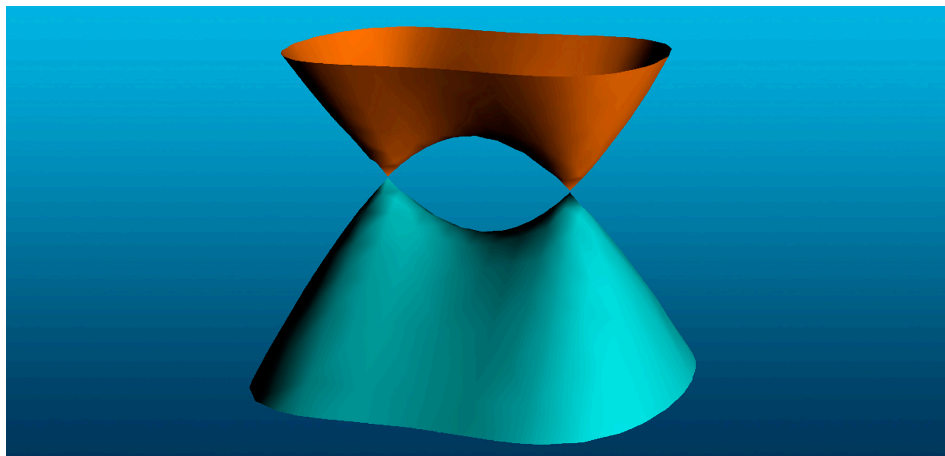


Strain Turns Tin into a 3D Topological Dirac Semimetal



Schematic illustration of the electronic structure of strained gray tin, showing cone-shaped regions that meet at Dirac points, hallmarks of a 3D topological Dirac semimetal.

A small amount of compressive strain turns a nonmetallic form of tin into a 3D topological Dirac semimetal (TDS)—a kind of “supermetal” with high electron mobility. Commonly known as “gray tin,” this material is the first experimentally confirmed 3D TDS composed of a single, simple element. In this work, ALS beamlines were used for material synthesis, structural studies, and electronic band-structure investigations. Combined with first-principles calculations, the results demonstrated that the conductive properties of gray tin can be tuned (from topological insulator, to ordinary semimetal, to Dirac semimetal) by varying the direction of an applied strain. With its rich topological phase diagram, the material shows promise for both novel physics studies and future device applications.

Properties such as conductivity (involving electron mobility) can be inferred from a material’s band structure. Overlapping valence and conduction bands indicate a metal in which electrons can move freely; insulators (and

semiconductors) exhibit a band gap (larger for insulators, smaller for semiconductors). Dirac semimetals constitute the special case where valence and conduction bands touch at discrete points. Furthermore, because electron velocity is proportional to band curvature, bands with tips that are V-shaped (or conical, in 3D) rather than U-shaped (or paraboloid) indicate higher electron mobility.

Three-dimensional TDSs are analogous to 2D graphene: their unusual electronic structures correspond to extraordinary physical properties (e.g. ultrahigh carrier mobility, giant linear magnetoresistance) that could be useful in developing next-generation electronics. They are also a versatile platform for exploring exotic electronic properties and topological phase transitions. However, 3D TDSs are rare. So far, only two others have been reported: Na_3Bi and Cd_3As_2 . The former contains sodium, which is unstable in air, and the latter contains arsenic, a toxic element.

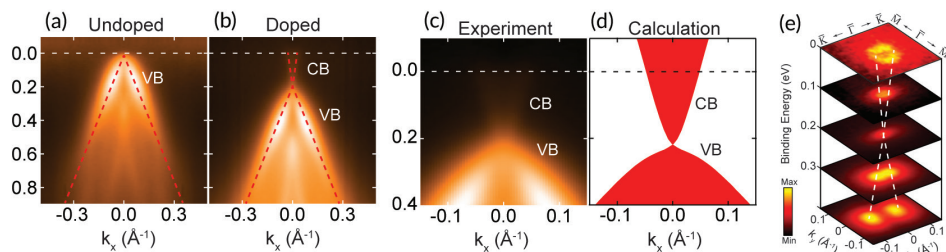
Humble Tin’s New Phase

Tin is a base metal that has been in use for thousands of years, since at least the Bronze Age (bronze is an alloy of copper and tin). It’s also a constituent of the alloys pewter (used for tableware) and solder (used for electronics). Before the advent of aluminum cans, tin-plated steel cans were used in the preservation of food. Pure, elemental tin comes in two forms: white and gray. White tin is a silvery, malleable metal that is stable at room temperature (55.8 °F and above). In colder temperatures, however, white tin transforms into gray tin, also known as “tin pest” because it decomposes into a brittle, powdery (useless) material. However, if a thin film of gray tin is grown on a substrate of indium antimonide (as Xu et al. did in this work), it can remain stable well above room temperature. The layering causes a strain in the gray tin, inducing a transformation to a new phase, with potential applications in ultrafast electronics or ultracompact storage. Given its ability to morph from one phase to another, gray tin could be an excellent platform for fundamental research of interest to many physicists.

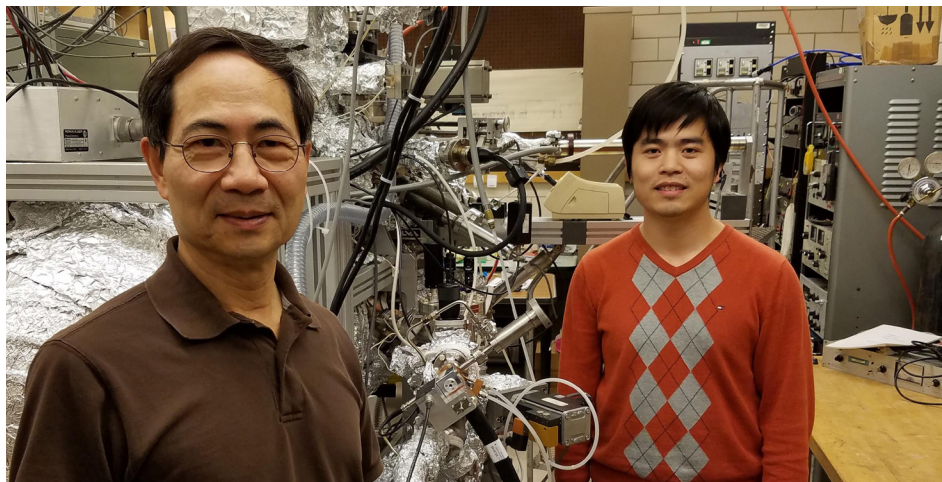
Gray tin is a well-known semimetal with a zero gap protected by the cubic symmetry of its crystal lattice. Previous studies by other groups had suggested that tensile strain, which breaks the cubic symmetry, opens a band gap, transforming the ordinary semimetal into a topological insulator. However, subsequent experiments were unable to verify the existence of a strain-induced band gap.

To investigate further, researchers came to the ALS, where the ready availability of sample preparation and characterization tools provided key contributions to the experiment. At Beamline 10.0.1, thin films of gray tin (6 to 30 bilayers thick) were grown in situ via molecular-beam epitaxy on a substrate of indium antimonide (InSb). Microdiffraction measurements at Beamline 12.3.2 showed that the lattices of the two materials were slightly mismatched, generating an in-plane compressive strain of 0.14%. Angle-resolved photoemission spectroscopy (ARPES) measurements of the electronic band structure were done at Beamline 10.0.1. As an electron-emission technique, ARPES only probes below the Fermi level (i.e., where the electrons are). In thin films of gray tin, the Fermi level sits right above the valence band. Therefore, to see the conduction band, the researchers electron-doped the sample with potassium to raise the Fermi level.

The results directly show linear band dispersions along all three momentum directions (i.e., Dirac cones) for both the valence and conduction bands, establishing gray tin as the first 3D TDS system based on a simple elemental material. The data were consistent with the researchers' first-principles calculations, which demonstrated that gray tin can be either a TDS or a topological insulator (as found in the earlier experiments), depending on the sign of the applied strain (compressive or tensile, respectively). Thus the system is a TDS for compressive strain, becomes a zero-gap semimetal at zero strain, transforms into a topological insulator at tensile strain, and finally becomes an ordinary semimetal at a sufficiently large tensile strain. The work makes clear that strain engineering can open up many new possibilities for controlling electronic properties. Like silicon, an elemental material at the foundation of semiconductor physics, gray tin as an elemental TDS may help realize important electronic devices in the future.



ARPES results for 6-bilayer gray tin. (a) Band dispersion before electron doping only probes the valence band (VB). (b) Band dispersion after electron doping provides access to conduction band (CB). (c) Close-up view of band dispersion in b around the zone center near the Fermi level (dashed line). (d) Calculated bands for comparison with c. (e) Stacking plots of constant-energy contours at different binding energies show a Dirac cone.



Physics Professor Tai-Chang Chiang and graduate student Caizhi Xu pose in Chiang's laboratory at the Frederick Seitz Materials Research Lab at the University of Illinois at Urbana-Champaign. Image courtesy of Physics Illinois.

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