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Multiscale Simulations of Lithium-Ion Batteries

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RCEU 2022 Project Proposal

Project Title

Multiscale Simulations of Lithium-ion Batteries

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I. Project Description

The use of lithium-ion batteries has significantly increased in electric vehicles and portable devices. However, higher energy density and fast charging still remain major challenges for this key energy storage technology. This project focuses on using model-based studies to determine the best routes to increase the energy density and fast charging capabilities of lithium-ion batteries. The energy density of a lithium-ion battery can be increased by using thicker electrodes, a design aspect that reduces electrochemically inactive battery components. However, thicker electrodes reduce the battery capacity when compared to thinner electrodes because lithium may not access all locations in the electrode during cycling. A thicker electrode also shows higher lithium-ion transport resistance when performing fast charging which creates a significant risk for lithium plating. Lithium plating poses problem related to battery performance, reliability, and safety and may result in catastrophic thermal runaway.

The Multiscale Transport and Energy Conversion group has developed lithium-ion battery models in the commercial finite element analysis software COMSOL Multiphysics. These models use existing baseline parameters and electrochemical properties to understand the effect of thickness, microstructure, and electrode geometry on battery energy density and fast charging capability. These modeling efforts are now being expanded to explore connections between battery performance, microstructure, and electrode shape.

II. Student Duties, Contributions, and Outcomes

a. Specific Student Duties

The student researcher will perform model-based analysis for this project using the open-source microstructure simulation software MATBOX, developed by the National Renewable Energy Laboratory, and the commercial finite element analysis software COMSOL Multiphysics. Simulation activities will be completed under the guidance of the PI and a graduate research assistant. Initially, the student will perform a brief literature review to assess and update the baseline parameters and electrochemical properties of lithium-ion battery materials. An initial set of sources will be provided. The student will be tasked with finding 4-5 additional journal papers related to the papers provided, and a brief review of these papers will be completed. Following the literature review the student will use the baseline parameters to generate thin and thick electrode microstructure geometry using MATBOX. Once the microstructure generation is completed the student researcher will apply characterization tools in MATBOX to extract average microstructural property data. This data will be used to perform battery simulations under varied charging conditions using a previously developed model in COMSOL Multiphysics. Depending on progress in the above tasks, the student researcher will develop their own set of electrode microstructures by tuning the microstructure parameters like electrode thickness, porosity, active material volume fraction, particle size and shape. Once the model-based studies are completed the student researcher will assist in developing a detailed report which may be used to support future publications.

b. Tangible Contributions by the Student to the Project *(10% of Review)*

The student will simulate a set of battery microstructures, analyze the synthetic microstructures, perform finite element analysis, and process data resulting from simulation efforts. The faculty advisor, graduate research assistant, and the selected RCEU student will develop an experimental plan for a set of studies that fit within the broader context of this research effort. In addition to these project specific contributions, the student will contribute to a potential publication related to the supported work.

c. Specific Outcomes Provided by the Project to the Student *(30% of Review)*

Several benefits can be expected from completion of this project. In the first task the student researcher will be introduced to the basics of literature reviews for research purposes. The selected student will receive training in characterization of image-based microstructures and the execution of finite element analysis models. This training will include improve the student's capabilities with Matlab and familiarize them with the use of a commercial finite element analysis software. In addition to these outcomes, the student will receive training in the documentation and presentation of research results and an introduction to fundamental concepts related to electrochemical energy storage.

III. Student Selection Criteria

Rising junior or higher standing is preferred for participation in this project. Experience with CAD software, Matlab, or Python is preferred.

IV. Project Mentorship *(30% of Review)*

The student researcher will work with the above faculty mentor and a graduate research assistant on the above project. The student researcher will have daily contact with the graduate research assistant during a standard work week. The student researcher will have several interactions with the faculty mentor during the week as well. These interactions will include a weekly one-on-one meeting with the faculty mentor, monthly research group meetings, and regular office work sessions with the faculty mentor and graduate research assistant present.

During one-on-one meetings the student researcher will be expected to provide a brief weekly update on progress, challenges, and plans for the coming week. Additional discussion of research methods and career interests will be handled during these meetings as well. At the end of the first three weeks of the research project the student will be expected to provide a brief presentation on their literature review efforts and planned activities for the remainder of the summer. This presentation will be given at a broader research group meeting. At the end of the summer, the student researcher will be expected to provide a presentation to the research group summarizing their efforts and findings.