（別紙様式２）

フォトンサイエンス国際卓越大学院プログラム（XPS）

光科学特別実習　報告書

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Research subject

Exploration of topological quantum phenomena in magnetic Weyl semimetal NdAlSi

Host researchers

I conducted a joint research project with the Strong Correlation Materials Research Group in Center for Emergent Matter Science (CEMS) at Riken as part of this program in XPS course. The group director is Taguchi-sensei, who kindly accepted this project. This group aims at obtaining gigantic cross-correlation responses, understanding their mechanisms, and developing new functions in strongly-correlated-electron bulk materials. Many experts of synthesis of high-quality crystals belong to this group. During my stay in this project, I worked together with Kikkawa-san, one of the experts of sample growth in this group, to synthesize single crystalline sample of magnetic Weyl semimetal NdAlSi.

Background

Topological quantum materials been extensively studied in condensed matter physics in recent years. In addition to the fundamental interest, topological quantum phenomena are also of interest from the viewpoint of applications to future power-saving devices, such as the creation of a new concept of electric current with low energy loss, called topological current. In particular, topological semimetals (Dirac or Weyl semimetals) host Dirac or Weyl electrons with linear band dispersion in the bulk, and their novel quantum properties due to their quantum topology are of great interest. In particular, it has been reported that a giant anomalous Hall effect due to the Berry phase at the band crossing point has been reported for magnetic Weyl semi-metals [E.Liu *et al*., Nature Physics **14**, 1125-11331 (2018)].

The purpose of this study is to clarify the physical properties of magnetic Weyl semimetals by observing the response of NdAlSi, which has been proposed as a magnetic Weyl half-metal, in relation to the topology of the band structure. It has been proposed that *R*AlSi, *R*AlGe (*R*=rare earth) is a magnetic Weyl half-metal with a crystal structure with broken spatial inversion symmetry [S. Y. Xu *et al*., Science Advances **3**:e1603266 (2017)]. In *R*AlSi, the Weyl point is generated by the spatial inversion symmetry breaking, regardless of the details of the magnetism, making it an ideal material for clarifying the relationship between magnetism and the Weyl electrons. In particular, as an optical response, a large magneto-optical effect is expected to appear due to the anomalous Hall effect originating from the Berry curvature. Also, the optical measurement is a powerful tool to observe the signature of topological materials, such as the angle resolved photoemission spectroscopy (ARPES) and optical conductivity measurements. In this project, I worked on the synthesis of high-quality single crystal of NdAlSi, which is necessary to move on to further study to observe physical properties related to the band topology in NdAlSi.

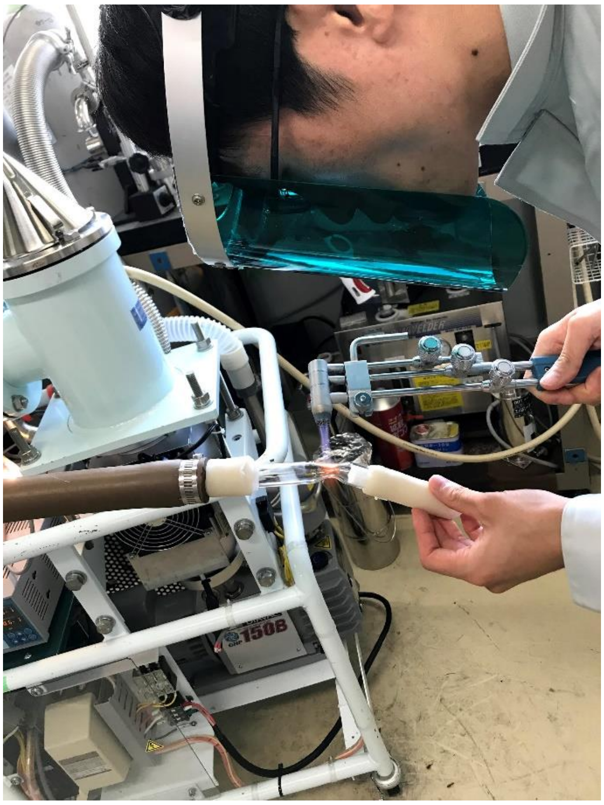
Project contents

I synthesize single crystalline sample of NdAlSi with the great help of Kikkawa-san. I used Al flux method, which is also adopted in the previous work [S. Bobev *et al*., Journal of Solid State Chemistry **178**, 2091-2103 (2005)]. I weighed the starting materials with the excess of Al, which is used as flux, and put them in an alumina crucible. Then the alumina crucible is placed inside a quartz tube. It is necessary to place the materials in vacuum before heating up because they become oxidized if placed in air. To make the inside of the quartz tube vacuum, I used the diffusion pump. A jet of diffused oil vapor heated by the heater at the bottom reaches supersonic speed and can capture molecules to create a vacuum of about 10^{-4} Pa. While pumping a vacuum, I sealed the quartz tube using oxyhydrogen burner. The picture of me sealing the quartz tube is shown in the bottom of this report. It was the first time for me to use this equipment so it scared me a little bit because it becomes very hot and shiny. It took me several times to master the sealing technique, but finally I found out how to do it. Then the sealed quartz tube is put into the electric furnace and heated up. After the treatment at high temperatures, the sample is slowly cooled down. I took the sample out above the melting temperature of Al (660 ℃), and removed the excess Al flux using a centrifuge. Finally, I got the single crystalline sample of NdAlSi. Later, I found that the quality of the sample changes depending on the synthesis condition, so I tried the growth by changing the treatment temperature and time, and the ratio of starting materials.

After the growth, I evaluated the sample quality by using X-ray diffraction and energy dispersive X-ray (EDX) and confirmed that the obtained crystal is the single crystal of NdAlSi. I also measured the magnetic and transport properties. Both of them roughly reproduce the results of previous research. Especially, the Hall resistivity shows anomaly at the transition field from ferrimagnetic phase to ferromagnetic phase, which is likely originating from anomalous Hall effect.

Achievement of this project

I successfully synthesized the single crystalline sample of NdAlSi in this project. The next step is to identify the Berry phase contribution to the physical properties through the transport and optical measurements to achieve the final goal to reveal the close relation between magnetism and Weyl electrons. At the end of this report, I would like to thank Taguchi-sensei and Kikkawa-san, who kindly accepted this project and taught me a lot during my stay.



Sealing of the quartz tube while evacuating the sample space with a diffusion pump.