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Microstructural Modeling and Design of Rechargeable Lithium Ion Batteries

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The properties of rechargeable lithium ion batteries are determined by the electrochemical and kinetic properties of their constituent materials as well as their underlying microstructure. Microstructural parameters such as lithium manganese oxide particle volume fraction and particle size distribution affect the power and energy density of the system. Prediction of the macroscopic response requires a model that incorporates the details of the microscopic arrangement of materials and treats pertinent spatial and crystallographic aspects of microstructure. Furthermore, models should account for coupled material effects such as stress development and local concentration changes. We have developed a method that uses microscopic information and constitutive material properties to calculate the macroscopic response of rechargeable lithium ion batteries (See Figures 1, 2, and 3). Previous attempts of incorporating microstructural effects on the properties of batteries have used mean-field approaches; such calculations will not capture potentially important effects such as localized electric shielding, stress development, or heat dissipation. The technique is demonstrated for a typical lithium-ion battery microstructure and demonstrates the beneficial effect of microstructural design on the compromise between power density and capacity.

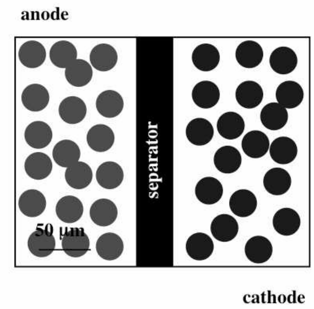

Figure 1. Hypothetical microstructure of a typical rocking-chair battery. Left electrode corresponds to anode, right electrode corresponds to cathode, and middle layer corresponds to separator.

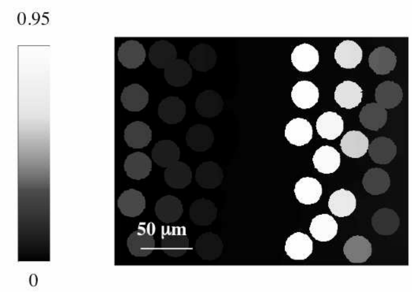

Figure 2. Normalized lithium concentration distribution for sandwich cell shown in Figure 1. Applied discharge rate corresponds to 1.5C. Lithium is extracted from anode (left) and intercalated into cathode (right). Concentration distribution corresponds to t=1560s, and is influenced by the local electrochemical potential gradients.

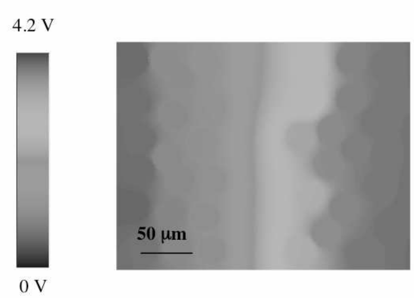

Figure 3. Predicted voltage distribution inside rocking-chair battery after 1560 seconds of galvanostatic discharge. Local electrostatic potential gradients influence the rate of intercalation at the surface of the electrode particles. Original microstructure and the corresponding lithium concentration distribution are shown in Figures 1 and 2.