



Influence of inter-particle resistance between active materials on the discharge characteristics of the positive electrode of lithium ion batteries

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ABSTRACT

We conducted multi-physics simulations of a composite electrode for lithium ion batteries (LIBs), considering four distinct electrode components as well as inter-particle resistance between the active materials. The physical properties of the simulation are determined by reference to well-defined single particle measurements from the literature, thereby avoiding the influence of the complex microstructure of the composite electrode as much as possible. The influence of inter-particle resistance between the active materials is explored to determine its influence on the discharge properties of the electrode.

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1. Introduction

Lithium ion batteries (LIBs) are playing key roles in many application systems such as mobile phones, laptop computers, and automobiles. Further, the application of LIBs to counter the unstable output from intermittent renewable energy systems is emerging as an important area of research and development [1]. In automobile applications, it is important to achieve both high storage density per unit weight for lighter vehicle weight and high output power density for acceleration. For this purpose, one valuable strategy is to design the microstructure of composite electrodes as well as to design materials or interfaces with superior properties. Because designing the inherently complex electrode microstructure is a significant engineering challenge, the empirical trial-and-error approach has been conventionally used to fabricate microstructures with superior properties. In this regard, much effort has been

invested in the rational design of LIB electrode microstructures [2–18]. In particular, Newman's model has been recognized as a pioneering work in this field [2–5]. While the model considers three components—active material, electrolyte, and electron conductive material—their microstructures are implicit in their one-dimensional or pseudo-two-dimensional models, thus further development is warranted. In terms of structural modeling, ordered or random packing is often an effective approach [6–11]. Goldin et al. have carefully discussed the influence of microstructure on the discharge characteristics of LIBs based on the electrode structures represented as orderly packed spheres [9]. Latz and Zausch have performed a multi-scale simulation of LIBs using a three-dimensional (3D) structure model based on the homogenization method [10]. Further extension of the modeling approach includes a stochastic modeling approach that enables reconstruction of a 3D structure from a two-dimensional image obtained from, for example, scanning electron microscopy [12]. Recent developments in X-ray tomography and FIB-SEM (focused-ion beam scanning electron microscopy) methods have enabled us to access 3D electrode models reconstructed from observations of real electrodes [13–20]. However, while active materials can be well distinct from the other phases in such a reconstruction approach, it is difficult to

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have good contrast for carbon-containing regions such as the electrolyte, conductive carbon, and binder. Because the charge-discharge characteristics of single particle of active materials are superior to actual multi-component electrodes [21–27], for example 75% capacity has been reported to be retained even at a high discharge rate of ca. 300C [24], explicit consideration of each component material in the simulation of a composite electrode is important to identify the knowledge gap between characteristics of ideal single particle electrodes and practical composite electrodes. As a first step to identify factors determining the characteristics of practical multi-component electrodes, we investigated the influence of inter-particle resistance between active materials on the discharge characteristics of a positive electrode consisting of four different phases. To avoid the difficulty in identifying the grain boundaries in the 3D reconstructed structures, we have started our effort using an artificial model constructed by packing particles of component materials represented by model shapes.

2. Computational details

2.1. Modeling the three-dimensional electrode structure

In this study we only focused on the microstructure of the positive electrode, assuming a larger capacity and faster kinetics of the negative electrode. Fig. 1 illustrates our schematic modeling process for an LIB positive electrode. First, spherical particles representing the active materials are randomly inserted into a cell with a specified volume ratio by using a porous structure simulator [6,8,28–30], as shown in Fig. 1(a). Note that particle overlap is permitted up to a specified ratio. Next, conductive carbon with a hexagonal planar shape is inserted into the cell (Fig. 1(b)). The

conductive carbon is placed on the surface of an active material or a conductive carbon randomly selected from those already inserted. The binder is then inserted onto a randomly selected surface of the active material, conductive carbon, or binder, as done with the conductive carbon (Fig. 1(c)). While the porous structure simulator [8] can generate structures comprising various particle shapes, we adopted a spherical active material and a hexagonal planar carbon to reduce the computational cost, as such complex particle structures require fine meshing, which is computationally demanding. In this study we treated the binder as an inhibition domain that does not contribute to lithium ion diffusion or electron conduction. For simplicity, the binder is represented as spherical particles. The pore region remaining after insertion of the binder particles is treated as the electrolyte phase in the model. Finally, a boundary layer is inserted between all the active materials in contact, as illustrated in Fig. 1(d), to investigate the influence of resistance between the active material particles and the electrode characteristics. Here, the boundary layer is represented as a disk with a thickness of $0.4\ \mu\text{m}$, which is the minimum necessary thickness to ensure a continuum boundary layer with the mesh size used in the present simulations.

To simulate the multi-physics based on the modeled electrode structure, a three-dimensional mesh is necessary. The mesh model is generated following the process shown in Fig. 2. First, a two-dimensional cross-section of the model is visualized with a specified slice pitch likewise a slice & view process in the microstructure observation by FIB-SEM. Images from the slice & view process are processed by a computer to reconstruct a 3D voxel model, which is further processed to a 3D mesh model suitable for the finite element simulations. A typical number of meshes is ca. 200,000 for a model size of $30 \times 30 \times 30\ \mu\text{m}^3$.

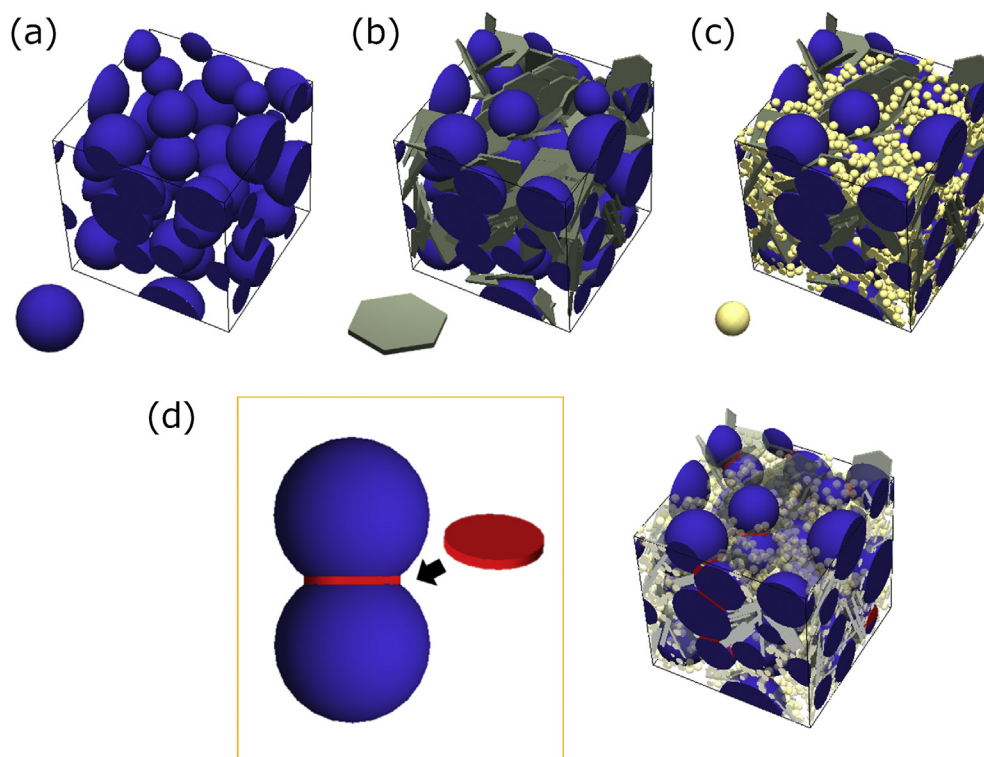


Fig. 1. Structure models at each step of modeling the three-dimensional LIB positive electrode for the finite element simulations: (a) Active material particles inserted into the simulation cell, (b) active materials with conductive carbon, (c) active material particles with conductive carbon and binder, and (d) the boundary layer inserted between active materials.

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