MERIT Internship REPORT

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Outline

- Period
  October 23, 2023 – November 24, 2023
- Place
  R&D Department of Frontier Technology, New Technology R&D Center, Corporate Technology & Business Development Unit, Murata Manufacturing Co., Ltd.
- Theme
  Study of dielectric material by using computational and data science

Background and contents

In recent years, machine learning and other data science have been increasingly applied to the real world. In particular, its usefulness in the field of materials science has been remarkable, making it possible to replace the conventional need for manual experimentation in the search for new substances and other areas. This methodology of materials science is called materials informatics, and it has become a new trend of the times. Murata Manufacturing, the host of this program, is also making efforts in this area, and has even implemented its own data-scientist-training program in cooperation with other IT-related companies.

Although material exploration has long been a subject of research, it is not realistic to investigate all material properties by experiment even for known materials, and there has always been demand for accurate prediction of material properties by numerical calculation, which has a relatively fast trial-and-error cycle. However, existing solid-state simulations based on first-principles calculations and molecular dynamics have the drawback that although their results are correct, they are computationally expensive. As a result of this disadvantage, the cell size could not be increased, and therefore, there was a fundamental problem that, for example, successive phase transitions in crystal structures could not be predicted correctly.

In this internship, we examined the effectiveness and universality of an alternative method for first-principles calculations [1], which has recently been implemented in a first-principles calculations package, called VASP. The alternative method skips first-principles calculations with larger cell sizes for finite-temperature solid simulations by machine learning data from first-principles calculations with smaller cell sizes. Using this method, we were not only able to reproduce the results for $BaTiO_3$, which had been studied earlier as an academically interesting

application, but also able to confirm both the effectiveness and the universality of the alternative method for other materials with important applications. I skip the details.

Impressions

It was very meaningful for me to see that the knowledge of condensed matter theory that I had learned in undergraduate is directly applied to materials exploration. In particular, the experience of absorbing new fields was unique, by utilizing all of my knowledge that I had not touched since undergraduate, such as linear response theory and simulations near phase transitions. Furthermore, I think that I was able to experience firsthand the special situation that it is difficult to confirm the validity of an analysis due to its characteristic of attacking areas where theoretical calculations are impossible. In addition, by listening to the research of various employees, I became clearly aware of how wide the range of specialized fields related to the search for material science is and the differences between each field, and I was able to reaffirm my own expertise as a theoretical physicist.

In addition, through this internship, I got the impression that the way of conducting research is not so different from that of academic research, at least in the department that I was assigned to. However, I was noted the fact that the position of the research department in a company has a considerable influence on this impression. Since I am currently considering a corporate research position as one of my career paths, I believe that this experience was useful for my future career choice.

Acknowledgements

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[1] R. Jinnouchi, F. Karsai, G. Kresse, Phys. Rev. B **100**, 014105 (2019)