# 論　文　の　要　旨

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）

氏　名　Cheng Zhang

The chirality-induced spin selectivity (CISS) effect is attracting attention for its potential in spintronics applications. It not only exists in some chiral organic molecules, but also has been observed in transport measurements of chiral inorganic materials $NbSi_2$ and $TaSi_2$. However, the microscopic production mechanism of spin-polarized electrons remains controversial. Spin-ARPES, as a direct and powerful experimental method for studying electronic states inside solids, provides the opportunity to examine the mechanism of the CISS and the effects of chirality from the electronic structure point of view.

In this thesis, the clean and atomically flat (0001) surfaces were obtained by cycles of argon ion sputtering and annealing after mechanical polishing of the single crystals $NbSi_2$ and $TaSi_2$, and the combination of spin-ARPES and DFT calculation is used to examine their electronic structures with spin properties.

The main conclusions are as follows:

1. The clear band structure of $NbSi_2$ was successfully observed by VUV-ARPES measurements, which mostly consistent with the bulk DFT calculation.
2. The photoelectron distribution of $NbSi_2$ exhibits as an unexpected spiral-shaped patterns, and the clarity of the spiral structures is related to the binding energy. The rotation direction of the spiral CEC patterns depends on the structural chirality, which is obtained by comparative measurements on the right- and left-handed crystal $NbSi_2$. In addition, the spiral electronic structure is not unique to $NbSi_2$, it also exists in the chiral crystal $TaSi_2$, which has the same crystal structure as $NbSi_2$.
3. The spiral pattern can emerge from the intrinsic band structure by DFT calculations considering surface contributions. In particular, the inherent bulk chirality and surface states that extend several layers into the bulk are essential ingredients that lead to the spiral pattern.
4. Soft X-rays ARPES experiment results show that surface electronic states have a non-negligible contribution to the formation of spiral structures. The result also shows that $k_z$ corresponding to $h\nu$=50 eV is determined about $0.1\times 2\pi/c$ from Γ point, which approximately is consistent with the result obtained by comparing VUV-ARPES and DFT calculation.
5. We have not observed spin polarization for the time being in the spin-ARPES experiment studying the CISS effect of $NbSi_2$. The possible reasons are as follows: (1) the spin polarization is too low for spin detectors to detect; 2) the escape depth of electrons is not deep; (3) the crystal is not homochiral but contains many domains of opposite chirality; (4) possible flowing electrons are a necessary condition for the formation of the CISS effect; (5) The current is so small that the spin signal is lost in the experimental noise.