Formation of $\text{Bi}_x\text{Se}_y$ phases upon heating of the Topological Insulator $\text{Bi}_2\text{Se}_3$: stabilization of in-depth Bismuth bilayers


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Bismuth Selenide ($\text{Bi}_2\text{Se}_3$) is a topological insulator compound with lamellar structure formed by the repetition of stacks of five atomic monolayers, each of them consisting of layers with either Se or Bi atoms. Each ensemble of five covalently bonded planes is connected to other quintuple-layers by van der Waals interactions, making this material potentially interesting for building novel devices. Its electronics properties are intimately related to other two-dimensional systems, presenting surface states with an electronic linear dispersion on selected points of the Brillouin zone.

The goal of this work was to observe and interpret the transformations that occur upon heating $\text{Bi}_2\text{Se}_3$ at temperatures up to $350^\circ\text{C}$. X-ray diffraction and Scanning Tunneling Microscopy (STM) techniques were used to observe these transformations. X-ray diffraction was measured following the 00L and 01L truncation rods. These measurements revealed that upon heating there is a coexistence of a major $\text{Bi}_2\text{Se}_3$ phase (a three-dimensional topological insulator) and a conducting phase with a structure composed of five $\text{Bi}_2\text{Se}_3$ quintuple-layers followed by a bilayer of Bismuth, leading to an overall $\text{Bi}_4\text{Se}_5$ stoichiometry.

Density Functional Theory calculations showed that whereas $\text{Bi}_2\text{Se}_3$ is a topological insulator, $\text{Bi}_4\text{Se}_5$ is a conventional conductor with several van Hove singularities near the Fermi level. STM measurements of the surface of this material showed the presence of hexagonal $\text{Bi}_4\text{Se}_5$ domains terminated in Bismuth bilayers embedded in a $\text{Bi}_2\text{Se}_3$ matrix. Low temperature scanning tunneling spectroscopy revealed that the bilayer termination exhibits a conducting behavior, with a corresponding conductor-like density of states, presenting no band gap. STS also showed that the bilayer and $\text{Bi}_2\text{Se}_3$ are in electrical contact, with the possibility of the presence of a topological state at the edge of the bilayer, since Bismuth islands are two-dimensional topological insulators.

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