Modification and Control of Topological Insulator Surface States Using Surface Disorder

Vincent Sacksteder
Nanyang Technological University, Singapore

Tomi Ohtsuki and Koji Kobayashi
Sophia University, Tokyo
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We numerically demonstrate a practical means of systematically controlling topological transport on the surface of a three dimensional topological insulator, by introducing strong disorder in a layer of depth $d$ extending inward from the surface of the topological insulator. The dependence on $d$ of the density of states, conductance, scattering time, scattering length, diffusion constant, and mean Fermi velocity are investigated. The proposed mechanism requires that the disorder strength be near the large value which is necessary to drive the TI into the non-topological phase. If the disorder depth $d$ is patterned using masks, gates, ion implantation, etc., then integrated circuits may be fabricated. This technique will be useful for experiments and for device engineering.

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Recently a new kind of material has been predicted and measured: topological insulators, which do not permit current to flow through their interior but do allow metallic conduction along their surfaces.[1,2] The conducting states residing on the topological insulator (TI) surface are of interest for their very strong spin-orbit coupling, their Dirac dispersions, and their potential for realizing Majorana fermions and states similar to the fractional quantum Hall effect. They are protected topologically, meaning that they are safeguarded by the bulk’s insulating property from local perturbations as long as a mobility gap is maintained between the bulk bands. In consequence the surface states are only weakly sensitive to fine details of the bulk Hamiltonian, such as lattice structure, details of atomic bonding, or interactions. They are, however, vulnerable to any conduction through the bulk at energies lying in the bulk band gap, and therefore demand a very high-purity bulk. Any engineering of TI devices for either practical or scientific applications will likely use a very pure and unaltered TI bulk, and utilize only the TI’s surface.

In this article we propose a way of engineering TI device properties to match engineering requirements. Our main contribution is the observation that introducing disorder only near the TI’s surface, in a region beginning on the TI surface and extending inward from the surface to a depth $d$, is a practical way of controlling the surface states. As the carrier moves across the surface of the TI, from time to time it becomes almost trapped at a particular site and dwells there for a while before continuing its journey. This trapping is unable to destroy or localize the in-gap surface state, but it does cause a localized increase in the surface state’s probability density, and our numerical results show a corresponding increase in the in-gap density of states $\rho$. Moreover, the increased dwell times at individual sites cause, on average, a decrease in the Fermi velocity $v_F$. The altered density of states and Fermi velocity change also the scattering time $\tau$, diffusion constant $D = v_F^2 \tau / 2$, and coupling constant $\alpha = e^2 / \hbar v_F$ controlling interactions, each of which is strongly sensitive to the disorder depth $d$. Therefore patterned surface disorder, with controlled variations of the disorder depth, can create channels with faster conduction and lower resistance, control points that are sensitive to a gating voltage, and the like.

We emphasize that there are several practical and achievable techniques for producing patterned surface disorder. Already many experiments have studied the effects on TI surfaces of disorder induced by atmosphere, by deliberate introduction of adsorbed molecules and dopants, and even by mechanical surface abrasion.[3,4] Numerous experiments have also demonstrated that capping can effectively protect a TI surface, so masking and etching techniques are promising, as is ion implantation.[5] Ion implantation in particular gives precise control of impurity concentration and depth, and allows control of the disorder average $\langle V \rangle$ by mixing ions.

We will numerically demonstrate that the topological state can be controlled by disorder depth $d$ only if the disorder strength $W$ is tuned near the value $W_c$, which causes the disordered TI to transit from the topological phase to the non-topological phase. $W_c$ is generally quite large, roughly the same as the bulk band width $E_B$, but it does depend on the Fermi level $E_F$, and reduces to zero when the Fermi level lies near the bottom of the conduction band.[6] The density of states and other surface state properties show a clear resonance at $W \approx W_c$ when graphed as a function of disorder.[7] This resonance mirrors the resonance that occurs at individual sites when the topological state becomes pseudo-trapped by disorder. At small disorder $W \ll W_c$, the topological state is pinned at the outer boundary of the disordered region and is therefore insensitive to the region’s depth. At large disorder $W \gg W_c$, the topological state is shifted inward to the boundary between the disordered region and the clean bulk, and is nearly untouched by the dis-
order, so the disorder depth again has little impact. Only at the resonance center $W \approx W_c$ does the topological state detach from the disordered region’s boundaries and fill the entire disordered region. It is only this de-pinned $W \approx W_c$ surface state which is sensitive to the disorder depth $d$, allowing the surface state control which is proposed here.

The depth dependence observed here is not caused by non-topological surface or bulk states. In-gap states can not occur inside the clean interior of the TI because the bulk band gap in the interior is independent of disorder located near the surface. Near $W_c$ the disordered region completely delocalizes, and therefore all in-gap states are mixed and participate in the topological conduction. In the parallel case of 2-D TIs with strong $W \approx W_c$ edge disorder, all in-gap states are confined to the disordered region, very few in-gap states are localized, and the conduction remains quantized.

Surface disorder with $W \approx W_c$ is a bona-fide way of modifying the topological surface states themselves, not of creating peripheral or additional effects distinct from the topological states.

The topological surface conduction which interests us is independent of any short-scale variation in the TI sample, including any microscopic details of the Hamiltonian. Because we are concerned with Fermi energies inside the bulk band gap, only a small number of parameters control conduction — the Fermi velocity, the density of states, and the scattering length. Therefore we study a computationally efficient minimal tight binding model of a strong $Z_2$ TI implemented on a cubic lattice with dimensions $l, w, h$. We leave the TI bulk pure, since the main effects of bulk disorder can be duplicated by narrowing the bulk band gap and increasing the penetration depth in a pure TI. In both cases the bulk states gradually delocalize and surface states are eventually destroyed by tunneling through the bulk.TI[27,32] With four orbitals per site, the model’s momentum representation is:

$$H = \sum_{i=1}^{3} \left[ \left( \frac{t}{2} \alpha_i - \frac{1}{2} \beta \right) e^{-ik_a} + H.c. \right] + (m + 3)\beta \tag{1}$$

$$\alpha_i = \sigma_x \otimes \sigma_i \text{ and } \beta = \sigma_z \otimes 1 \text{ are gamma matrices in the Dirac representation, } t = 2 \text{ is the hopping strength, } m = -1 \text{ is the mass parameter, } a = 1 \text{ is the lattice spacing, and the penetration depth is of the same order of } a.$$ This non-interacting model exhibits a bulk spectral width $E_B = 10$, a bulk band gap in the interval $E_F = [-|m|, |m|]$, and a single Dirac cone in the bulk gap. It belongs to symmetry class $AIII$ for non-zero disorder and $DIII$ for vanishing disorder[33]. To this model we add uncorrelated white noise disorder $\delta(x)$. On each individual site the disorder is proportional to the identity and its strength is chosen randomly from the interval $[-W/2, W/2]$, where $W$ is the disorder strength. In the 3-D limit this model’s topological phase transition occurs at $W_c \approx 7.5$ when the Fermi energy is at the Dirac point[27]. In our study the disorder is confined to the quasi-2-D boundary, which may alter $W_c$. Our results (see also Ref. 20) remain consistent with the 3-D value.

We will present numerical results about the global density of states $\rho(E)$ as a function of energy, and also about the conductance $G(E)$. The density of states is defined as $\rho(E) = Tr(\delta(E - H))$, where $\delta$ is the matrix version of the Dirac delta function. Our numerical calculation of this quantity is performed using the highly scalable Kernel Polynomial method, which is reviewed in Ref. 33. $Tr(\delta(E - H))$ is approximated with an expansion in its Chebyshev moments, the resulting sum over moments is truncated at some maximum number of moments, and this truncation is smoothed using the Jackson kernel. We verified convergence by systematically recalculating our results with different numbers of moments, going as high as 10,000 moments. We calculated large $400 \times 400 \times 20$ slabs, with periodic boundary conditions in the slab plane. We found that the density of states is self-averaging so that 10 samples were sufficient to obtain high accuracy results.

We also calculate the conductance between two leads using the Landauer formula $G = G_0 \ Tr(t^\dagger t)$, averaging over 100 disorder realizations, where $G_0 = e^2/h$ is the conductance quantum. $t$ is the TI’s transmission matrices, which we compute using the transfer matrix method[34][35]. We employ a periodic QR decomposition of the transfer matrix to avoid loss of accuracy, as discussed in Refs. 37[38]. We minimize effects from external leads by using metallic leads. Each TI site adjacent to the leads is connected to a perfectly conducting 1-D wire, similarly to network models.

Our conductance calculations use a slab of height $h = 20$, length $l = 40$ between the two leads, and width $w = 40$ with periodic boundary conditions along this transverse axis. The scattering length is less than 40 for all disorder strengths greater than $W > 2$, so finite size effects from the sample width and length are small. Moreover, because we study disordered boundaries whose maximum depth is $d = 5$ layers, the two disordered boundary layers are always separated by at

FIG. 1: Schematic of the sample geometry. The shaded region is disordered. In the calculation of the density of states, periodic boundary conditions (pbc) are imposed in the $x$- and $y$-directions. In the case of conductance calculation, pbc are imposed in the $y$-direction with $x$ the current direction. In both cases, fixed boundary conditions are imposed in the $z$-direction.
least ten layers of pure non-disordered bulk. Changing the clean bulk’s depth from 10 to 15 while keeping \( d = 5 \) fixed confirms that the conductance is unchanged when the disorder in the boundary is not too large (\( W = 3,6 \) at \( E_F = 0,0.25 \)), but that at larger disorder the conductance increases. Since the clean bulk's depth is equal to \( h - 2d = 20 - 2d \), and our numerical results keep \( h = 20 \) fixed, our results on the conductance’s depth dependence underestimate the behavior of a thick slab. This does not affect our qualitative conclusions.

In Figure 2, we focus our attention on the bulk gap \( E_F = [−1,1] \), where the topological surface states are found. We show the normalized density of states in the gap for six values of the disorder strength, with smaller disorder at the bottom and larger disorder at the top. The smallest-disorder curves are linear in \( E_F \), i.e. \( \rho \propto |E_F| \), which is a hallmark of the 2-D Dirac fermions which ride the TI’s outer boundary. As seen in the inset, the slope grows with increasing disorder, which indicates that disorder causes a decrease in the Fermi velocity \( v_F = dE/dk \). At larger disorder \( W \geq 3 \) the DOS departs from the linear Dirac form in two intervals near \( E_F = ±1 \), and by \( W \geq 6 \) these intervals expand to fill the whole band gap. The cause of this nonlinear behavior depends on the disorder strength: when \( W < W_c \), the 2-D topological state remains pinned to the TI’s outer boundary but its plane-wave character and Dirac cone are destroyed by strong scattering\[19\][22] while near the phase transition \( W \approx W_c \) the state depins and fills the disordered region.

We focus first on the density of states. When the DOS is independent of \( d \), since the clean TI bulk always ensures the existence of a conducting topological state regardless of the disordered region. Panels (a) and (d) show two contrasting behaviors which are sensitive to conducting state’s topology and position: at small disorder \( \rho \) and \( G \) are independent of \( d \), while at larger disorder they are not. The \( d \) dependence is always roughly linear, as seen in panels (c) and (f). Panels (b) and (e) allow us to pinpoint the transition from no \( d \) dependence to linear dependence by plotting the magnitude of the change when \( d \) is changed from 2 to 4, and from 3 to 5.

We focus first on the density of states. When the DOS is sensitive to the disorder depth, it reveals that the topological state is depinned and fills the disordered boundary region. If instead the DOS is independent of \( d \), the topological state is pinned to the TI’s outer boundary. Figure 4(b) shows that at \( E_F = 0,0.25 \) the topological state depins from the TI surface starting at \( W \approx 6.5,5.5 \), and the depinning becomes large around \( W \approx 7.0,6.5 \). At smaller disorder the topological state is pinned, and its conduction parameters are all independent of the disorder depth \( d \). We have summarized this trivial scaling in the first row of Table 1.

Turning to the conductance data, if \( G \) is independent of \( d \) then it is determined by a two-dimensional not
three-dimensional conductivity: $G = 2w \sigma_{2D}/l$. When instead the conductance is linear in $d$, transport is three-dimensional. We concentrate first on the latter, linear, case. Here the disorder is large $W > W_c$ and strongly disordered non-topological states fill the disordered region. Their diffusion constant, 3-D density of states, Fermi velocity, etc., are insensitive to the disorder depth $d \geq 2$ because $d$ is larger than the scattering length $l$, which is comparable to the lattice spacing. In other words, the scattering energy $h/\tau$ is much larger than the kinetic energy, producing truly 3-D diffusive transport, which is the source of $G$’s linear dependence on $d$. We have summarized the conduction parameters of these non-topological states in the last line of Table I.

More interestingly, panel (e) shows that $G$ is constant in $d$ at $W = 6$ for $E_F = 0$, and nearly constant also at $W = 7.5$, $E_F = 0$. These large disorder strengths indicate that conduction is purely topological, since any strongly disordered nontopological states would produce a conductance linear in $d$. Comparing to the DOS data in panel (b), we find that at $E_F = 0,W = 6,7.5$ the conducting state is depinned, but its conductance is still insensitive to $d$; it is a depinned topological state. This is the state which is our focus, because it can be manipulated and controlled by changing $d$. The depinned state’s topological nature is confirmed by its robust conduction under strong disorder.

The depinned topological state is guaranteed to conduct over large distances, and therefore must have a long-wavelength limit where the average parameters of 2-D surface transport are well-defined, including the 2-D density of states $\rho_{2D}$, average Fermi velocity $v_F$, etc. We will show that these quantities are strongly dependent on $d$, beginning with the Fermi velocity $v_F = dE/dk$, the eigenvalue’s derivative with respect to $k$. Its scaling can be determined from the fact that the depinned topological state is not localized. Therefore the eigenvalues within the gap repel each other according to Wigner-Dyson level repulsion, and the energy scale $dE$ in $v_F = dE/dk$ is set by the level spacing $\Delta E$. The depinned state’s 2-D DOS $\rho_{2D}$ is proportional to $d$, and therefore $\Delta E = 1/(\rho_{2D} A)$ scales with $1/d$, where $A$ is the surface area. In strongly disordered samples the momentum scale $dk$ in $v_F$ is controlled by the inverse of the lattice spacing $a$ and is not sensitive to $d$. Therefore $v_F \propto 1/d$.

We turn to scattering and its scaling. Since the disorder is strong enough to depin the topological state from the TI surface, it is near the unitary scattering limit where impurities create bound states at energies far from the Fermi level. In this limit the scattering time $\tau \propto \rho_{2D} n$ is determined only by the impurity density $n$ and not by the disorder strength $W$. This scaling can be combined with the Einstein-Smoluchowski relation $\sigma_{2D} \propto e^2/\rho_{2D} D$ and with $D = v_F^2 \tau/2$ to obtain the conductivity $\sigma_{2D} \propto e^2(\rho_{2D} v_F)^2/2n$. Since our numerical results show that the depinned state’s conductivity $\sigma_{2D}$ is constant in $d$, we conclude that the impurity density $n$ seen by 2-D transport also must be constant in $d$.

Table I summarizes the depinned topological state’s transport parameters. We include the dimensionless coupling constant, which controls interaction effects, as $\alpha = \frac{\pi^2}{\hbar v_F}$.

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* Electronic address: vincent@sacksteder.com

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