論文 / 著書情報
Article / Book Information

題目(和文)	強いスピン軌道相互作用を持つ層状ビスマス化合物の単結晶における超伝導および磁気輸送特性
Title(English)	Study on Superconducting and Magnetotransport Properties in Single Crystals of Layered Bismuth Compounds with Strong Spin-orbit Coupling
著者(和文)	大川顕次郎
Author(English)	Kenjiro Okawa
出典(和文)	学位:博士(理学), 学位授与機関:東京工業大学, 報告番号:甲第10422号, 授与年月日:2017年3月26日, 学位の種別:課程博士, 審査員:笹川 崇男,東 正樹,中村 一隆,舟窪 浩,吉本 護
Citation(English)	Degree:Doctor (Science), Conferring organization: Tokyo Institute of Technology, Report number:甲第10422号, Conferred date:2017/3/26, Degree Type:Course doctor, Examiner:,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

（博士課程）
Doctoral Program

論 文 要 旨

THESIS SUMMARY

専攻： Department of	物質科学創造 専攻	申請学位（専攻分野）： Academic Degree Requested	博士 Doctor of （ 理学 ）
学生氏名： Student's Name	大川 顕次郎	指導教員（主）： Academic Advisor(main)	笹川 崇男 准教授
		指導教員（副）： Academic Advisor(sub)	東 正樹 教授

要旨（英文800語程度）
Thesis Summary（approx.800 English Words ）

Relativistic effects on electronic states in solids have attracted much attention in recent years. In particular, strong spin-orbit coupling (SOC) originated from relativistic effects can induce exotic superconducting states (e.g. the topological superconductivity) and magnetotransport effects (e.g. the extremely large magnetoresistance (XMR)). The majority of the studies has been on superconducting states induced in topological insulators by intercalating, applying pressure, or utilizing proximity effects, all of which involve experimental difficulties, such as chemical instability and complex electronic structures. Thus, it is of great importance to establish stoichiometric materials, in particular, having good cleavage planes.

The exploration for new candidate materials with topological metallic phases, which exhibit the exotic physical properties beyond the topological insulator, was proposed in this thesis. Based on a topological semimetal-based strategy, screening of candidate materials was performed from the crystal structure database. As a result of the screening, three layered bismuth-based semimetals, in which bismuth should introduce the strongest atomic SOC among the stable elements into the compounds, α-PdBi, β-$PdBi_2$, and InBi were chosen for the detailed study in this thesis. By growing single crystals, we performed magnetotransport measurements at low temperatures. The electronic structures were evaluated using relativistic first principles calculations. In common with three bismuth-based compounds, it was verified that the SOC played essential roles in bulk and surface properties.

The normal and superconducting properties of the noncentrosymmetric superconductor α-PdBi were evaluated. From the relativistic first principles calculations, the large Rashba-split bands were confirmed, suggesting this material can be a suitable platform for the unconventional superconductivity such as spin-singlet/triplet mixed paring states. In fact, the signatures (the upward curvature near T_c in H_{c2}-T phase diagram, and the two-step superconducting transition) were experimentally observed in a pure α-PdBi crystal. This suggests that the multi-gap superconductivity and the spin mixed pairing state may be realized in this systems. However, H_{c2} at absolute zero was well below the Pauli limit, indicating the conventional orbital pair-breaking mechanism will be applied for α-PdBi. Even if the spin mixed paring state is realized, it seems that the component of the spin-triplet is relatively small.

Next, the superconducting properties in a centrosymmetric superconductor β-$PdBi_2$ were evaluated. By performing the relativistic first principles calculations, the topologically non-trivial surface states were found to be emerged across the Fermi level. It strongly suggests that β-$PdBi_2$ is a good and first stoichiometric candidate material as a topological superconductor. β-$PdBi_2$ has a comparably high T_c and the good cleavage plane between Bi-Bi layers, indicating that it can be an excellent material as the candidate of a topological

superconductor. Substitution effects in β-$PdBi_2$ were examined for further revelation of the bulk superconducting states. The substitution of magnetic and non-magnetic elements for Bi in β-$PdBi_2$ was systematically performed up to the solubility limit. It was found that T_c decreased in all the substituted samples, and the suppression rate of T_c was appreciably larger for magnetic doping than that for non-magnetic one. The results indicate that the pair breaking effects of the magnetic impurities severely suppress T_c. This suggests the possibility of realizing fully gapped superconducting states in bulk β-$PdBi_2$. In the case of fully gapped superconducting states in bulk, Majorana fermions are expected to appear in the surface vortex states of the topological superconductor. Therefore, the direct probes to detect the Majorana fermions in the surface vortex states such as STM/STS should be performed. β-$PdBi_2$ can serve as a guideline for searching for a new candidate material for the topological superconductors.

Finally, the compensated semimetal InBi was focused, and the magnetotransport measurements were performed. It was found that InBi was a new XMR semimetal (MR ~ 12000 % at 1.8 K and 7 T). The MR showed a classical parabolic dependence on the magnetic field and was not saturated. In addition, the field-induced metal-insulator like transition was observed at low temperature. Using several single crystals with different residual resistivity ratio (*RRR*), it was found that the MR in InBi strongly depended on the *RRR* (sample quality). Assuming no change in effective mass and carrier concentrations in these single crystals, this dependency was explained in terms of the change in the carrier mobility by the semiclassical two-carrier model. By performing the relativistic first principles calculations, it was found that InBi had compensated electron and hole carriers and “hidden” 3D-Dirac bands. This Dirac bands were appeared at M-point and R-point as a result of the strong SOC. At this symmetry points, it is required that the orbital degeneracy cannot be solved by the crystal symmetry in the tetragonal structure. This is a new strategy for the exploration of 3D-Dirac semimetals. It was experimentally and theoretically confirmed that InBi was a new compensated XMR semimetal.

The semimetal-based strategies will lead to diversity in topological electronic materials. Superconductors that have been overlooked may realize topological superconducting states. In fact, another layered superconductor $PdTe_2$, which was selected using the proposed semimetal-based strategy in this thesis, was found to have topological surface states. The electronic structures and superconducting states are also revealed. Likewise, it is expected that many candidate materials will be discovered by the strategy proposed in this study. By finding the materials suitable for experiments, the further elucidation of the topological superconductivity, such as detecting Majorana fermions is expected.