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Material Selection for Minimizing Direct Tunneling in Nanowire Transistors

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Material Selection for Minimizing Direct Tunneling in Nanowire Transistors

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Abstract—When the physical gate length is reduced to 5 nm, direct channel tunneling dominates the leakage current for both field effect transistors (FETs) and tunnel field effect transistors (TFETs). Therefore, a survey of materials in a nanowire (NW) geometry is performed to determine their ability to suppress the direct tunnel current through a 5 nm barrier. The materials investigated are InAs, InSb, InP, GaAs, GaN, Si, Ge and carbon nanotubes (CNTs). The tunneling effective mass gives the best indication of the relative size of the tunnel currents when comparing different materials of any type. The indirect gap materials, Si and Ge, give the largest tunneling masses in the conduction band, and they give the smallest conduction band tunnel currents within the range of diameters considered. Si gives the lowest overall tunnel current for both the conduction and valence band and, therefore, it is the optimum choice for suppressing tunnel current at the 5 nm scale. A semi-analytic approach to calculating tunnel current is demonstrated which requires considerably less computation than a full-band numerical calculation.

Index Terms—nanowire, FET, tunneling, leakage, Si, Ge, InAs, InSb, InP, GaAs, GaN, CNT

I. INTRODUCTION

Many different materials are being considered for field effect transistor (FET) applications. Examples include Si, Ge, III-Vs, carbon nanotubes (CNTs), and graphene [1]–[6]. For both standard FETs [7] and tunnel FETs (TFETs) [8], [9], direct tunneling through the channel limits the off-current as the channel lengths drop below 10 nm. Therefore, it is timely to assess and compare the ability of different channel materials to block the direct tunnel current at the sub 10 nm scale.

At this length scale, extremely tight gate control over the channel potential is required. Nanowires offer the tightest gate control of the channel not only because of the proximity of the gate to the channel, but also because nanowires allow access to the quantum capacitance limit [10]. Recently, promising results have been experimentally demonstrated for scalable nanowire FETs in developing complex nanoprocessors [11]. Therefore, the nanowire geometry is considered for a variety of materials and diameters for both n-type (NMOS) and p-type (PMOS) channels. The materials investigated are InAs, InSb, InP, GaAs, GaN, Si, Ge and CNTs. The primary purpose of this work is to survey a broad range of materials and diameters and compare their ability to block the tunnel current both in the conduction and valence bands. A secondary objective is to demonstrate a semi-analytical approach to calculating the tunnel current which requires considerably less computation than a full-band numerical calculation.

Previous studies have focused on issues of electrostatics and gate control of the channel which are clearly critical issues. These studies also focused on planar structures, and they used either effective mass models [7], [12], [13] or full-band models [14]. The most recent study compared 5 nm gate, n-type FETs of different geometries and materials including Si, carbon nanotubes (CNTs), graphene nanoribbons, and In0.75Ga0.25As, using atomistic, full-band models [15]. It was found that all materials could provide good transistor performance provided that two conditions were met. The first condition is that their bandgaps must be sufficiently large to block the interband tunneling current. The second condition is that, for materials with smaller effective masses, the gate must modulate the potential of the source and drain extensions increasing the effective gate length. As acknowledged in [15], the second condition is identical to using source and drain underlaps to effectively increase the channel region. It has been shown that long source and drain underlaps can block both the direct tunneling current and the interband tunneling current of a CNTFET, so that even with a 2 nm metal gate, good on-off current ratios can be achieved [16]. However, this is not the device geometry of interest now. In this paper, we answer the question, ‘How well do different materials block the direct tunneling current in both n-type and p-type nanowire FETs or CNTFETs with actual 5 nm channels?’

II. COMPUTATIONAL APPROACH

To focus on the single issue of channel tunneling and to make a clearly-defined, even comparison across a wide range of materials, a uniform, square, 5 nm long tunnel-barrier is considered. The actual potential barrier in appropriately designed structures can closely approximate this shape [15]. As will be shown in Sec. III, the currents for different materials differ by up to 6 orders of magnitude. While a potential discontinuity reduces transmission, the reduction is of order unity. Therefore, the abruptness of the barrier does not affect the material comparisons or final conclusions.
The III-V materials are simulated for 3, 6 and 10 nm diameters, and their Hamiltonian matrix elements are calculated using the discretized three dimensional 8-band \( \text{k} \cdot \text{p} \) model as described in Ref. [17], [18]. All the compound semiconductors are considered zinc blende and their material parameters are taken from Ref. [19]. The \((100)\) Si and Ge nanowires are simulated atomistically using a \(sp^3 s^* d^x\) tight-binding model as implemented in the newly developed code NEMOS [20]. Due to the heavier computational burden involved with such simulations, the H-passivated Si and Ge nanowires are simulated only for 3, 4, 5 and 6 nm diameters. Hamiltonians for \((7,0), (10,0)\) and \((25,0)\) zigzag CNTs are calculated using an empirical \(\pi\)-bond model [21].

The tunnel barrier and source Fermi level for an n-type channel are shown in Fig. 1. The barrier and Fermi level for p-type channels are the same with the sign of all energies reversed. The total barrier height is 0.4 eV, and the height above the source Fermi level is 0.3 eV. The Fermi level in the source side is set to 0.1 eV above the conduction band edge for NMOS and 0.1 eV below the valance band edge for PMOS. In the off-state of a digital FET, the drain bias is the supply voltage, \(V_{DD}\), so injection from the drain can be ignored. Therefore, the drain Fermi function is set to 0 for the n-FETs and 1 for the p-FETs.

Intraband tunnel current through the potential barrier is calculated coherently using the non-equilibrium Green’s function (NEGF) formalism implemented in a recursive Green function algorithm [22]. The temperature is \(T = 300\) K. Full-band, self-consistent calculations including phonon scattering have been performed for Si NW FETs with channel lengths of 15 nm. In the off-state, the current calculated coherently exceeded the current calculated with phonon scattering by a ratio of 1.35 for a 3 nm diameter wire, and the trend indicated that the ratio decreased towards unity as the diameter increased [23]. For 5 nm channels, the coherent tunneling process will be exponentially enhanced and thus be the dominant tunneling mechanism pushing the ratio very close to unity justifying a coherent tunneling calculation.

For wider diameter nanowires, full-band calculations of the current can be quite numerically demanding. Therefore, we assess two semi-analytical approaches to calculating the intraband tunnel current in nanowires. The first method uses the standard analytical expression of transmission through a finite potential barrier [24],

\[
T_{SB}(E) = \frac{4k^2\kappa^2}{4k^2\kappa^2 + (k^2 + \kappa^2)^2 \sinh^2 \kappa d}, \tag{1}
\]

where \(d\) is the barrier width, and \(k\) and \(\kappa\) are the magnitudes of the real and imaginary wavevectors, outside and inside of the barrier, respectively, at energy \(E\). The wavevectors are calculated numerically from the full-band models.

The imaginary wavevectors \(\kappa\) in the bandgap are the decay constants that have an exponential effect on the tunnel current, and, thus, they govern its order-of-magnitude [25]. The imaginary wavevectors are calculated following Ref. [26] for the Si and Ge nanowires and Ref. [27] for the rest of the materials. For direct gap materials, like the III-Vs and CNTs, one single imaginary band connecting the bottom of conduction band and top of valance band can be found as shown by the red solid line in Fig. 2(a) for InAs.

Si and Ge have an indirect gap bulk bandstructure that results in a considerably more complex bandstructure in the bandgap. In Fig. 2(b), the bandstructure for the 6 nm Si nanowire is plotted. Although the bandgap of the Si in nanowire form becomes direct [28] there is no single imaginary band that connects the band edges. Therefore, the minimal values for \(\kappa\), as shown by the red solid line in Fig. 2(b), which give the least action for tunneling, are used for evaluating Eq. (1). Since the tunneling barrier height is 0.4 eV, only the upper imaginary branch contributes to the electron tunneling, and only the lower imaginary branch contributes to the hole tunneling. Thus, in contrast to interband tunneling (tunneling from the conduction to the valence band or vice versa), phonon assistance is not required.

The bandstructure for the 6 nm Ge nanowire is shown in Fig 2(c). The conduction band edge is at \(X\) in the one-dimensional
Brillouin zone. This connects to the minimal imaginary band at the top of the bandgap. The values for $k$ and $\kappa$ used to evaluate Eq. (1) are the ones indicated in red (solid lines). As with Si, the minimal values for $\kappa$ are used. However, in contrast to Si, the imaginary band connecting to the conduction band minimum crosses the imaginary band connecting the direct bandgap at $\Gamma$ a few hundred meV below the bandedge. To move from one branch to another requires phonon assistance. Nevertheless, the coherent tunneling expression (1) for electron tunneling will be shown to give good agreement with the numerical calculations. For hole tunneling, the real $k$ is taken from the light hole valence band since it connects to the direct-gap imaginary band at $\Gamma$. Having chosen the real and complex bands for tunneling, $k$ and $\kappa$ are calculated at each energy and used in Eq. (1) for transmission.

The second semi-analytic method uses the WKB expression for tunneling in which the energy dependent transmission coefficient $T_{WKB}(E)$ is

$$T_{WKB}(E) = \exp\{-2\kappa d\}. \quad (2)$$

In this approach, the transmission is calculated only from the complex bandstructure in the bandgap. Even though this method has been successfully used previously to calculate the interband tunneling current [30, 33, 34], we find that Eq. (1) provides better agreement with the numerical calculation of the intraband tunneling current. The same imaginary bands as described earlier and shown in Fig. 2 are used to evaluate Eq. (2).

The tunneling current, $I_D$, is calculated from

$$I_D = M \frac{S q}{\hbar} \int_{E_c}^{E_c+0.4} dE T(E) f(E-E_{FS}) \quad (3)$$

for n-type channels or from

$$I_D = M \frac{S q}{\hbar} \int_{E_v}^{E_v-0.4} dE T(E) \left[1 - f(E-E_{FS})\right] \quad (4)$$

for p-type channels where $S$ is 1 or 2 depending on whether or not spin is explicitly included in the Hamiltonian. $M$ is the number of propagating modes, and it is automatically included in the Hamiltonian in the numerical (NEGF) calculations. For the analytical calculations, its value is set to 4 for the Si and the Ge conduction bands and to 1 for all other cases. $E_c$ is the conduction band edge, $E_v$ is the valence band edge. The transmission $T(E)$ is calculated either from Eqs. (1) or (2) or numerically from NEGF.

To focus solely on the tunnel current, all currents are calculated by integrating the transmission coefficient over the energy range from the band edge of the source to the top of the barrier as given in Eqs. 3 and 4. This is sufficient to capture 84% of the total current for GaN and 99.8% for the other materials except for Si and Ge. These two materials block the tunneling current so effectively that a significant fraction (as high as 72%) of the total current can flow above the barrier.

### III. RESULTS

The NEGF calculated currents versus diameter for the different materials are shown in Fig. 3(a) and (b) for electrons and holes, respectively. As might be expected, the off current is slightly lower for PMOS than for NMOS for most of the materials since holes tend to have heavier effective masses. For the Ge nanowires, the currents are slightly larger for the PMOS devices because Ge has a small light-hole effective mass. Si has the lowest tunnel-currents for both NMOS and PMOS except for the smallest diameter NMOS where Ge has slightly lower current. Electron and hole currents are same for the CNTs because their Hamiltonians are calculated from a $\pi$-bond model that produces symmetric bandstructure with respect to the middle of the bandgap. Also, it is worth mentioning that, for the largest diameter CNT, the bandgap ($E_g = 0.397$ eV) is smaller than the 0.4 eV barrier height assumed here. This would mean a large current due to band-to-band tunneling through the valance band in the channel. For the range of diameters considered, all of the other materials have bandgaps that are greater than the barrier height.

Insight can be obtained from the tunneling effective masses, $m^*$, and the bandgaps plotted in Figs. 4 and 5. The tunneling masses are calculated from

$$m^* = \frac{\hbar^2}{2(E_c - E_v)(E - E_v)} \quad (5)$$

following Kane’s two-band model [35], where $E_g$ and $\hbar$ are the bandgap and the reduced Planck’s constant, respectively. Energy, $E$, is taken to be at the source Fermi energy. Note that as $E$ approaches a band-edge, such as, for example, $E_c$, $E_v$ in the numerator cancels $E_v$ in the denominator, and Eq. 5 reduces to the usual expression for parabolic dispersion, $E_c - E = \frac{\hbar^2 k^2}{2m^*}$, as it should. As shown in Fig. 6, the single value of $m^*$ combined with Eq. (5) provides a good fit to the $E - k$ relations within the energy ranges of interest.

Comparing the tunneling masses in Fig. 4 with the tunneling currents in Fig. 3, it is clear that the order of the magnitudes of the tunneling currents correlate closely with the order of the magnitudes of the inverse of the tunneling masses in Fig.
4. In other words, the larger the tunneling mass, the smaller the tunneling current. The CNTs provide the one discrepancy in which the tunneling mass of the smallest CNT is heavier than the tunneling hole mass of GaAs and InP; however, the tunnel current is slightly larger.

Comparing the bandgaps of the direct gap semiconductors shown in Fig. 5, the order of the bandgaps correlate closely with the order of the tunneling masses (there is a small reversal for GaAs and InP). Thus, the bandgaps give a good indication of the ordering of the tunnel currents, i.e. the larger the bandgap, the smaller the intraband tunnel current. However, this trend cannot be used to compare the direct bandgap semiconductors with CNTs. For example, even though the bandgaps of InP and GaAs are greater than the smallest CNTs, the tunneling masses are less. Most notably, the indirect gap materials, Si and Ge, stand out amongst themselves. When comparing them with the other direct-gap materials, only the tunneling masses matter. Once the indirect gap materials are included, the bandgaps can no longer be used to predict which material gives the smallest intraband tunnel current. Finally, for all but the smallest diameters, Si has the heaviest tunneling mass and the lowest tunnel current both for electrons and holes.

The energy distribution of the electron and hole currents are shown in Fig. 7. The energy distribution of the smallest (GaN) and largest (InSb) direct gap currents are shown along with the indirect gap (Si and Ge) currents. In the tunneling region, \( |E| < 0.4 \text{ eV} \), the conduction-band tunnel currents of Si and Ge are an order of magnitude smaller than the closest direct gap material, GaN. Immediately above the barrier, there is a resonance effect present in Si and Ge that is significantly stronger than that observed in any of the other direct gap materials. This could be related to the fact that the degeneracy of the conduction band edge in both Si and Ge \( \langle 100 \rangle \) nanowires is 4, i.e. there are 4 propagating modes at the conduction band edges [29], [36]. In contrast, the conduction band of the direct-gap materials consists of one propagating mode. At higher energies, the Si and Ge current distributions converge to those of GaN. For those three materials, many modes contribute to the current at the energies above the barrier. This is in contrast to InSb which is still single moded at those energies, and this accounts for the difference in the magnitude of the curves above the barrier. The valence band shows similar trends. The tunnel current of Si is smallest everywhere while Ge and GaN are comparable.

A comparison of the tunneling currents calculated from the semi-analytical transmission coefficients, Eqs. (1) and (2), and the NEGF calculation are shown in Figs. 8 and 9. The current calculated from the exact analytical expression, Eq. (1), gives good agreement with the full numerical calculation with the largest error being a factor of 4.8 for the Si valence band. Also, the error is usually large for the narrower gap materials, and this is not unexpected. For bandgaps less than 0.8 eV, electrons from the source are tunneling through the barrier below midgap. Thus, the intraband tunneling becomes a virtual interband tunneling process which is outside of the validity of Eq. (1). In our case, the 6 and 10 nm InAs and InSb nanowires have bandgaps less than 0.8 eV, and these are the two other cases which also do not give good agreement between the numerical calculations and Eq. (1).

The agreement with the WKB expression, Eq. (2), is generally worse for all of the semiconductors except InSb. It does, however, capture the correct order-of-magnitude, and this is to be expected, since the order-of-magnitude is determined by the imaginary wavevector in the bandgap and the exponential decay factor [37].

The good agreement between the full numerical calculation
Fig. 7. (a) Electron and (b) hole current density versus energy where 0 eV indicates the band edge and 0.4 eV is the top of the barrier for electrons and -0.4 eV is the top of the barrier for holes. All the NWs have the same diameter of 3 nm.

Fig. 8. Electron current calculated analytically and numerically. Transmission calculated from Eq. (1) is plotted with the dashed line and transmission calculated from Eq. (2) is plotted with the dotted line. Solid lines are from NEGF calculations.

Fig. 9. Hole current calculated analytically and numerically. Transmission calculated from Eq. (1) is plotted with the dashed line and transmission calculated from Eq. (2) is plotted with the dotted line. Solid lines are from NEGF calculations.

and the semi-analytic calculation of the transmission coefficient given by Eq. (1) indicates that Eq. (1) can be used to calculate the tunnel current in larger diameter structures which are difficult to simulate fully numerically. Since we have demonstrated that Eq. (1) is valid for a single square barrier, it can also be used to obtain the transmission through a spatially varying barrier. Spatially varying barriers can be approximated as a series of thin square barriers, and the transmission for each thin square barrier can be cascaded to obtain the total transmission [24].

While this discussion has focused on intraband tunneling through the channel of a standard FET in the off-state, the results are also relevant to the off-state leakage current in sub-10 nm channel TFETs. In standard FETs, the source-to-drain tunneling is an intraband tunneling process. For a TFET in the off-state with a p-type source, an electron in the source valence band undergoes interband tunneling through the source-to-channel, high-field region into an evanescent conduction band state a few hundred meV below the conduction band edge of the channel. At this energy, it can tunnel through a low-field, 10 nm channel into the drain. The process of tunneling through the low-field channel region is determined by the evanescent wavevector \( \kappa \) in the channel, and this \( \kappa \) is identical to the \( \kappa \) governing the source-to-drain tunneling process in a standard FET. The injection mechanisms are different, but the tunneling transport through the channel region is the same governed by the same evanescent wavevector \( \kappa \). Thus, the current and effective mass comparisons shown in Figs. 3 and 4 also indicate the effectiveness of different materials in blocking the off-state leakage current in sub 10 nm channel TFETs.

IV. CONCLUSION

For a 5 nm physical gate length, direct channel tunneling dominates the leakage current for both FETs and TFETs. Therefore, we have performed a survey of materials to determine their ability to suppress the direct tunnel current through a 5 nm barrier. The tunneling effective mass gives the best indication of the relative size of the tunnel currents when comparing two different materials of any type. For direct gap III-V materials, the bandgaps are correlated with the tunneling masses, so the relative size of the bandgaps can also be used to determine the relative size of the tunnel currents. However, this only holds within the direct-gap, III-V subset of materials. The indirect gap materials, Si and Ge, give the largest tunneling masses in the conduction band, and they give the smallest conduction band tunnel currents within the range of diameters considered. Si gives the lowest overall tunnel current for both the conduction and valence band and, therefore, is the optimum choice for suppressing tunnel current at the 5 nm
scale. The semi-analytic expression for the tunnel current given by Eq. (1) gives good agreement with the numerical result. Therefore, this expression can be used to calculate the tunnel current in wider diameter NWs which, using a full band model, are intractable or very difficult to simulate fully numerically. The transmission coefficients can also be cascaded to simulate spatially varying barriers.

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