Modeling Volume Expansion in Lithium-Ion Batteries

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Volume expansion is an important phenomenon observed in many electrode materials of interest to lithium-ion batteries.[1-4] As mentioned in Ref. 2, a variety of mathematical models exist in the literature describing the various aspects of lithium-ion battery behavior, but none of them include volume expansion. Recently, Botte[2] modeled volume expansion in a single electrode particle by allowing its radius to vary in proportion to the intercalation flux at the particle surface. This model assumes uniform expansion at all radial positions even though the local lithium concentrations are different.

Here, we present a rigorous volume expansion model of a single particle, treating expansion at every radial position as a function of the local lithium concentration. The figures show the predicted effect of the expansion factor, which is defined as the percentage by which the host particle expands as its lithium content changes from zero to its theoretical maximum. Fig. 1a shows the change of particle radius with time as lithium deintercalates from a carbon particle at a constant current equivalent to a 2C discharge. Since lithium content decreases during discharge the particle radius also decreases. Further, the decrease in radius is greater for higher expansion factors. The corresponding evolution of potential with time during discharge is shown in Fig. 1b. A significant increase in discharge capacity is seen with increase in expansion factor. This arises from the fact that greater the expansion factor smaller the particle size at the end of discharge, and consequently, lesser the moles of lithium remaining in the particle. This means that with increase in expansion factor more moles of lithium deintercalates resulting in greater discharge capacity.

We use the model to study the effect of volume expansion on a single particle in response to a variety of inputs (*e.g.,* current step, voltage step, linear voltage sweep). Further, we develop a methodology to estimate the lithium diffusion coefficient and the volume expansion coefficient from DC and AC polarization experiments. Finally, we incorporate the single particle model into a lithium-ion battery model and analyze its performance, especially, at high rates of discharge. In doing so, the battery model is also modified to account for electrode thickness and/or porosity changes arising due to particle expansion.

References

1. X.Wang, Y. Sone, and S. Kuwajima, *J. Electrochem. Soc.,* **151**, A273 (2004).
2. G.G. Botte, *Meeting Abstracts*, 204th ECS Fall Meeting, Orlando, Florida, October, 2003, The Electrochemical Society Inc., p.314.
3. L.M.L. Fransson, J.T. Vaughey, K. Edstrom, and M.M. Thackeray, *J. Electrochem. Soc.,* **150**, A86 (2003).
4. L. Fransson, E. Nordstrom, K. Edstrom, L. Haggstrom, J.T. Vaughey, and M.M. Thackeray, *J. Electrochem. Soc.,* **149**, A736 (2002).
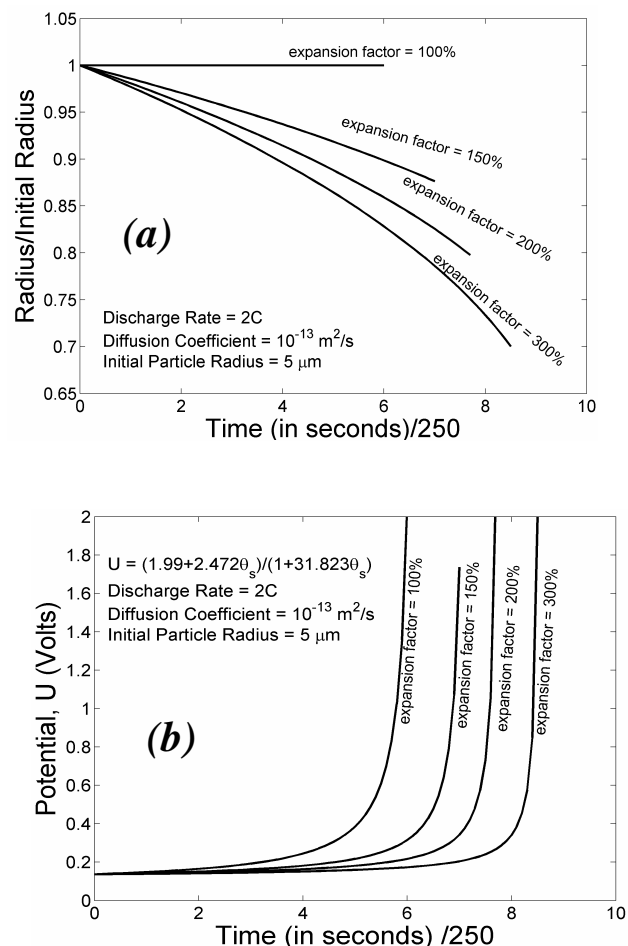
Fig. 1. The effect of expansion factor on the potential and particle radius during a 2C discharge of a single particle.