Simplified Multiphysics Model for All-Solid State Microbatteries

M.S. Nesro[1], I.M. Elfadel[1]

[1]Masdar Institute of Science and Technology, Masdar City, Abu Dhabi, UAE

Abstract

Introduction: Lithium microbatteries are replacing conventional power sources in different microsystems application areas such as wireless sensor networks and biomedical applications. In many of these application areas compact models of microbatteries are needed in the embedded power management program or during the design stage of the overall system[1,2,4]. These compact models are typically derived from physics-aware finite element descriptions. In this paper we develop a simplified Multiphysics FEM for all-solid state Li metal microbattery.

Use of COMSOL Multiphysics®: The existing all-solid state battery in the COMSOL Model Library is modified by assuming local and global electro neutrality of the solid state electrolyte[3]. This assumption will help us reduce the complex nonlinear Nernst-Plank-Poisson (NPP) equation for the electrolyte domain to a linear diffusion equation. In COMSOL Multiphysics®, the Transport of Diluted Species interface is used to model the diffusion of lithium in the electrolyte. A linear diffusion equation is used to model the transport of lithium inside the cathode both in the full nonlinear and simplified model.

Results: The simplified model uses the same battery parameters as the COMSOL Model Library full nonlinear model. Both models are solved with COMSOL Multiphysics®. The discrepancy between our model and the nonlinear model is within 5% and runs six times faster than the nonlinear model. Figure 1 shows the steady state Lithium concentration profile in the electrolyte for discharge rate of C=1.6 as a function of position. Finer meshing is required at the boundaries to decrease the maximum error due to Neumann boundary conditions imposed at the two ends of the electrolyte. Since linear diffusion equation is used in both cases, lithium concentration profile inside the cathode matches with the nonlinear full model with zero relative error.

Figure 2 shows voltage discharge profile for discharge rate for C=1.6 as a function of battery capacity in µAh. The discharge curve is within 1.5% of the full nonlinear model discharge profile. The nonlinear NPP equation accounts both for diffusion and migration components. The potential drop due to the migration term dominates near the cliff of the curve. Maximum error is observed near the cliff of the curve because the approximation was actually done to the migration term in the original nonlinear model. Similar agreement was also found for higher discharge rates. Other parameters like electrolyte potential drop, charge transfer over-potentials at the interfaces and diffusion over-potential in the cathode follow a similar trend.

Conclusion: Based on the electro neutrality assumption, our simplified model is able to predict the discharge profile of an all-solid state battery within 5% of the full nonlinear model available in the COMSOL Model Library. Such a simplified FEM model will be the basis of a compact model that can be used in embedded battery management program and in battery-circuit co-design work flow.

Reference

[1] D. Danilov, R.A.H. Niessen and P.H.L. Notten "Modeling All-Solid-State Li-Ion Batteries," J. Electrochem. Soc 158, A215-A222(2011)

[2] S.D. Fabre, D.Guy-Bouyssou, P. Bouillon, F. Le Cras, and C. Delacourt "Charge/Discharge Simulation of an All-Solid-State Thin-Film Battery Using a One-Dimensional Model," J. Electrochem. Soc 159 A104-A115(2012)

[3] D. Danilov and P.H.L. Notten "Mathematical modeling of ionic transport in the electrolyte of Li-ion batteries," Electrochimica Acta. Soc 159 5569-5578(2008)

[4] L.L.Z. Shi and G. Ceder. "Solid State thin film lithium microbatteries." http://ceder.mit.edu/publications.php,MIT Publication, 2003.

Figures used in the abstract

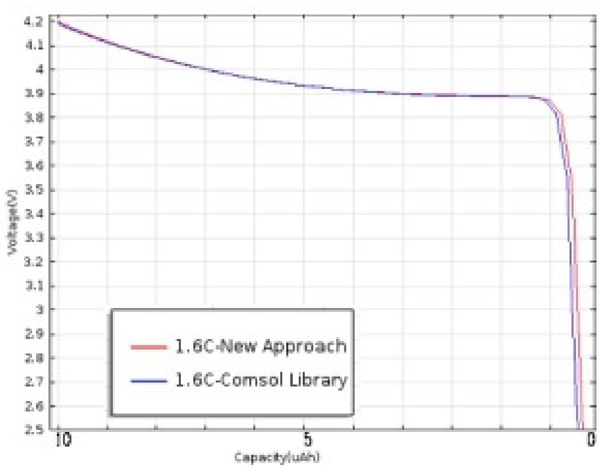

Figure 1: Concentration profile for C=1.6

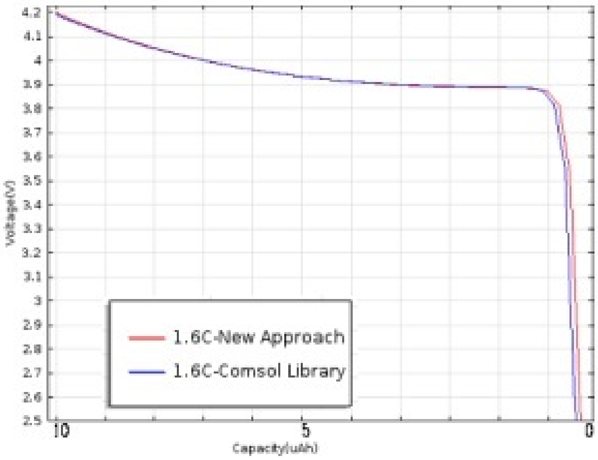
4.2
4.1
4
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3
2.9
2.8
2.7
2.6
2.5
Voltage(V)
1.6C-New Approach
1.6C-Comsol Library
10
5
0
Capacity(uAh)

Figure 2