

# Thickness-Dependent Conductivity Scaling of B20-Type Chiral Topological Semimetals for Beyond-Cu Interconnect Applications

Sukhyeong Youn  
Department of Materials Science and  
Engineering  
Yonsei University  
Seoul 03722, South Korea  
[suknjong@yonsei.ac.kr](mailto:suknjong@yonsei.ac.kr)

Hyeuk Jin Han  
Department of Materials Science  
and Engineering  
Sungshin Women's University  
Seoul 01133, South Korea

Jiwon Chang\*  
Department of System Semiconductor  
Engineering  
Yonsei University  
Seoul 03722, South Korea  
[jiwonchang@yonsei.ac.kr](mailto:jiwonchang@yonsei.ac.kr)

**Abstract**— The resistivity size effect that degrades conventional metals such as Cu at nanoscale dimensions has driven the search for alternative interconnect metals. Topological semimetals are promising candidates because their Fermi-arc surface states can suppress the rise in resistivity as the film is thinned, in contrast to the behavior of conventional metals. Using a density functional theory (DFT)–Wannier–Kubo framework, we investigate the thickness-dependent resistivity of four B20-type chiral topological semimetals, CoSi, AlPt, AlPd, and GaPd, separating the surface and bulk contributions and including the effect of surface vacancies over a range of defect densities. Without surface vacancies, suppression of the resistivity increase occurs only in CoSi and AlPt, whereas AlPd and GaPd stay bulk-dominated and their resistivity instead rises slightly toward smaller thickness. Under surface disorder, however, the resistivity of AlPt increases most steeply, while CoSi remains the least affected among the semimetals which exhibit the surface-dominated regime. CoSi is the only semimetal to satisfy both conditions, making it the best of the four materials with respect to thickness scaling and defect tolerance.

**Keywords**—topological semimetal, conductivity scaling, first-principles, interconnect

## I. INTRODUCTION

As interconnect dimensions are scaled down, the resistivity of conventional metals such as Cu increases steeply, because electron scattering from surfaces and grain boundaries becomes to dominate at the nanoscale [1,2]. This size effect is a fundamental obstacle to further scaling and has motivated the search for alternative conducting materials which resist performance degradation in ultra-thin films[3,4].

Topological semimetals (TSMs) have emerged as promising candidates for beyond-Cu interconnects[5,6]. Their nontrivial band topology guarantees Fermi-arc surface states which are protected against backscattering[7]. And the number of these surface conduction channels is determined by the bulk topology rather than by the film thickness [5,8]. In contrast to the conventional size effect, the surface-state fraction of the total conduction increases as the slab is thinned, leading to a decrease in resistivity. Consistent with this expectation, the resistivity of the Weyl semimetal NbAs in its nanobelt form has been reported to fall to less than one-tenth of its bulk value [6]. Such unconventional scaling has been investigated in detail for the chiral TSM CoSi [9], which has served as the representative system for this behavior.

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It remains unclear whether this favorable scaling and its robustness against surface disorder extend to other B20-type TSMs. Both issues are essential for assessing TSMs as interconnect materials. In this work, we examine four B20-type chiral TSMs, CoSi, AlPt, AlPd, and GaPd, within a density functional theory (DFT)–Wannier–Kubo framework. We analyze their resistivity as a function of slab thickness and surface defect density. The four TSMs are isostructural and exhibit nontrivial band topology[10,11,12,13]. They differ widely, however, in their bulk electronic band structure. Our results show that unconventional conductivity scaling emerges in CoSi and AlPt, but not in the other materials, under defect-free conditions. However, when surface disorder is introduced, only CoSi retains its unconventional scaling behavior, demonstrating remarkable robustness against surface defects.

## II. METHODS

The overall calculation workflow is summarized in Fig. 1. DFT calculations were performed using the Quantum ESPRESSO package [14] with the Perdew–Burke–Ernzerhof generalized gradient approximation [15] for the exchange–correlation functional and optimized norm-conserving Vanderbilt pseudopotentials [16]. Spin–orbit coupling was included in all calculations, since the heavy elements present in several of the TSMs, such as Pt and Pd, make spin–orbit coupling significant for the band structure. Self-consistent and non-self-consistent calculations were carried out on a  $20 \times 20 \times 20$   $k$ -point mesh. All structures were geometrically optimized by minimizing the total energy with respect to the atomic positions and lattice parameters. The computational parameters are summarized in Table I.

From the converged DFT wavefunctions, maximally localized Wannier functions were constructed with the Wannier90 package [17], using transition-metal d-orbitals and Si/Al/Ga p-orbitals as initial projections, to obtain tight-binding Hamiltonians that accurately reproduce the DFT band structures. Slab models of the (100) surface were built by truncating the bulk tight-binding Hamiltonian along the

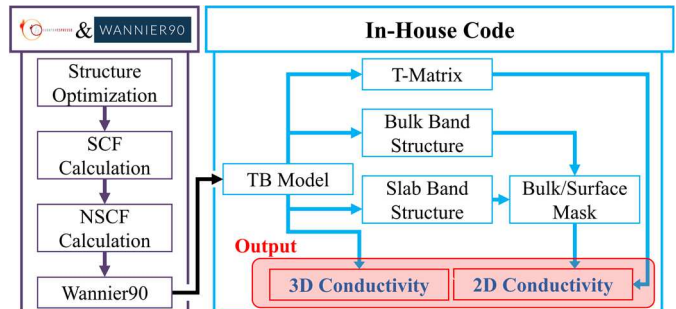


Figure 1. Workflow of the conductivity calculation.

TABLE I. INPUT PARAMETERS USED FOR QUANTUM ESPRESSO CALCULATIONS

| Parameters                      | Values        |
|---------------------------------|---------------|
| Kinetic energy ( $E_k$ ) cutoff | 90 Ry         |
| Charge density cutoff           | 360 Ry        |
| Ionic minimization threshold    | $10^{-4}$ Ry  |
| Self-consistent field threshold | $10^{-12}$ Ry |

surface-normal direction, with the thickness varied from 3 to 16 layers. To classify the slab states, the three-dimensional (3D) bulk bands were projected onto the (100) surface, and slab states located within the projected bulk continuum were assigned to the bulk region, while those in the projected bulk gap were assigned to the surface region. The Fermi-arc surface spectra were obtained using WannierTools [18].

Surface vacancies were introduced on both surfaces of each slab to model surface disorder. For each TSM, the constituent element with the lower vacancy formation energy was selected as the vacancy species, specifically Co, Al, Pd, and Ga for CoSi, AlPt, AlPd, and GaPd, respectively. A vacancy was represented by removing the hopping terms to and from the vacancy site and shifting its on-site energy to 10 eV above the Fermi level. The resulting impurity scattering was incorporated by modifying the slab Green's functions with a T-matrix self-energy. The surface defect density  $N$  is defined as the average number of vacancies per surface unit cell.

The conductivity was computed from the Kubo-formula, with a constant energy broadening  $\eta = 1$  meV representing scattering sources other than the surface vacancies. The surface and bulk contributions to the conductivity were obtained by integrating over the corresponding regions of the two-dimensional (2D) Brillouin zone, and the slab resistivity was normalized to that of the infinite bulk,  $\rho_0$ .

### III. RESULTS & DISCUSSION

The four B20-type TSMs investigated in this work, CoSi, AlPt, AlPd, and GaPd, crystallize in the chiral cubic structure with space group  $P2_13$  (No. 198) (Fig. 2). Because all four share this chiral structure, their bulk band structures host symmetry-protected Weyl nodes at the same high-symmetry points,  $\Gamma$  and R, carrying opposite topological charges that give rise to Fermi-arc surface states spanning the surface Brillouin zone. Evaluating transport across so many slab thicknesses directly with DFT would be computationally demanding, so we employ the tight-binding Hamiltonians constructed from the maximally localized Wannier functions described above. Fig. 3 compares the Wannier-interpolated band structures with the directly computed DFT band structures along the high-symmetry path of the 3D Brillouin zone for all four TSMs. The interpolated bands closely reproduce the DFT bands throughout the Brillouin zone,

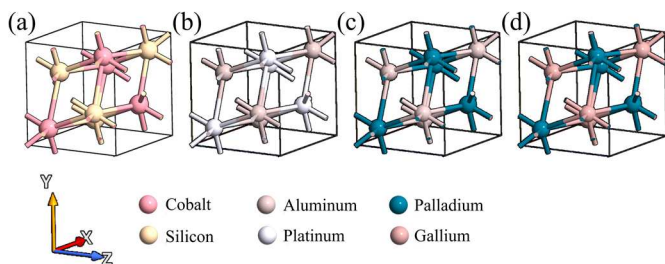


Figure 2. Primitive unit cell structures of (a) CoSi, (b) AlPt, (c) AlPd, and (d) GaPd.

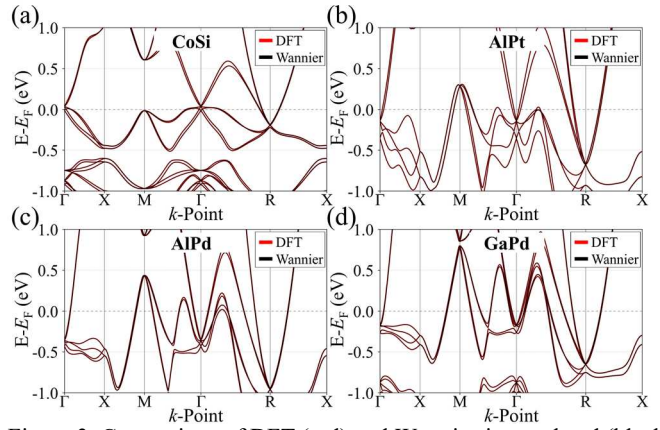


Figure 3. Comparison of DFT (red) and Wannier-interpolated (black) band structures for (a) CoSi, (b) AlPt, (c) AlPd, and (d) GaPd.

including at the Weyl nodes at  $\Gamma$  and R, confirming that the Wannier Hamiltonians accurately describe the electronic band structure used in the subsequent transport calculations.

Because surface and bulk states are both present near the Fermi level in a finite slab, we separate them in  $k$ -space before computing their respective conductivities. For each TSM, we overlay the projected 3D bulk band continuum on the (100) slab band structure, as illustrated in Fig. 4. Applying the classification described above at the Fermi level partitions the 2D Brillouin zone into a bulk region and a surface region. Fig. 5 shows the Fermi-level surface-state spectrum of each TSM, where topologically protected Fermi arcs are observed across all four.

The fraction of the 2D Brillouin zone occupied by the bulk region differs markedly among the TSMs and correlates with the bulk conductivity. Table II lists this bulk region fraction together with the conductivity of the infinite bulk,  $\sigma_0$ , for each TSM. The two quantities follow the same trend, with CoSi having the smallest bulk region fraction and the lowest  $\sigma_0$ , and GaPd the largest values of both. A larger bulk region implies that more bulk bands cross the Fermi level and contribute carriers, so TSMs with a small bulk region are expected to depend more strongly on surface conduction. This distinction explains the thickness-dependent transport behavior analyzed in the following paragraphs.

We first examine the thickness dependence of the resistivity for defect-free slabs ( $N = 0$ ), shown as the normalized resistivity  $\rho/\rho_0$  in Fig. 6. For CoSi and AlPt,

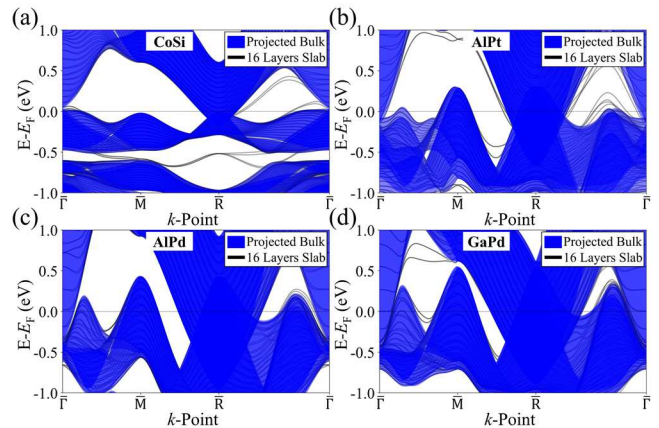


Figure 4. Overlay of (100)-oriented slab band structures (black) and the projected 3D bulk band structures (blue) for (a) CoSi, (b) AlPt, (c) AlPd, and (d) GaPd.

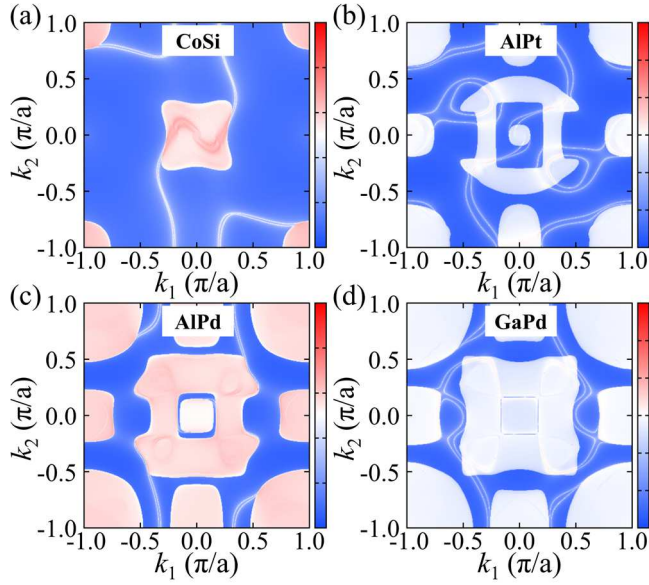


Figure 5. Surface state spectrum in 2D Brillouin zone at the Fermi level for (a) CoSi, (b) AlPt, (c) AlPd, and (d) GaPd.

resistivity falls as the slab is made thinner, the unconventional trend characteristic of TSMs. AlPd and GaPd behave oppositely and show no such reduction. Rather, their resistivity edges upward only slightly toward the smallest thicknesses. This contrast originates from the competition between the bulk and surface contributions identified above. Because the surface states are confined to the two surfaces, their contribution to the conductivity is nearly independent of slab thickness, so as the slab thickness decreases, it becomes a larger proportion of the 3D conductivity. CoSi and AlPt have small bulk regions, so this surface contribution comes to dominate the thinned slab and drives the resistivity downward. AlPd and GaPd have much larger bulk regions, so bulk conduction remains dominant at all thicknesses, and the increasing surface contribution never surpasses it. The resistivity therefore does not decline.

The existence of this surface-dominated regime is determined by the occupation of the bulk bands near the Fermi level. As the slab is thinned, quantum confinement progressively shifts the bulk subbands away from the Fermi level. In CoSi and AlPt, the bulk bands cross the Fermi level down to seven and six layers, respectively, and in thinner slabs they no longer reach it, as shown by the slab band structures in Fig. 7(a, b) and 7(c, d). Below these thicknesses, transport proceeds mainly through the surface states. In AlPd and GaPd, by contrast, the bulk bands continue to cross the Fermi level down to the thinnest slabs considered, as shown in Fig. 7(e) and 7(f), respectively, so no surface-dominated regime emerges. The surface-to-bulk conductivity ratio, shown in Fig. 6(b, d, f, h), quantifies this competition directly. For CoSi and AlPt, the ratio exceeds unity in thin slabs, confirming that surface conduction exceeds the bulk where the resistivity drops. For AlPd and GaPd, it remains below unity at all thicknesses, consistent with their bulk-dominated transport.

TABLE II. BULK REGION FRACTION AND INFINITE-BULK CONDUCTIVITY OF THE FOUR TSMs

| TSM  | Bulk Frac. | $\sigma_0 (\times 10^4 \text{ S/cm})$ | TSM  | Bulk Frac. | $\sigma_0 (\times 10^4 \text{ S/cm})$ |
|------|------------|---------------------------------------|------|------------|---------------------------------------|
| CoSi | 13.31%     | 4.81                                  | AlPd | 61.34%     | 109.44                                |
| AlPt | 38.13%     | 47.56                                 | GaPd | 68.85%     | 136.53                                |

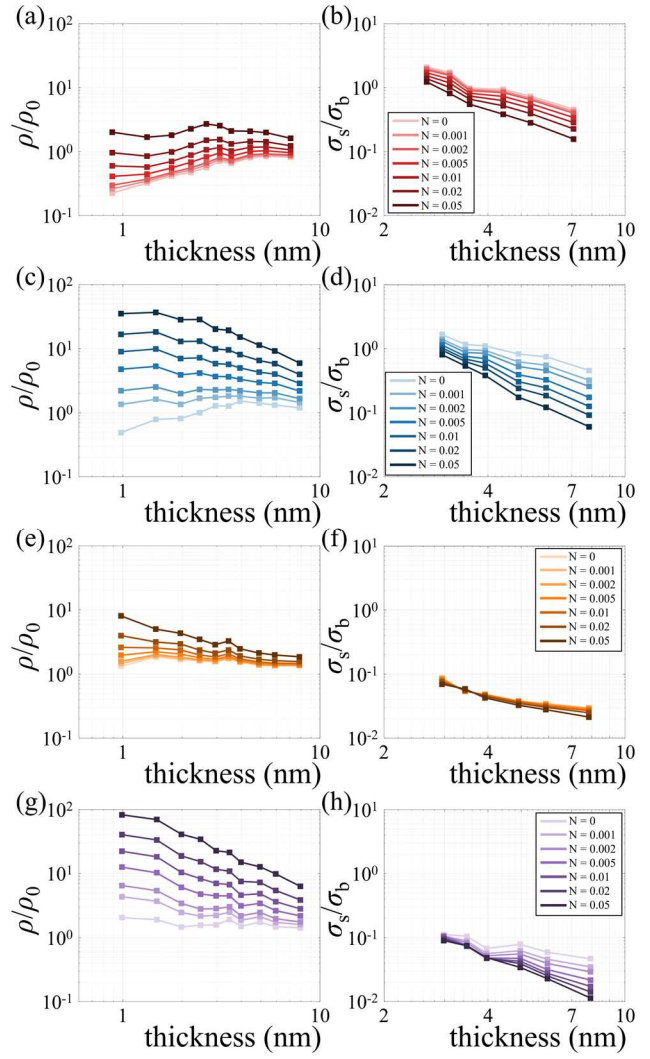


Figure 6. Normalized resistivity  $\rho/\rho_0$  as a function of slab thickness for (a) CoSi, (c) AlPt, (e) AlPd, and (g) GaPd, and the surface-to-bulk conductivity ratio  $\sigma_s/\sigma_b$  for (b) CoSi, (d) AlPt, (f) AlPd, and (h) GaPd, at various surface defect densities  $N$ .

We next examine the robustness of the unconventional scaling against surface vacancies, introduced at a density  $N$  on both surfaces of the slab. Fig. 6 shows the resistivity as a function of thickness for increasing  $N$ . Although surface vacancies raise the resistivity in all four TSMs, the magnitude of the resistivity increase at a given thickness exhibits significant material dependence. CoSi and AlPd are less sensitive to surface vacancies, showing only modest resistivity increases even at the highest defect density considered. In contrast, AlPt and GaPd are considerably more sensitive, with their resistivity increasing much more steeply. At the thinnest slab (3 layers), going from  $N = 0$  to  $N = 0.05$  raises the resistivity by only about  $5\times$  and  $3\times$  for CoSi and AlPd, but by roughly  $47\times$  and  $36\times$  for AlPt and GaPd. Notably, this sensitivity ordering does not follow the bulk region fraction of Table II. AlPt has a small bulk region but shows the largest resistivity increase, whereas AlPd, with a large bulk region, is the least affected. The bulk region fraction that determines the pristine thickness scaling therefore does not predict the response to surface disorder.

The presence of a surface-dominated regime and robustness against surface disorder are two independent properties of these TSMs. The former is set by the defect-free

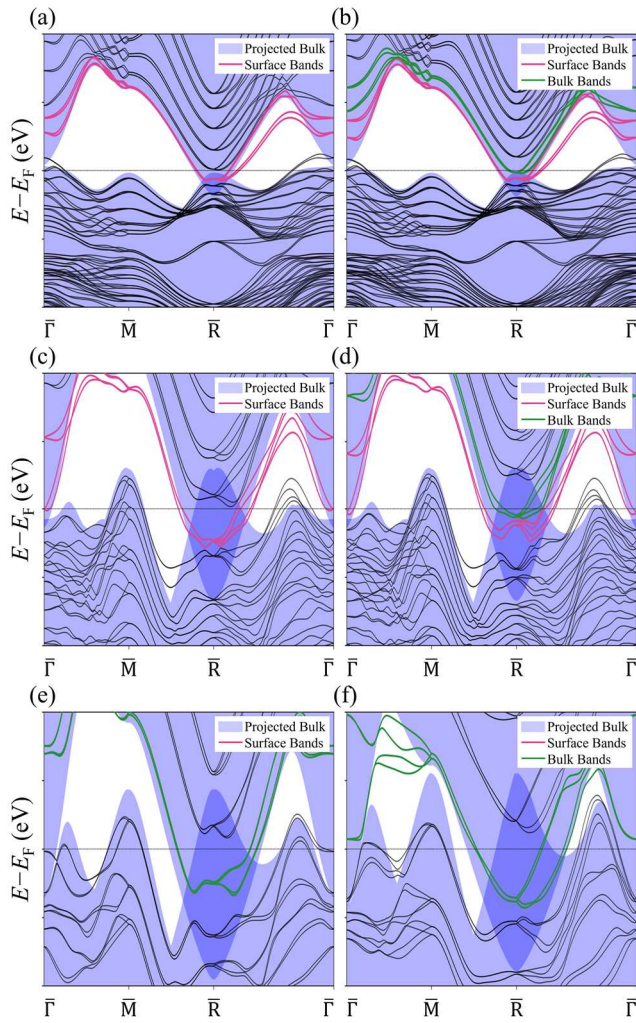


Figure 7. Slab band structures near the Fermi level for (a, b) CoSi at 6 and 7 layers, (c, d) AlPt at 5 and 6 layers, and (e) AlPd and (f) GaPd at 3 layers.

electronic structure, whereas the latter reflects how strongly the conduction channels are disrupted when vacancies are present. AlPt illustrates their independence. It shows the surface-dominated regime characteristic of unconventional scaling, but exhibits the most significant degradation under surface defects. A favorable interconnect material must satisfy both. These two criteria place the four TSMs into the four possible combinations. CoSi has the surface-dominated regime and resists disorder, whereas AlPt has the regime but is highly sensitive to it. AlPd resists disorder but lacks the regime, and GaPd has neither. CoSi alone falls in the favorable category, and among the materials with the regime it also shows the smallest resistivity increase under disorder.

#### IV. CONCLUSION

We investigated the thickness-dependent resistivity of four B20-type chiral TSMs, CoSi, AlPt, AlPd, and GaPd, within a DFT–Wannier–Kubo framework. In defect-free slabs, CoSi and AlPt exhibit unconventional scaling in which the resistivity decreases with reduced thickness, sustained by surface-dominated conduction, whereas the resistivity of AlPd

and GaPd increases only weakly or remains nearly constant owing to their larger bulk contribution. When surface vacancies are introduced, however, CoSi and AlPt show different trends, with AlPt degrading sharply while CoSi withstands the disorder better. Among the TSMs studied, only CoSi combines a surface-dominated regime in the pristine limit with robustness against surface disorder, two distinct requirements, making it the strongest of the four semimetals in these respects.

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