MERIT Internship (Domestic) Report

Department of Chemistry, School of Science
Doctoral course 2nd year, 8th student
Takumi Sakamaki

Recipient

Mitsubishi Chemical Corporation, Science & Innovation Center, Materials Design Laboratory (MDL)

Outline

Period: October 1st, 2021 – November 5th, 2021.
Place: Materials Design Laboratory (MDL) of Mitsubishi Chemical Corporation,
Research theme: "Prediction of physical properties and improvement of prediction accuracy in amine and epoxy cured polymers with materials informatics (MI)".
Report on internship study : November 4th.

Background

I decided to do this internship for the following three reasons.
(1) To feel the atmosphere of the research in the company.
(2) I expected that I could developed my research from deferent perspective.
(3) I wanted to try research using MI because I'm interested in MI.

The MDL proposes solutions to problems faced by various departments from the perspective of computational science. The purpose of this internship was to predict the physical properties of epoxy and amine curing systems based on the structure and composition of starting materials and the curing conditions, aiming to speed up the proposal of the physical properties desired by customers.

Research

Since the contents of this report are confidential, the specific contents are not described.

In the amine-epoxy curing system, amine and epoxy react sequentially to form a three-dimensional network structure. In general, when predicting the physical properties of a simple structure such as a linear polymer, it is easy to predict from the physical property information of the monomer unit, but in this work, there is no unit because of random structure. So it was necessary to predict from the composition and structural information of starting materials. However, when predicting from composition and structure information, there is no method to organize the data. Therefore, optimization of this method can improve the prediction accuracy.

In this work, I thought that the prediction accuracy could be improved by examining the processing method of the descriptor data of amine and epoxy. I have conducted various methods for processing the data, such as combining the features of amine and epoxy into one, and optimizing the averaging method when combining composition data. As a result, I have successfully improved the accuracy of prediction compared to previous results. When I analyzed this results, I discovered tendency in the amount of features influencing each physical property. From this result, I found the possibility of further improving the prediction accuracy by selecting features that have an impact on physical property prediction.

During the internship period, I was able to participate in the weekly discussions "MI small talk meeting" where researchers conducting research using MI in the department shared information with each other.

Impressions Through Internship

Since I had no previous experience with programming languages, I struggled a lot at first. But, thanks to the careful and easy-to-understand explanations of MDL researcher Dr. Momose who directly instructed me on the theme of this internship, I was able to achieve sufficient results and propose a direction for my research during internship. Due to the coronavirus, I could not have a relationship with other researchers. But I could visit experimental facility in MDL department on November 4th.

Acknowledgement