Abstract

題　目 Spin- and Angle-Resolved Photoelectron Spectroscopy Studies of Chiral Crystals $NbSi_2$ and $TaSi_2$
（スピン角度分解光電子分光によるキラル結晶 $NbSi_2$ および $TaSi_2$ の電子状態の研究）

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The chirality-induced spin selectivity (CISS) effect, in which a spin-polarized current is generated when an electric current is passed through a material with a chiral structure, has been observed in some chiral organic molecules, and is attracting attention because of its potential in spintronics applications. However, the microscopic mechanism of the production of spin-polarized electrons is still controversial.

Besides the organic molecules, the CISS effect has been observed in transport measurements in the inorganic chiral materials $NbSi_2$ and $TaSi_2$. The robust and stable crystal structure provide the opportunity to experimentally examine the mechanism of the CISS and the effects of chirality from the electronic structure point of view. In this thesis, the combination of spin- and angle-resolved photoemission spectroscopy (spin-ARPES) and density functional theory (DFT) calculation is used to examine the electronic structures with spin properties of $NbSi_2$ and $TaSi_2$, thereby complementing the transport and structural studies of these classes of materials.

This thesis mainly includes the following parts:

1. A brief introduction of the research about CISS and Weyl semimetals. Some basic concepts are described.
2. The basic principles, the experimental techniques and instruments of spin-ARPES are introduced.
3. The growth and preparation of single crystals $NbSi_2$ and $TaSi_2$ are described in detail. We successfully observed the electronic structure of these materials and found the spiral shaped constant energy contour (CEC) pattern by ARPES measurements and discussed its origin.

Our comparative experiments on left- and right-handed crystals $NbSi_2$, DFT calculations, and symmetry arguments reveal that the spiral CEC patterns can be caused by the intrinsic crystal structure, i.e., the inherent bulk chirality and surface states that extend several layers into the bulk are essential ingredients that lead to the profound spiral pattern. The relation between the observed spiral CEC pattern and the CISS effect is not obvious at present. In the transport CISS effect, however, the voltage applied across them may play a role analogous to the role of the surface in the spiral CEC in terms of symmetry reduction. Further studies, spin-ARPES measurement will experimentally reveal the spin texture and may help to understand the relation between present findings, the CISS effect and the spin-electronic structure.

Key words: Chiral crystal, Spiral band structure, Spin-ARPES, DFT calculation.