Report on MERIT Long-term Overseas Dispatch

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From the end of September 2019, I stayed in a research group called PLASMANT in the University of Antwerp in Antwerp, Belgium for two months. PLASMANT, as the name suggests, is a group that focuses on research to synthesize materials using plasma. The group is working on efficient material synthesis using not only experiments but also computer simulations. This time, Associate Professor Erik Neyts who leads the atomic level simulation in the group supported me for the stay.

There are some differences from Japan when we live abroad. For me, water was the most different things from Japan. In Belgium we can drink tap water as well as Japan, but the taste was different. Even I usually don't care about my hair, I felt something wrong with my hair after taking shower with Belgium water. The origin of these differences is the "hardness" of water. Hardness is the concentration of calcium ions or magnesium ions dissolved in water. In Belgium, water is "harder" than that in Japan. Hardness also affects washing and special detergent is required to keep salt from clogging. Of course, water also affects cooking. In Belgium, eating in restaurant is expensive. For example, if you order hamburgers, French fries (in fact, "French" fries have its origin in Belgium) and beer, it costs around 2000 yen. Thus, I cooked by myself often to save money. The hardness of water is related to "equilibrium state" and "kinetics". Equilibrium is the final ion concentration when a stone is placed in the water of a beaker and left for decades or hundreds. It is the maximum concentration that can be dissolved. However, the water with maximum concentration of calcium or magnesium is not for drinking use. Thus, kinetics is important in tap water case. Kinetics is related to the "amount that dissolves per unit time" and "time in contact with water". In Europe, there may be more rocks that are more soluble than in Japan, or it may take some time to reach the water treatment plant after it rains.

My research in Antwerp is related to this "equilibrium state" and "kinetics". The target is a reaction process that carbon atoms dissolved in a metal form bonds between carbon

atoms. This is the initial reaction when a material called carbon nanotubes is formed. We want to discuss the equilibrium state and kinetics of the reaction using a simulation called molecular dynamics calculation, however, the time range that can be handled by molecular dynamics is as short as nanoseconds, which is insufficient to observe the reaction. Therefore, an acceleration method called metadynamics was used to accelerate the reaction. I chose Antwerp University as a place to stay because Prof. Erik is an expert in molecular dynamics and my supervisor, Prof. Shibuta has done many collaboration researches with him and because Dr. Kristof, doing post doc in the group, specializes in molecular dynamics acceleration methods. Although it was a short period of two months, I was able to have a fulfilling research life. A new molecular dynamics acceleration method developed with Erik and Kristof prior to the two-month stay is already submitted to a journal, and the results of the two-month stay are currently being prepared.

Acknowledgement

I would like to appreciate Prof. Erik Neyts and Dr. Kristof Bal for supporting my stay and daily discussions. I would also like to appreciate Prof. Yasushi Shibuta for his great support for this dispatch, including financial aspects. Currently, the MERIT program cannot provide any financial support for long-term overseas dispatch due to the cutting of the leading graduate school budget. I hope the financial support from MERIT program will recover in the future, and more students will be able to experience overseas research.

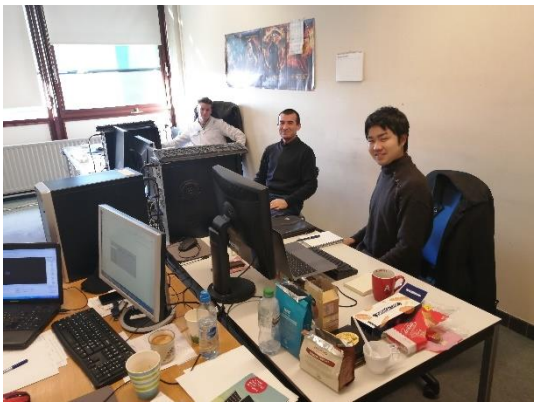

Fig.1. Picture of the room I conducted research. A master student from Antwerp, a faculty member who came to study from Uzbekistan for the short term, and me. The group has members of various nationalities.

Fig.2. Lunch with group members. I had lunch for two months every day at this university cafeteria. The second man from the right is Kristof.