Report on Long-term Overseas Dispatch

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Abstract

I studied in Prof. Adam Foster's group at Aalto University in Finland for 80 days from Aug. 12 to Oct. 30 as a Long-term Overseas Dispatch of the MERIT program. My purpose was to learn the use of molecular dynamics simulations to study the structure of a water/solid interface. My specific target was to simulate the hydration structure on the surface of a $SrTiO_3$ photocatalyst.

Selection of the host laboratory

My research is related to the study of water splitting photocatalysts. I have studied the interface between liquid water and a photocatalytic semiconductor to understand the reaction field of photocatalysis, especially the role of the hydration structure and the surface electronic structure. So far, my work on $SrTiO_3$-based photocatalysts has shown that an unusual electronic structure is formed at the water/$SrTiO_3$ interface and that the hydration structure drastically changes after UV light irradiation. However, the interpretation of the physical and chemical phenomena is still difficult based only on spectroscopic or local probe analysis techniques. I therefore wanted find another complementary technique that was not available in my laboratory but would let me look at the photocatalysis process from another viewpoint that I had not considered before. To select a suitable host laboratory, I first thought that a laboratory with very special and cutting-edge experimental instruments would be the best choice. However, on further consideration I realized that the overseas dispatch program would be a good chance to obtain new experience in a type of research that I usually have less contact with. I therefore decided to visit a theoretical research group that specializes in simulating liquid/solid interfaces. Computational science has been developing very rapidly in recent years and the reliability and reproducibility are becoming good enough for direct comparison with experimental results. It would therefore be quite a valuable experience for an experimentalist to join a theoretical research group and fuse the experimental and theoretical studies.

Prof. Adam Foster is a leading researcher in the study of liquid/solid interfaces by multiscale methods using first-principles calculations and molecular dynamics simulations. His group has published many papers on the water/solid interfaces of NaCl,

CaF_2, $CaCO_3$, Mica, and p-nitroaniline. Prof. Hiroshi Onishi in Kobe University, who is my research collaborator, has a long collaboration history with Prof. Adam Foster. His recommendation to visit Prof. Adam Foster's group helped me to finally decide to join his group for studying the water/$SrTiO_3$ interface.

Work done during the stay

Since I didn't have experience with computational physics before, there was a certain level of apprehension to join a theoretical group. Fortunately, there was a chance to participate in a Summer School of Molecular Dynamics Simulations from Aug. 18 to 20, just after my arrival at Aalto University. This was a very good way to start to learn how to carry out computational simulations.

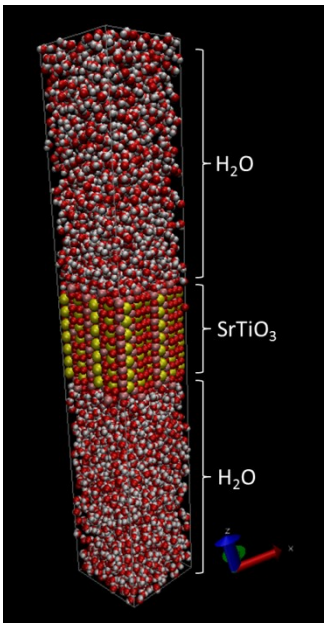

Fig.1. Simulation of a water / $SrTiO_3$ interface

In my study, I calculated the hydration structure on a $SrTiO_3$(001) surface using molecular dynamics simulations. To run the simulations, I used a molecular dynamics simulation program "LAMMPS" [1]. LAMMPS is based on Newtonian equations of motion and simulates the classical motion of atoms. The atomic coordinates, bonds, angles, pair-potentials, and thermodynamic ensembles are required to run a LAMMPS simulation. The most important parameter is the pair-potential for each atomic pair. In the system of water and $SrTiO_3$, I obtained the appropriate pair-potentials from published literature [2]. In the first step, I simulated the hydration structure for the simplest $SrTiO_3$(100) (1×1) model and successfully obtained a reasonable simulation results by using the published pair-potentials [2]. However, in experiments, I often use a reconstructed $SrTiO_3$(100) ($\sqrt{13}\times\sqrt{13}$) surface. This surface structure is much more complicated and it was difficult to obtain a stable slab model for $SrTiO_3$ ($\sqrt{13}\times\sqrt{13}$). However, by modifying the ionic charges of $SrTiO_3$, it was possible to create a stable ($\sqrt{13}\times\sqrt{13}$) slab model and obtain a reasonable hydration structure on the slab (Fig.1).

I learned many things in these three months by joining a theoretical research group. Before this visit, I found it quite challenging to understand the details in papers on theoretical surface studies. Simulating the water/$SrTiO_3$ interface on my own during this stay was very helpful for getting a much deeper understanding of what is discussed in such papers and I am planning to continue the simulation work after returning to Japan.

Life during the stay

Prof. Adam Foster's group is a part of the laboratory of Computational Nanoscience (COMP) in the department of applied physics. There were three theoretical research laboratories on the same floor of the building where I worked. Students and postdoctoral fellows belonging to different research groups share the same room and interact with each other. There were many international students and the COMP group had a very international atmosphere. It was interesting to hear about the cultures in different countries during lunchtime conversations.

In a theoretical research group, each researcher focuses on their own computer display and their own research subject. When there is a question that a student cannot solve on his own, it is easy to consult with others and more experienced people can give advice on appropriate calculation methods. Other than that, the study basically tends to become quite individual. To improve group communication Adam's group had at least one social party in a month, which was quite helpful. They enjoyed a few drinks and played various board games (Fig.2). Professors, research fellows, and students from different countries could all join to play the games, talk, and joke. I also enjoyed the parties a lot.

Fig.2. Photo of a monthly party.

Fig.3. Photo of a Finnish forest.

I also had an opportunity to join a Finnish language class. It was really interesting to study Finnish in English. The lecture style was focusing on improving our communication skills. It was also a good chance to reflect on the style of English lectures in schools in Japan.

Finland is a country with a rich nature, where 70% of the country is covered by forests and 10% by lakes and seas. I walked in a forest (Fig.3) and enjoyed taking a sauna on holidays. In particular, it was an exciting experience to go to a sauna (80°C) until the sweat comes out and then jump into a lake (0°C) that is frozen on the surface. I missed Japanese food during the stay, but the traditional Finnish foods, especially the salmon soup and the reindeer meat, were quite delicious.

Acknowledgements

I appreciate the MERIT program for giving me a valuable experience of studying abroad. I am grateful to Prof. Adam Foster and his colleagues for accepting me in their laboratory. I am especially grateful to Dr. Peter Spijker who helped me a lot with the simulations and gave me a lot of valuable advice during the stay. I also appreciate Prof. Hiroshi Onishi in Kobe University and my supervisor Prof. Mikk Lippmaa for helping to prepare the trip to Finland.

References

[1] http://lammps.sandia.gov/index.html (LAMMPS)

[2] S.I. Lukyanov *et al.*, *Surf. Sci.* **611**, 10-24 (2013).