Internship Report

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company	Nissan ARC, Ltd.
department	device analysis
period	October 16 2017-December 15 2017
subject	simulation of electrode-electrolyte interfaces

Backgrounds

For the further spread of electric vehicles, it is highly required now to improve the safety and power density of lithium-ion secondary batteries. All-solid lithium ion batteries, where one employs solid-state electrolytes, are being intensively developed. They are free of liquid leakage and volatilizing materials, leading to the drastic reduction of combustion risk. Further, since they do not include a separator, they are expected to have improved output densities. Researches toward all-solid-state batteries with the advantages above are conducted by automakers all over the world in order to realize the safety and a long cruising distance of electric vehicles.

During the internship, we studied systems composed of a metal anode and a solid electrode in an all-solid lithium ion battery by using first principle calculation. There are two important properties of all-solid batteries; ionic conductivity and electrochemical window, that is, the range of voltage against which the materials are stable. These characteristics of individual materials are naturally important, but equally those on interfaces, if one considers that batteries are always composite systems. It is not easy, however, to experimentally observe solid-solid interfaces in detail and *in situ*. To understand such systems, simulations in real space will play an important role.

Simulations and results

After I learned how to use the softwares and simulation codes employed in Nissan ARC, I applied the softwares to construct simulation models, and utilized the codes for geometry optimizations and molecular dynamics simulations of those models.

Analyses of the simulation results revealed that the structure and reaction rate on interfaces widely vary depending on the anode material. For a certain material, precursors of a solid-electrolyte interphase (SEI), which may reduce the ionic conductivity, were produced. By analyzing the charge and electronic density of states for atoms on the interfaces, we revealed the origin of such variation from the viewpoint of electrostatics and molecular orbitals.

Impressions

I was able to discuss in depth our researches with the skilled members of the department, which was quite meaningful. Moreover, I saw people who had taken a PhD or even a postdoc and then succeeded in industry. Not only did these experiences encourage me, but they also made me notice that I should think about my career plan without any bias for academia and industry. After finishing the internship, I feel that I have much more future paths than previously because I have learned not only the simulation techniques of classical systems but also quantum ones.

Acknowledgments

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