

## **Report for MERIT Overseas Dispatch**

MERIT-WINGS 11<sup>th</sup>

Department of Chemistry, School of Science

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Name of hosting research institute: University of Illinois

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Research project title: Integrating Data Science to Enhance Quantitative Electron Microscopy Analysis of Molecular Dynamics

### **【Research】**

Self-assembly is a phenomenon widely found in materials science, biology, chemistry, and other fields, and is an important process that plays a fundamental role in the construction of functions. However, the mechanism has not been elucidated even with current science, and precise control of crystallization and flexible design of materials have not been realized.

In our laboratory, single-molecule atomic-resolution time-resolved electron microscopy (SMART-EM) have been developed to directly elucidate the molecular dynamics. I apply this technique to elucidate the mechanism of order formation in amorphous materials. However, in amorphous materials without structural descriptors, it is not easy to evaluate transient structures and dynamic behaviors that appear in aperiodic structures before nucleation and during aggregation. Therefore, I attempt to acquire pioneering techniques, including molecular recognition, at Qian Chen's laboratory, which is developing a method of analysis based on transmission electron microscopy observation in liquid (LP-TEM) and machine learning.

In general, LP-TEM images have a larger background effect than images taken in vacuum, making it difficult to identify the observed objects. Therefore, I learned a segmentation method using deep learning in LP-TEM images. A program was run to track the movement of each particle on the segmented sequential images, and it became clear that the nanoparticles aggregated and aligned from the disorderly distribution observed in the early stages of the observation.

Next, I attempted to detect crystalline regions formed in amorphous materials by

applying the analytical methods of this laboratory. As a result, I succeeded in classifying them according to their periodic structures. By unifying the classification criteria across multiple frames, it was possible to analyze where and when the same structure was formed in a time-evolving manner. In the future, I would like to develop a detailed discussion based on the identification of the crystal structures detected here.

### **【Research Environment】**

The rules and management systems at the universities in the U.S. were more robust than I had imagined because the equipment was basically shared throughout the university. Access to electron microscopes required the completion of a training program strictly regulated by the university with a resident technician specializing in each instrument. In addition, instrument reservations were generally booked up, including on weekends. Furthermore, the reservation form required detailed input of specific sample preparation conditions and the purpose of the measurement, making it difficult to have a brief touch-up during a stay of only a few months. It was an opportunity for me to learn the advantages and disadvantages of the different organizations in Japan, which are operated by different departments or laboratories.

In the host laboratory, analysis was basically performed on each individual's own PC. Therefore, in order to learn new analysis, I had to start by installing the software and programs used for the analysis, even if it was commonly performed in the laboratory. In particular, I struggled to build an environment for using software that was incompatible between windows and mac OS. However, thanks to this process of trial and error, I gained the knowledge, experience, and confidence that I can do almost anything with a single notebook PC.

### **【About Life】**

The campus is located in Urbana-Champaign, an idyllic area about 2.5 to 3 hours by car or 4 to 5 hours by chartered bus from Chicago, a large city in Illinois. On campus, there are supermarkets, banks, and restaurants in a compact area, which is convenient for students who live in dormitories or on-campus residences. There are also many libraries and cafes, and students have many options for places to study and work on PCs other

than lecture halls and laboratories without having to worry about seating.

On the other hand, outside of the campus town, there was no supermarket within walking distance. In particular, there was no bus service to my accommodation on weekend, so I faced difficulties in the American car society.

### 【Acknowledgments】

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