Report of 2019　MERIT internship

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Accepting company：Nissan ARC Co., ltd., Analysis PF Department, Device analysis Laboratory

Training period：2019/9/16-2019/11/15

Research theme：　Density Functional Theory (DFT) analysis on surface and interface

Purpose：　Nissan ARC Co., Ltd. has a high level of technical power in computational materials science and has achieved results applying electrochemical interface system analysis technology based on first-principles calculations to lithium-ion battery materials. Through a two-month internship at this company, I aimed to learn large-scale DFT analysis techniques, to gain deep insight into computational materials science, and to experience styles of company's R&D positions.

Results and discussion：

Lithium-ion batteries (LIB) are important functional materials for realizing the IoT society that are equipped with electric vehicles as well as electronic devices such as smartphones. However, dissolution of Mn into the electrolyte in $LiMn_2O_4$, a LIB cathode material often used in electric vehicles, is known as one of the causes of battery deterioration. Therefore, establishment of a method for suppressing dissolution of Mn is desired for extending the life of the battery.

In this study, microscopic simulation of the positive electrode / electrolyte interface of LIB was performed using the ESM-RISM (Effective screening medium – Reference interaction site model) method in which the electrode is treated by DFT and the electrolyte is treated by classical solution theory. The analysis of the mechanism of Mn dissolution process into the electrolyte and the guidelines for suppression of dissolution were discussed.

First, a positive electrode material surface model was created using Materials Studio owned by Nissan ARC, and the ESM-RISM method implemented PWscf package was used for calculation by using a supercomputer. The electrolyte introduced $LiPF_6$ and ethylene carbonate (EC) molecules at a concentration of 1M, respectively. Here, the ESM-RISM method implements a constant-μ method that can set the electrode potential (electron chemical potential) as a parameter. The reaction at a potential of zero charge and an equilibrium potential was reproduced. From the analysis, active barrier and charge transfer of the dissolved Mn ions were considered.

As a result of simulating the process of dissolution of Mn from the positive electrode material,

it was found that the dissolved Mn became divalent ions. Moreover, when the ground potential of the dissolved process was plotted, two activation barriers derived from Mn dissolution were confirmed. To investigate the origin of these activation barriers, the distribution of RISM was analyzed from the converged electronic structure. As a result, it was found that the first barrier is a barrier due to nearest octahedrally coordinated oxygen, and the second barrier is a barrier due to the electric double layer induced on the electrode surface.

Impression：

Through this internship, I think that the above objectives have been achieved. In particular, the model for which I was assigned had a lot of conditions that had to be taken into account, and the convergence of the calculation was extremely difficult. For that reason, I was not getting the results I wanted, but I was bothering my head, but if I thought positively, I was able to reconsider the conditions that I had never looked at so far, and reconsidered them one by one. I think that the knowledge and skills of computational science have been greatly improved. In addition, discussions with the same talented team members were very meaningful and I learned a lot. When I had many things to do, my supervisor told “Decide on priorities to do and proceed from the ones that are likely to produce important results.” There was also a sense of speed unique to company’s R&D positions. I have tried to do it first rather than asking to people, so the style of asking anything before executing is fresh, and the strategy of doing business efficiently would be useful on conducting my future research.

Acknowledgement：

During the 2 month internship program, I was very thankful to Dr. Ohwaki, Dr. Ishino, and Dr. Ikeshoji in Nissan ARC, Co., Ltd.. I was also very grateful to the Secretariat for Professional development Consortium for Computational Materials Scientists (PCoMS), who has made efforts to introduce the company and adjust the accommodations for 2 months internship program. I am also grateful for the Materials Education program for the future leader in Research Industry and Technology (MERIT), which gave me an opportunity that I would not be able to experience in an ordinary doctoral program. Finally, I would like to express my deep appreciation to my supervisor, Prof. Kimura, who allowed me the internship for two months.