学位論文の要旨

Abstract of Thesis

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学位論文題目 Title of Thesis（学位論文題目が英語の場合は和訳を付記）

Pressure-driven superconductivity in topological insulators
（トポロジカル絶縁体の圧力誘起超伝導）

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The introduction of concept of topology into condensed matter physics has led to a great success in physics and materials science, as evidenced by winning of Novel prize (physics) in 2016, and it has led to a new understanding of quantum phase beyond Landau's theory of spontaneous symmetry breaking [1-3]. The topological concept has been utilized to classify numerous quantum matters, including insulators, metals, superconductors, and bosonic systems. Topological insulators, which are quantum electronic matters that have a bulk insulating gap accompanied by the topologically protected gapless surface states or edge states. In analogy with topological insulators, topological superconductors possess a bulk superconducting gap together with the gapless Majorana bound states (Andreev bound states) [4-5]. Beyond the fundamental interests from view of condensed matter physics and materials science, the primary motivation for studying topological materials would originate from that they may provide an ideal platform for detecting and manipulating Majorana fermions. Actually, the topological materials are expected as a building block for realizing the fault-tolerant quantum computation system. Many theoretical and experimental studies have been devoted to obtain a crucial evidence for clarifying the existence of Majorana fermions in realistic materials.

In this Doctor thesis, the author reports novel physical properties of topological insulators under pressure. This Doctor thesis consists of eight chapters. In chapter 1, the author explains the starting point toward topological insulator, *i.e.*, quantum Hall effect and quantum spin Hall effect. Characteristics of topological insulators and topological superconductors, as well as recent progress of study on topological insulators under pressure are also summarized in chapter 1. In chapter 2, the motivation and purposes of this study are fully described, in relation to the background described in chapter 1. The concrete purposes of this study are to precisely clarify the structural behavior of tetradymite-type (A_2B_3) topological insulators under pressure, and to investigate their physical properties under pressure, in particular to search for novel quantum phases such as superconductivity.

In chapter 3, pressure dependence of crystal structure in Ag-doped Bi_2Se_3, $Ag_{0.05}Bi_{1.95}Se_3$, is

fully investigated by use of synchrotron X-ray diffraction (XRD) measurement, and the XRD data are analyzed by Le Bail fitting to determine the lattice constants at 0 – 30 GPa. The pressure-dependent XRD patterns show the presence of two structure phase transitions at 8.8 and 24 GPa; three structure phases, rhombohedral structure ($R\bar{3}m$, No. 166), monoclinic structure ($C2/m$, No. 12), and tetragonal structure ($I4/mmm$, No. 139)), exist at 0 – 30 GPa. Discontinuous changes of lattice constants and unit cell volume (V) are observed for each structural transition, indicating the first order structural phase transition.

In chapter 4, pressure dependence of physical properties of Ag-doped Bi_2Se_3 is reported at 0 – 26 GPa, in particular the emergence of superconductivity is confirmed at 11 GPa. Two superconducting phases (superconducting transition temperature (T_c) = 4 – 5 K, and T_c ~ 7 K) are found at 11 – 26 GPa. In Ag-doped Bi_2Se_3, Ag is substituted for Bi, as evidenced from X-ray fluorescence hologram, and recent study on fluorescence holography and photoelectron holography suggested that Ag was substituted for Bi, and intercalated into the space between Se layers, indicating that the Fermi level is located near the bottom of conduction band or the top of surface states. In Ag-doped Bi_2Se_3, no superconductivity is observed at ambient pressure, which is consistent with hole-doped Bi_2Se_3 system [6]. From magnetic field (H) dependence of T_c at 11 and 20.5 GPa for Ag-doped Bi_2Se_3, the reduced magnetic field (h^*) - t plots are obtained, in which $t = T / T_c$, suggesting a possible p-wave pairing in superconductivity.

In chapter 5, the author reports pressure dependence of crystal structure of $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (x = 0, 0.25, 0.5, 1.0, and y = 1.0) clarified from synchrotron XRD patterns at 0 – 30 GPa. The crystal structure is analyzed by Le Bail fitting for the XRD patterns of these four samples. Three or four phases are found in $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (x = 0, 0.25, 0.5, 1.0, and y = 1.0). All samples have phase I (rhombohedral structure ($R\bar{3}m$, No. 166)), phase II (monoclinic structure ($C2/m$, No. 12)), and phase III (9/10-fold monoclinic structure (9/10 fold-$C2/m$, No. 12)). An additional 8-fold monoclinic structure (phase II') is often present together with phase II and phase III. To be precise, phase II' is observed in $Bi_{2-x}Sb_xTe_{3-y}Se_y$ at $x \neq 0$. From the XRD patterns, the author finds that the pressures causing the first and second structure phase transitions gradually increase with increasing x value (amount of Sb).

In chapter 6, the author reports the electric transport properties of $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (x = 0, 0.25, 0.5, 1.0, and y = 1.0) up to 15 GPa. At ambient pressure, all samples show no superconductivity down to 2.0 K. With increasing the pressure, the superconductivity emerges in phase I, and the T_c value gradually increases. The H dependence of T_c is measured for $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (x = 0, 0.25, 0.5, 1.0, and y = 1.0) in phase I and phase II. The h^* - t plots are followed by p-wave polar model, indicating a possible p-wave superconducting pairing.

The author further performs the structure analysis by Rietveld refinement for XRD patterns of $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (x = 0, y = 1.0), and calculates the band structures at different pressures. At 2.37 GPa (phase I), the Z_2 invariant of Bi_2Te_2Se is 1;(000) at the Fermi level, indicating the strong topological insulator. At 14.4 GPa (phase II), Z_2 = 0;(000) is provided, suggesting topologically trivial, but the Z_2 invariant is very sensitive to the structure. Therefore, the topological nature is still under debate. At

28.6 GPa (phase III), the Z_2 invariant suggests a strong topological nature. From the calculation of Z_2 invariant, the *p*-wave pairing may be understandable at least for phase I.

In chapter 7, the author simply reports the structure and electric transport properties of $BiSbTeSe_2$ ($Bi_{2-x}Sb_xTe_{3-y}Se_y$ (x = 1.0, and y = 2.0)) under pressure. $BiSbTeSe_2$ shows two structural phase transitions at 0 - 29 GPa. Namely, three structural phases are observed at 0 – 29 GPa, in the same manner as Bi_2Te_2Se (rhombohedral structure ($R\bar{3}m$, No. 166), monoclinic structure ($C2/m$, No. 12), and 9/10-fold monoclinic structure (9/10 fold-$C2/m$, No. 12)). It was previously reported that the Fermi level in $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (x = 1.0 and y = 2.0) crossed the Dirac point [7]. Actually, our data of transport properties also suggest that the Fermi level does not cross the conduction band but the surface states. With increasing pressure, the superconductivity is observed in phase II. This behaviour is different from that of $Bi_{2-x}Sb_xTe_2Se$ (x = 0, 0.25, 0.5, and 1.0), but is similar to those of Bi_2Se_3 [8], and Ag-doped Bi_2Se_3 in this study. From these results, it is suggested that the Te amount in $Bi_{2-x}Sb_xTe_{3-y}Se_y$ closely relates to the phase in which superconductivity emerges.

The results and discussion obtained in this study are summarized in chapter 8, and the author points out the future tasks necessary to clarify the superconducting properties of topological insulators. This Doctor thesis provides a systematic study on physical and structural behaviors of topological insulators under pressure. New findings on pressure-induced structural phase transition and pressure-driven superconductivity are reported in this thesis, and the detailed strategies in future study are presented for pursuing topological nature of superconductivity.

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