Advancing Manufacturing Science and Technology through Convergence and Big Data Analytics for Lithium Ion Batteries and Beyond

Basic Idea

In the past 30 years, much progress has been made in discovering new material compositions and structures for lithium ion batteries (LIBs), resulting in a growing number of publications that proclaimed, based usually on laboratory scale experiments, significantly increased specific energy and specific power, as well as prolonged cycle life of LIB electrodes. In contrast, there is little change in the way LIBs are manufactured. It has been recognized, however, that advances in battery manufacturing science and technology can significantly reduce the cost and improve the quality of LIBs for applications ranging from potable electronics, electric vehicles, to stationary energy storage systems.

The proposed project aims at accelerating the pace of manufacturing science and technology through convergence and big data analytics. Taking a convergence approach of integration of historically distinct disciplines and technologies, relatively mature manufacturing methods in membrane fabrication and dry powder paint industries will be further investigated and translated to fabricate battery electrodes with the goal of significantly reducing the cost and environmental impact of battery manufacturing. Taking the advantage of a large amount of data in battery materials characterization, testing, and modeling, methods in big data analytics will be used and, if necessary, developed to establish processing-structure-property-performance relationships with the goal of shortening the time to turn laboratory innovations into products. Since a convergence process typically is followed by a process of divergence, the knowledge and methodologies developed through the convergence and big data analytics approach to battery manufacturing are expected to further advance manufacturing science and technology in diverse fields, including membrane and paint industries.

The basic ideas/hypotheses of this proposal, illustrated in Figure1, are:

(1) Significant reduction in the cost and environmental impact of battery manufacturing can be made by translating and improving manufacturing technologies used in other more mature fields, such as membrane manufacturing and dry powder paint industry.
(2) Shortening the duration between discoveries made in the lab and manufactured products can be accomplished using big data analytics and knowledge discovery to establish the relationships between processing parameters and the performance of LIBs.
(3) The approaches and methodologies developed in this project are general and applicable to manufacturing of other products, including selective and reactive membranes and multi-functional and self-healing paint.

The project is expected to help Kentucky (KY) become not only a leader in battery materials research but also in battery manufacturing which is crucial to maintaining and growing KY's automobile industry - the third largest in the US in terms of number of vehicles produced annually. While LIBs are mainly produced in Asia, a recent study found that the total cost of making LIBs in the US and China is comparable because battery manufacturing processes are highly automated. Furthermore, battery manufacturers want to be near their R&D facilities and close to their ultimate consumers in the US. Since the proposal seeks to further reduce the cost of battery manufacturing, the project is expected to help establish domestic battery manufacturing plants and create jobs. The project will also help advance two of the "Ten Big Ideas for Future NSF Investments," namely "Harnessing Data for 21st Century Science and Engineering" and "Growing Convergent Research."

Background and motivation

With strong support from NSF, DOE, and the automobile industry, KY has made, in the past ten years, significant progress in battery materials research and established unique battery R&D capabilities, including scale-up battery cell fabrication and characterization facilities. Specifically, KY researchers have developed nanostructured silicon-based electrodes with theoretical capacity ten-times larger than that of the graphite electrodes used in today's LIBs. Much progress has also been made in developing high power electrochemical capacitors based on graphene and biomass-derived high surface area porous carbon. A wide range of materials characterization tools and electrochemical test instruments have been acquired for battery research. In addition to making and testing coin cells, a complete pouch cell fabrication line has recently been installed in a unique dry room facility at the Center for Applied Energy Research for battery scale-up and manufacturing R&D. Recently, KY researchers have demonstrated the possibility of translating manufacturing processes used in membrane and dry powder paint industries to battery manufacturing with the potential of significantly reducing the cost and environmental impact. Coupled with innovative thermal processing and atmosphere plasma processing, the possibility of revolutionizing battery manufacturing by converging three distinct technologies, e.g., membrane manufacturing, dry powder coating, and intense light and plasma processing, forms a meaningful and reachable goal for this proposed project. If successful, the project will make the conventional wet slurry mixing and casting process of making battery electrodes obsolete, eliminating the cost and environmental impact associated with the use and release of toxic organic solvents and chemicals, and making high energy and high powder density, fast-charging electrodes that cannot be made by the conventional wet manufacturing method.

To accelerate the pace of materials discovery to manufactured products, the project incorporates the latest advances in Materials Informatics and Big Data, known in some literature as the "Fourth Paradigm" of materials science.[1] More specifically, the Big Data and Knowledge Discovery techniques can help reveal the processing-structure-property-performance relationships by performing "inverse analysis" with measured data on performance, property, and structure of materials as inputs and processing parameters as output.[1] Battery manufacturing research is particularly suited for this kind of inverse analysis because there is much information obtained during battery testing, e.g., the voltage *vs.* capacity, capacity *vs.* cycle number, and capacity *vs.* charge rate. Detailed information on the structure and composition of battery materials can also be obtained using a range of characterization tools, such as optical microscopy, focused ion beam (FIB)/scanning electron microscopy (SEM), transmission electron microscopy (TEM), x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), x-ray micro-tomography (micro-CT), and *in situ* nanoindentation that provide unprecedented details on the structure and composition, as well as mechanical and electrochemical properties of battery materials. By employing *in situ* vibrational spectroscopic techniques (e.g., Raman and FT-IR) at the interface between battery electrode and electrolyte, battery degradation mechanisms and irreversibly formed electrochemical products can be tracked. Atomic-scale and nanoscale chemical information, morphology, and interfacial chemistry can be investigated by integrating surface-enhanced Raman spectroscopy (SERS) and atomic force microscopy (AFM) characterization. The vast data generated from battery testing and structural characterization provide a fertile ground for applying Materials Informatics and Big Data analytics techniques, such as Bayesian inference, principal component analysis, and machine learning, to uncover the engineering relationships that are necessary for designing and optimizing manufacturing processes.

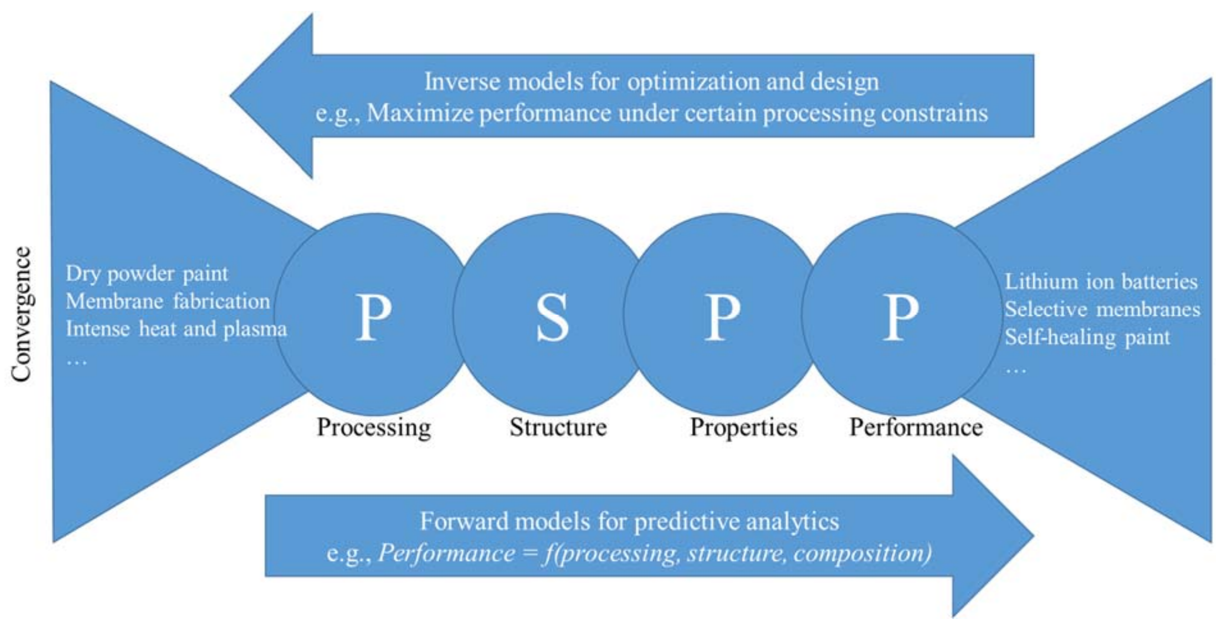

Figure 1. Convergence and Big Data Analytics approach to manufacturing batteries and beyond (adopted and modified from ref. [1])

1 Ankit Agrawal and Alok Choudhary, "Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science," APL Materials **4** (5), 053208 (2016).