Performance of Topological Insulator Interconnects

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Abstract—The poor performance of copper interconnects at the nanometer scale calls for new material solutions for continued scaling of integrated circuits. We propose the use of three dimensional time-reversal-invariant topological insulators (TIs), which host backscattering-protected surface states, for this purpose. Using semiclassical methods, we demonstrate that nanoscale TI interconnects have a resistance 1-3 orders of magnitude lower than copper interconnects and graphene nanoribbons at the nanometer scale. We use the nonequilibrium Green function (NEGF) formalism to measure the change in conductance of nanoscale TI and metal interconnects caused by the presence of impurity disorder. We show that metal interconnects suffer a resistance increase, relative to the clean limit, in excess of 500% due to disorder while the TI’s surface states increase less than 35% in the same regime.

Index Terms—Topological Insulators, Interconnects, Non-Equilibrium Green Functions (NEGF)

I. INTRODUCTION

Electronic packaging is constantly evolving in order to achieve the lower power consumption and reduced circuit delays demanded by the scaling of microelectronic circuits. Copper is an effective solution for technology nodes in the near future, but finite-size effects in metals increase copper interconnect resistivity dramatically as dimensions decrease to the nanoscale [1]. By 2025, Metal 1 pitch is predicted to reach tens of nanometers [2], where increased line edge roughness and grain boundary scattering in copper raise resistivity, and thus dissipation and signal delay, to unacceptable values [3], [4]. A materials change will hence be necessary to avoid the "interconnect bottleneck" [5], [6], whereby the poor performance of nanoscale interconnects inhibits further scaling.

Zigzag graphene nanoribbons (GNRs) have been proposed as next generation interconnect materials because of their high electron mobility [7]. Unfortunately, reliable fabrication of GNRs is difficult due to defects in growth and line edge roughness, both of which increase scattering and degrade electron mobility [8], [9]. In addition, finite-width GNRs develop a band gap [10]–[12], further reducing their conductance.

We propose the use of time-reversal-invariant topological insulators (TIs) for use in nanoscale interconnects. Topological insulators are a recently discovered class of materials that are gapped in their bulk spectrum but have surfaces that host massless, metallic Dirac fermions [12]. Time-reversal symmetry protects TI surface states from backscattering caused by charged disorder and edges, resulting in high conductance even in the presence of these scattering mechanisms. Therefore, TI interconnects will not suffer as much as copper interconnects and GNRs from scaling-induced resistance increases.

In this letter, we investigate the transport properties of metals, GNRs, and TIs to benchmark these materials for future nanoscale interconnects. We theoretically demonstrate that below 6 nm, TI interconnect resistance is multiple orders of magnitude lower than the resistances of copper interconnects and GNRs due to the TI’s backscattering protection. Using the non-equilibrium Green function (NEGF) formalism, we show that metal interconnects greatly increase in resistance with scaling-induced disorder, while transport through TI interconnects is comparatively insensitive. Having shown that TI interconnects continue to conduct well at the nanoscale while GNRs and copper do not, we conclude that TIs are excellent candidates for a future interconnect material.

II. SEMICLASSICAL TRANSPORT

Although the widths of interconnects are decreasing, their lengths are often longer than the mean free path (MFP) of electrons and, as such, semiclassical calculations provide a useful picture of longitudinal transport [13]. We use Matthiessen’s rule to calculate the conductance of the TI Bi$_2$Se$_3$ and GNRs, assuming that all scattering mechanisms are independent of each other [14]. We consider Bi$_2$Se$_3$ because it is the most practical candidate for engineering purposes due to its bulk band gap of 0.3 eV [12]. Under Matthiessen’s rule, the conductance is given by

$$G = G_0 \sum_n \frac{1}{1 + L \left( \Lambda^{-1} + \ell_n^{-1} \right)}.$$

where $G_0$ is the conductance quantum, $L$ is the length of the wire, and $\Lambda$ is the experimentally measured, room temperature MFP. In this work, we use an MFP of 1 µm for GNRs [7] and two MFPs of 10 nm and 100 nm for Bi$_2$Se$_3$ [15], [16]. The edge scattering length $\ell_n$ in [1] is the distance that the $n$th transverse mode travels before scattering off an edge and is calculated from a modified form of the equation in [17]:

$$\ell_n = \frac{W}{W} \left[ \frac{E_F^2 - E_g(W)^2}{(2\pi \hbar v_F n/2W)^2} \right] - 1.$$

Here, $W$ is the width of the wire, $E_F$ is the Fermi energy, $E_g(W)$ is the width-dependent band gap of the material, $\hbar$ is the reduced Planck constant, and $v_F$ is the Fermi velocity. The modification in [17] accounts for the band gap observed in both narrow GNRs and the surface states of thin Bi$_2$Se$_3$ [9]. [17]. We use experimentally observed Fermi levels of 0.26 eV and 0.21 eV for Bi$_2$Se$_3$ and GNR, respectively [12], [18]. Because the topological surface states of Bi$_2$Se$_3$ are insensitive...
the GNR, regardless of the MFP. Copper’s resistance rapidly grows due to the increased grain boundary and surface scattering, while GNRs suffer from high resistance due to the increasing band gap in small-width ribbons.

to scattering off crystalline edges [19], [20], we exclude the $\ell_n$ term from its calculation. Additionally, the one-dimensional $n = 0$ edge mode in GNRs is susceptible to weak localization making it nonconducting [21], thus we begin the sum in (1) at $n = 1$ for GNRs. We model the resistance of copper using a combined Fuchs-Sondheimer [22] and Mayadas-Shatzkes [23] model for wires of aspect ratio 2 [2] to accurately capture both sidewall reflections and grain boundary scattering [19], resulting in values that agree well with experiments [24]. The integration of copper into CMOS manufacturing requires a diffusion barrier of a minimum width of 2 nm [3]. In order to account for the liner in copper interconnects, we also calculate resistance where the line width includes the added total liner width of 4 nm. Since the diffusion coefficients for bismuth and selenium are orders of magnitude smaller than that of copper, it does not require a diffusion barrier for Bi$_2$Se$_3$ [25]–[27].

Fig. 1 illustrates that the lower resistance of pure copper makes it the optimal material for interconnects, but accounting for the required 2 nm diffusion liner shows it to be highly resistive below a physical interconnect width of 6 nm. Above 6 nm, surface scattering is insignificant, resulting in copper’s high conductance. Despite having high mobilities, both GNRs and Bi$_2$Se$_3$ are far more resistive than copper at this scale because their conductances are limited by their two-dimensional density of states. The especially poor performance of GNRs below 40 nm is caused by the lack of an $n = 0$ mode, which, combined with their band gap, significantly reduces the number of conduction channels and dramatically increases their resistance. Below 6 nm, the resistance of copper increases rapidly, attributable to increased surface scattering [24]. We see that Bi$_2$Se$_3$ with either MFP clearly outperforms copper and GNRs at this scale because it does not require a diffusion liner and has no edge scattering.

### III. Influence of Disorder

While Matthiessen’s rule is useful for longer wires, we require a quantum description for interconnect lengths below the MFP, where impurity-induced weak localization has a strong deleterious effect on conductance [28]. We employ the NEGF formalism to understand the transport properties of materials below the MFP in the presence of disorder-induced, phase-coherent scattering. Using NEGF, we calculate the percent increase in resistance, relative to the clean limit, of both TI and metal interconnects as a function of impurity disorder strength. Although copper nanowires have been shown to have highly anisotropic conductance [29], [30], the resistance change due to uniform disorder is independent of direction [31], and thus we do not consider anisotropy here. We use TI and metal models that accurately display the qualitative transport characteristics of Bi$_2$Se$_3$ and copper but do not consider GNRs because of their previously demonstrated insulating behavior at the nanoscale.

We use a Hamiltonian that accurately models the low energy behavior of TIs on a cubic lattice, defined by [32]–[34]

$$
H_{\text{TI}} = \sum_{r,\delta} \psi_r^\dagger (H_m + d_\delta I_4) \psi_r + (\psi_r^\dagger H_3 \psi_{r+\delta} + \text{H.c.}),
$$

(3)

The annihilation operator $\psi_r$ is a spinor with two orbital and two spin degrees of freedom. The vectors $\delta = (\pm a \hat{x}, \pm a \hat{y}, \pm a \hat{z})$ are the distances between nearest neighbor atoms on the lattice, spaced by the lattice constant $a = 3\,\text{Å}$. The matrices $\Gamma_i (i \in \{0, x, y, z\})$ are the Dirac gamma matrices, $\Gamma = (\Gamma^x \hat{x}, \Gamma^y \hat{y}, \Gamma^z \hat{z})$, $I_4$ is the $4 \times 4$ identity matrix, and $M = m - 3b/a^2$. In this work, we set $m = 1.5\,\text{eV}$, $b = 9\,\text{eV}\,\text{Å}^2$, and $\gamma = 3\,\text{eV}\,\text{Å}$ to put the insulator in the strong topological phase with a bulk band gap of 1eV. This large band gap results in highly localized surface states that do not hybridize, allowing the simulation of smaller structures while maintaining the qualitative behavior of larger devices. In (3), $d_\delta$ is the disorder potential, which is randomly distributed in the range $-D/2 \leq d_\delta \leq D/2$, representing impurities introduced during growth and fabrication [35]. Conductance calculations are averaged over ten trials for each disorder strength $D$, where each trial has a different random disorder potential configuration. The disorder range studied, $0\,\text{eV} \leq D \leq 5\,\text{eV}$, corresponds to a surface state MFP down to 0.32 nm, using the relation $\Lambda = 12h^3 / (\alpha D^2 E_F^c) [36]$, covering the range of experimentally measured MFPs in TIs [15], [16]. The metal is modeled by a 3D tight-binding Hamiltonian with nearest-neighbor hopping $t_0 = 1.5\,\text{eV}$ [37], such that the metal has the same bandwidth as the TI. The chemical potential is set to 0.8 eV, although qualitative trends are independent of specific value. Random impurity disorder is added to the metal in the same fashion as for the TI. Grain boundary scattering is not relevant here as the device dimensions are smaller than typical grain sizes. Both materials are modeled using a wire with dimensions $(10a \hat{x}, 5a \hat{y}, 5a \hat{z})$, where transport is simulated along $\hat{x}$ with a bias of 1 mV and temperature at 300 K.

Fig. 2 shows the percent increase in resistance, relative to the clean limit, of each interconnect versus disorder strength.

| Width (nm) | Resistance (Ω/µm) |
|-----------|--------------------|
| Cu        | Cu + Liner         |
| GNR       | Bi$_2$Se$_3$ (10 nm) |
| Bi$_2$Se$_3$ (100 nm) |
For the metal interconnect, on-site impurity disorder increases elastic scattering, resulting in more than a 450% increase in resistance above 2 eV of disorder. We plot the resistance of the TI at three different chemical potentials ($\mu_1$, $\mu_2$ and $\mu_3$), illustrated by the inset of Fig. 2. For conduction through the Dirac point at $\mu_1$, the presence of disorder decreases resistance by 76% at $D = 5$ eV. Disorder-induced mid-gap states increase the number of conduction channels, as is evident in Figure 3, resulting in the TI transitioning into a diffusive metal phase. Transport at $\mu_2$, crossing solely through the TI surface states, results in a slight decrease in resistance as transport occurs at higher energies than most of the disorder-induced mid-gap states. The small change in resistance for the TI at $\mu_1$ and $\mu_2$ compared to the dramatic rise for the metal demonstrates the benefit of the topological protection of the TI surface states. Chemical potential $\mu_3$ crosses both the surface states and the bulk bands, which results in the resistance increasing by 30% at $D = 5$ eV due to the localization of the unproctected bulk electrons. Continued conduction through the surface states, however, limits the resistance increase in the TI. Because the Fermi level of as-grown Bi$_2$Se$_3$ crosses both the bulk and surface bands, our calculations at $\mu_3$ are of particular interest as they indicate that Bi$_2$Se$_3$ can benefit from both bulk conductance and surface backscattering protection.

### IV. ADDITIONAL CONSIDERATIONS

Recent theoretical work suggests that inelastic scattering by acoustic phonons greatly reduces the mobility of TIs [41]. Although this is true for long lengths, TI interconnects with lengths less than or equal to the MFP may not suffer such a large degradation. To investigate inelastic scattering, we add a phenomenological on-site self-energy to the TI Hamiltonian. The scattering self-energy $\Sigma_S = -i\hbar/2\tau$ [37] is characterized by the mean free time $\tau = \Lambda/v_F$. Here, the MFP $\Lambda$ is 23.8 nm [16] and the Fermi velocity $v_F$ is $5 \times 10^5$ m/s [32], resulting in $\tau = 47.6$ fs and a scattering self-energy $\text{Im}\{\Sigma_S\} = -0.014$ eV. Simulated transport shows only a 20% resistance increase over that without inelastic scattering, a much smaller reduction than was reported in [41]. As such, we see that inelastic phonon scattering is not a significant source of performance degradation in nanoscale TI interconnects.

Another concern in the use of TI interconnects is that they would be in the presence of time-reversal-breaking electromagnetic fields from nearby lines, which could destroy their topological protection. We estimate the influence of this crosstalk by using Ampere’s law for a wire carrying a current of 1 mA at an interconnect pitch of 5 nm resulting in a magnetic field strength $|B| = 40 \text{ mT}$. Such a field creates a Zeeman energy gap $E_Z = g\mu_B|B|$, where $g \approx 32$ is the g-factor for Bi$_2$Se$_3$ [42] and $\mu_B = 57.9 \mu\text{eV-T}$ is the Bohr magneton. Using this relation, we obtain a Zeeman energy splitting of 74.1 $\mu$eV. Therefore, even in the presence of many other lines, this gap will be smaller than 1 meV, resulting in an immeasurable impact on the TI’s topological properties.

### V. CONCLUSION

We have performed a numerical study to explore the use of TIs as future interconnects. Using semiclassical techniques, we find that copper is much less resistive than the Bi$_2$Se$_3$ or GNRs above line widths of 6 nm. Below this width, however, the increased surface scattering in copper and the observed band gap in GNRs cause both to rapidly rise in resistance above Bi$_2$Se$_3$, making the TI the best candidate in this regime. Using NEGF, we also observe that disorder causes the metal’s resistance to increase by orders of magnitude but has no negative impact on the TI’s backscattering-protected surface states. Because TIs maintain their conductive properties under the effects of scaling microelectronics, they are excellent candidates for next-generation interconnect materials.

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