The 97th GREEN Seminar

Digital-Twin Battery Modeling and Simulations for Understanding the Structural, Electrochemical, and Mechanical Behaviors of Next-Generation Batteries

Chair: Dr. Toshihiko Mandai (GREEN)

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Digital-twin-driven 3D modeling is very useful and impactful in understanding sophisticated composite electrodes for next-generation batteries. Once 3D structures are generated with reasonable resolution, they can be utilized to analyze structural, electrochemical, and mechanical behaviors in various conditions like mechanical roll pressing and electrochemical testing. However, the first hurdle is how to generate 3D structures as precise as possible through reconstructing the actual electrodes or creating virtual electrodes with limitedly provided information. Furthermore, depending on available time and computing resources, we have to choose the best method for specific system.

In this work, we will first introduce how the digital-twin 3D modeling has been utilized for all-solid-state battery studies: visualizing the microstructures of composite electrodes; quantifying specific contact area between electrode components; calculating effective electronic or ionic conductivity; and simulating voltage profiles, overpotentials, and lithium ion concentrations during cycling. And then, we will present that mechanical behaviors of single electrode particle can be also simulated successfully with digital-twin-driven 3D structure during charging and discharging process. Furthermore, simulations on structural deformation of composite electrodes are being compared in different manners of finite element method, finite volume method or discrete element method.

Venue: Auditorium, 1F, WPI-MANA Bldg., Namiki-site

Date: Tuesday, February 6th, 2024

Time: 10:00-12:00

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