. (d) Sensitivity for pH sensing for different pH values. \( \phi_{\text{bio}} \) is tuned for TFET and CFET so that they operate in the subthreshold regime. The bandgap and the effective masses used in the simulations are 0.4 eV and 0.15 eV respectively (where \( m_0 \) denotes the mass of a free electron) and the diameter of nanowire is taken as 5 nm. (e) Sensitivity as a function of subthreshold swing averaged over 4 orders of magnitude of current for both CFET and TFET based biosensors. Surface potential change due to attachment of biomolecules \( (\phi_{\text{bio}}) \) is taken to be 0.1 V. Sensitivity increases substantially with the decrease in subthreshold swing. The shaded region shows the sensitivity values for CFET biosensors, indicating that there is a restriction on the maximum achievable sensitivity since the subthreshold swing in CFETs cannot be minimized below 60 mV/dec at room temperature. All simulations in this figure are performed through self-consistent solutions of Poisson’s and Schrodinger’s equations within the framework of non-equilibrium Green’s function formalism. (f) Surface density of biomolecules \( (N_{\text{bio}}) \) required to be attached to the sensor surface for both CFET and TFET biosensors in order to achieve the same sensitivity value in both, as a function of subthreshold swing. It is observed that \( N_{\text{bio}} \) decreases significantly with decrease in the subthreshold swing. (g) 2D colormap showing the response time (in seconds) of the biosensor as a function of the subthreshold swing and the molar concentration of the biomolecules in the solution.
Fig. 3(b) shows the current as a function of the drain voltage for both CFET and TFET biosensors before and after the biomolecule conjugation. It is observed that for similar currents in both biosensors before biomolecule conjugation, the current in TFET biosensors can be more than 2 orders of magnitude higher than that in CFETs after the attachment of the biomolecules, which obviously indicates significant increase in sensitivity. Comparison of the performance of CFET and TFET biosensors, for biomolecule as well as pH sensing, clearly shows that the sensitivity of TFET biosensors can surpass that of CFET biosensors by several orders of magnitude (Figs. 3(c) and 3(d)). The dependence of \( S_n \) on SS can be derived as

\[
S_n = 10 \left( \int_{0}^{\phi_{bio}} \frac{dx}{\pi x^{2}} \right) - 1, \tag{5}
\]

which depicts the strong relation between the two. Thus, TFETs can harness the benefits of the substantial increase in sensitivity (up to more than four orders of magnitude) with decreasing subthreshold swing and lead to ultra-sensitive biosensors while CFET biosensors are strictly restricted to a higher limit on the maximum achievable sensitivity as highlighted in Fig. 3(e).

In the following discussions, we show that TFET biosensors not only lead to substantial increase in sensitivity, but also provide significant improvement in terms of the response time, which is defined as the time required to obtain a desired sensitivity (more specifically the time needed to capture a certain number of biomolecules in order to achieve a desired change in electrical signal). First, we derive an analytical formula for the surface density of biomolecules \( N_{bio} \) that is required to be captured in order to obtain a particular sensitivity. \( N_{bio} \) can be related to \( \phi_{bio} \) as \( \phi_{bio} = ((1/C_{ox} + 1/C_{NW})^{-1} + 1) \phi_{0} \), where \( C_{ox} \), \( C_{NW} \), and \( C_{DL} \) represent the oxide, the subthreshold swing, as (\( \ln (S + 1) \), where \( S_{avg} \) denotes the average value of subthreshold swing over the range \( \phi_{0} \) to \( \phi_{bio} \). In the subthreshold region \( (1/C_{ox} + 1/C_{NW})^{-1} + C_{DL} \approx C_{DL} \) and hence, \( N_{bio} \) can be written as

\[
N_{bio} = \frac{\pi \varepsilon_{r} R_{NW} K_{1}(R_{NW}/\lambda_{DH}) S_{avg}}{\lambda_{DH} K_{0}(R_{NW}/\lambda_{DH})} \log_{10}(S + 1). \tag{6}
\]

In the above equation, we have used the expression for \( C_{DL} \) as \( \pi \varepsilon_{r} R_{NW} k_{1}(R_{NW}/\lambda_{DH})/K_{0}(R_{NW}/\lambda_{DH}) \). Here, \( \lambda_{DH} \) denotes the Debye–Hückel screening length, \( \varepsilon_{r} \) is the dielectric constant of the electrolyte, \( R_{NW} \) is the radius of the nanowire, and \( K_{0} \) and \( K_{1} \) are the zero- and first-order modified Bessel functions of the second kind. It is clear that \( N_{bio} \) decreases with decreasing values of the swing (Fig. 3(f)). This can be easily explained by the fact that, better the response of the sensor to the gating effect, lower would be the required change in oxide surface potential (\( \phi_{bio} \)) and hence in the required \( N_{bio} \) for achieving the same sensitivity. The response time \( (t_{r}) \) can be related to \( N_{bio} \). Now, using Eq. (6), the dependence of response time to the subthreshold swing is derived as

\[
t_{r} = \frac{\pi \varepsilon_{r} R_{NW} K_{1}(R_{NW}/\lambda_{DH}) \log_{10}(S + 1) S_{avg}}{\lambda_{DH} K_{0}(R_{NW}/\lambda_{DH}) D N_{ave} \rho_{o}}. \tag{7}
\]

where \( \rho_{o} \) is the concentration of biomolecules, \( N_{ave} \) denotes the Avagadro’s number, and \( D \) is the diffusion coefficient of the biomolecules in the solution. Since the CFETs are plagued by the Boltzmann tyranny effect, there exist fundamental limitations to the minimum response time that can be obtained from biosensors based on them. This lower limit in CFETs can be derived using Eq. (7) as

\[
t_{r_{min}} = \frac{\pi \varepsilon_{r} R_{NW}^{2} K_{1}(R_{NW}/\lambda_{DH}) \ln(S + 1) K_{0} T}{\lambda_{DH} K_{0}(R_{NW}/\lambda_{DH}) D N_{ave} \rho_{o}}. \tag{8}
\]

In Fig. 3(g), the response time is plotted as a function of both the subthreshold swing and the biomolecule concentration in the electrolyte. Since TFET biosensors are not bound by a lower limit on the subthreshold swing, they can be highly advantageous for reduction of response time (up to more than an order of magnitude) and detection of biomolecules at low concentrations.

It is to be noted that in this Letter we have presented the results for n-TFET assuming a positive charge of the biomolecules, which obviously indicates significant increase in the sensitivity but can also lead to significant reduction in response time, thereby facilitating detection at low biomolecule concentration, that is critical for preventing biological accidents or attacks. Thus, we believe that the proposed ultra-sensitive TFET biosensors could pave the way for a paradigm shift in biosensing applications.

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