Control of Nanoscale Transport with a Novel Size Effect

From an emergence of quantization on a nanometer scale, the QSE allows flexible control of matter and is a rich source of advanced functionalities. A complete picture of the QSE with a new class of size effects can dominate the nanoscale transport in systems with metallic surface states, typically topological materials.

Quantized electronic states generated by the quantum size effect (QSE) in nano-confined systems enable a unique tunability for a wide range of phenomena such as superconductivity, light-matter interaction and non-equilibrium carrier dynamics. Modulations of the bandgap and the density of states further improve functionalities in catalysts and information devices. A QSE-induced transition into an insulating phase in semi-metallic nanofilms was predicted for bismuth a half century ago and has reignited interest with regard to its surface states exhibiting non-trivial electronic topology. In the case of a system having metallic surface states as typically observed in topological materials, the transition is marked by the disappearance of conducting channels in the film interior; thereafter, electric current flows only through the surfaces. This transition was first predicted a half century ago for bismuth (Bi). A Bi single crystal is a typical semimetal with small carrier pockets and three-dimensional Dirac dispersions. Moreover, because of a large spin-orbit coupling, Bi surfaces host spin-polarized metallic states that have been intensively examined in the context of electronic topology. The QSE-driven metal-insulator transition in Bi nanofilms originally received great attention as a nanoscale path to achieve a substantial thermoelectric figure of merit, and is now of interest to enhance surface-state-induced exotic phenomena. Evidence of the metal-insulator transition in Bi films was obtained only in this decade through transport measurements on epitaxially grown samples. A recent angle-resolved photoemission spectroscopy (ARPES) measurement on Bi films furnishes a clear contrast to the transport results showing only the interior-insulating phase below a threshold thickness. Although this strange contradiction between metallic and insulating signatures observed in completely the same system implies the presence of an intriguing mechanism, essential quantization information was lacking in previous experiments.

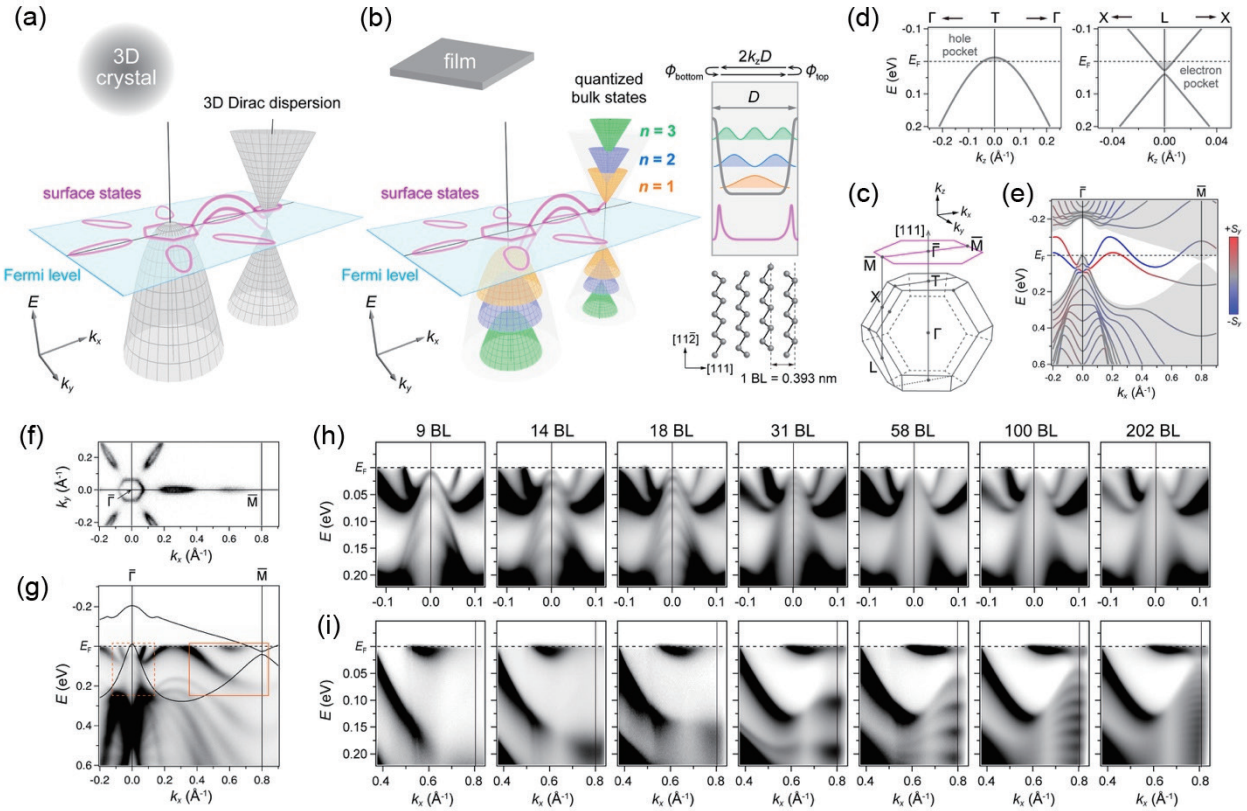


Fig. 1: Direct observation of a QSE-induced metal-insulator transition. (a,b) Schematic of the metal-insulator transition in a Bi nanofilm. (c) Bulk and surface Brillouin zone of Bi in direction [111]. (d) Bi bulk band structures calculated around the hole and electron pockets with a tight-binding method. (e) Band structures obtained from a tight-binding calculation for a Bi(111) slab (14 BL). (f,g) Experimental Fermi surfaces and band structures measured on a Bi(111) film (14 BL) grown on a Ge(111) substrate. Shaded areas in (e) and solid curves in (g) show the calculated bulk projections. (h,i) Experimental band structures magnified inside dashed and solid boxes in (g), respectively, for each thickness. [Reproduced from Ref. 1]

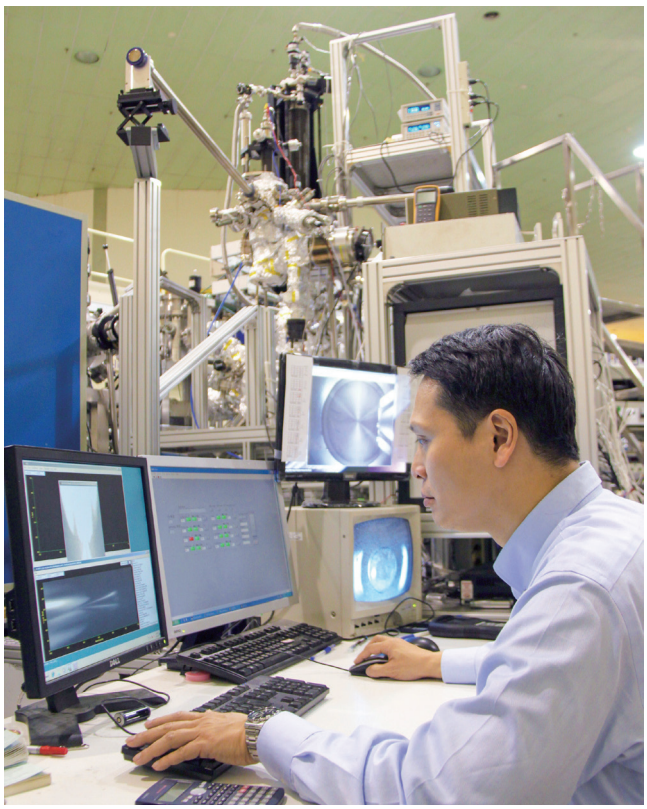
To solve the contradiction existing in transport and ARPES results, Suguru Ito and Iwao Matsuda from the University of Tokyo, Japan, Shu-Jung Tang from National Tsing Hua University, Cheng-Maw Cheng from NSRRC and their teams investigated the evolution of the electronic structure of high-quality Bi nanofilms. With high-resolution ARPES measurements at **TLS 21B1**, these authors performed a detailed and systematic study of the electronic structure of Bi nanofilms of varied thickness; they reported the first direct observation of a QSE-induced metal-insulator transition. As shown in **Fig. 1**, the visualization of an anomalous level evolution contrasted with tight-binding simulations to highlight an additional mechanism beyond a simple QSE. In addition, an unexpected degeneracy of the top two quantized energy levels detected from ARPES completely breaks a standard quantization rule. This tendency is totally opposite a well known effect of hybridization between top and bottom surface states and reconciles a contradiction among previous experiments in an unprecedented manner. An important question is the nature of the central mechanism responsible for the anomalous behaviors. To combine with density function theory (DFT) and the ARPES result, these typical modulations of quantized bulk states can be fully explained only when we consider the deformation of a quantum confinement potential, which is triggered by enhanced effects of Coulomb repulsion with decreasing system size, centering on a size-independent contribution from the surface states.

In summary, Ito and Matsuda systematically revisited the strange contradiction among recent studies on the metal-insulator transition in Bi films. They revealed an unexpected mechanism of the transition by high-resolution ARPES combined with DFT calculations. Anomalous evolution and a degeneracy of quantized energy levels indicate that the increased Coulomb repulsion from the surface states deforms a quantum confinement potential with decreasing thickness. The potential deformation strongly modulates the spatial distributions of quantized wave functions, which leads to an acceleration of the transition beyond the original QSE picture. Their presented study not only solves a serious controversy about a transition discussed for half a century but also introduces a novel size effect that can be universally present in a system with metallic surface states, typically topological materials.[1,2,3] (Reported by Cheng-Maw Cheng)

*This report features the work of Suguru Ito, Iwao Matsuda and their collaborators published in Science Advances **6**, eaaz5015 (2020).*

TLS 21B1 U90 – (CGM) ARPES

- High-resolution Angle-resolved Photoemission Spectroscopy
- Materials Science, Condensed-matter Physics



References

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