Computational Process Material Design Simulation of the Slurry Coating Process

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Objectives
Fuel cell and Li-ion battery electrodes are made by a slurry coating process. The slurry coating is a process to obtain a porous structure by evaporating the solvent from a slurry containing small particles and the polymer. The process has been widely used, and also has great influence on the electrode performance. Since what is happening during the process is not well understood, the coating is carried out by trial and error on the basis of experiences. This is the reason that there is no methodology that can deal with the material and drying process. Therefore, we developed the simulation model to deal with the material at molecular level and the evaporation of the solvent, and the model was applied to investigate the phenomena of the coating process and also to increase the electrode performance.

Outline of Results
The solvent-evaporation model was developed by using coarse-grained molecular dynamics, which includes molecular-scale information. Large-scale calculation on the K computer made it possible to calculate the slurry coating process directly and also to predict porous structure. After the solvent evaporation, by connecting the porous structure obtained by molecular simulation with macro CAE seamlessly, electrode performance was able to be evaluated. As a verification, the developed method was applied to positive electrode of catalyst layer in the fuel cell, and we confirmed qualitative agreement with experimental results, in regard to polymer coverage of small particles and diffusion property of oxygen gas. In order to investigate slurry coating phenomena, the effect of material properties and process conditions on porous structures were also discussed.