MERIT Internship Report

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Period of implementation

December 6, 2021 - February 9, 2022

Host company

Advanced Technology Research and Development Department, New Technology Center, Technology and Business Development Division, Murata Manufacturing Co.

Theme

Research on screening of ferroaxial materials by utilizing symmetry

Background

The symmetry of a material dominates the various physical properties that shows. In my PhD research, I have focused on the symmetry of mainly magnetic structures in materials and observed them using resonant X-ray diffraction.

Recently, a symmetry called ferrroaxial has been attracting attention. In actual crystal structures, this symmetry is realized by rotation of a part of the structure around the principal axis with respect to the primary structure. A material with this symmetry exhibits electrogyration, which is proportional to the first order of the applied electric field. It is known that the angle of rotation depends on the direction of the applied electric field and the sign of the ferroaxial domain. Using this property, our group has successfully observed the ferroaxial domain in a material by using a technique to measure the small angle of rotation in two dimensional space[1]. In order to explore new physical properties based on symmetry, our laboratory is conducting a joint research with Murata Manufacturing Co. We planned and implemented the MERIT internship at Murata Manufacturing Co., as an opportunity to learn the process of searching for new physical properties and implementing them in products.

The purpose of this internship was to learn how to search for materials using high-throughput screening, how to evaluate physical properties using computational science, how to synthesize materials, and how to implement them in experimental devices.

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[1] Hayashida, T. “Visualization of Ferroaxial Domains in an Order-Disorder Type Ferroaxial Crystal.” *Nature Communications*, 11, 4582 (2020).

Activities

We constructed a system for screening and searching for materials that can exhibit electrogyration from among the approximately 250,000 materials registered in the Materials Database. First, materials with ferroaxial symmetry were extracted by symmetry determination, and as a result, about 200 candidate materials were obtained. These candidates were evaluated by first-principles calculations and visual confirmation, and the extraction conditions were determined by comparing them with empirical facts, finally filtering down to about 50 promising candidates.

Among these candidates, many of which have already been reported to undergo the ferroaxial-nonferroaxial phase transition, which is the key to the expression of electrogyration, were included, suggesting the validity of this screening method. Some of these materials have not been focused on as electrogyration materials, and the discovery of these new materials is one of the major achievements of this internship. Finally, we examined the feasibility of single crystal synthesis and optical measurement based on past literatures, and obtained several promising candidate materials to be tested. In the future, we will conduct actual material synthesis and optical evaluation, and provide feedback to the search method, which will lead to the search for electrogyration materials with greater optical effects and the construction of material design guidelines.

Impressions

In this internship, I was able to put myself in the field of research and development at a company for a certain period of time, which I had not imagined in my previous research activities, and intensively conduct research in relatively inexperienced fields such as material exploration and computational science. In addition, I was able to observe the research environment and facilities at the company, and was often surprised by the scale of the company, which was very different from the life at the university, and the daily life at work. On the other hand, the atmosphere of the research site was close to that of my own laboratory, and I was very impressed by the environment of casual discussions around an open desk.

Acknowledgments

I would like to express my gratitude to Dr. Hirose of Murata Manufacturing Co., Ltd. for setting up the internship at the local office in the Corona disasterous days. I would also like to express my gratitude to Mr. Murata, Dr. Hirai, and the other members of the department to which I was assigned for their direct guidance. Thank you very much.

Finally, I would like to express my gratitude to my supervisor, Professor Kimura, and my deputy supervisor, Professor Katsumoto, for giving me the opportunity to do this internship.