

Accepted Manuscript

Title: Electrochemical Model for Ionic Liquid Electrolytes in Lithium Batteries

Author: Kisoo Yoo Anirudh Deshpande Soumik Banerjee
Prashanta Dutta



PII: S0013-4686(15)30070-0
DOI: <http://dx.doi.org/doi:10.1016/j.electacta.2015.07.003>
Reference: EA 25279

To appear in: *Electrochimica Acta*

Received date: 1-5-2015
Revised date: 26-6-2015
Accepted date: 1-7-2015

Please cite this article as: Kisoo Yoo, Anirudh Deshpande, Soumik Banerjee, Prashanta Dutta, Electrochemical Model for Ionic Liquid Electrolytes in Lithium Batteries, *Electrochimica Acta* <http://dx.doi.org/10.1016/j.electacta.2015.07.003>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Electrochemical Model for Ionic Liquid Electrolytes in Lithium Batteries

Kisoo Yoo, Anirudh Deshpande, Soumik Banerjee, and Prashanta Dutta^s

School of Mechanical and Materials Engineering

Washington State University, Pullman, Washington 99164-2920, USA

ABSTRACT

Room temperature ionic liquids are considered as potential electrolytes for high performance and safe lithium batteries due to their very low vapor pressure and relatively wide electrochemical and thermal stability windows. Unlike organic electrolytes, ionic liquid electrolytes are molten salts at room temperature with dissociated cations and anions. These dissociated ions interfere with the transport of lithium ions in lithium battery. In this study, a mathematical model is developed for transport of ionic components to study the performance of ionic liquid based lithium batteries. The mathematical model is based on a univalent ternary electrolyte frequently encountered in ionic liquid electrolytes of lithium batteries. Owing to the very high concentration of components in ionic liquid, the transport of lithium ions is described by the mutual diffusion phenomena using Maxwell-Stefan diffusivities, which are obtained from atomistic simulation. The model is employed to study a lithium-ion battery where the electrolyte comprises ionic liquid with mppy⁺ (*N*-methyl-*N*-propyl pyrrolidinium) cation and TFSI⁻ (bis trifluoromethanesulfonyl imide) anion. For a moderate value of reaction rate constant, the electric performance results predicted by the model are in good agreement with experimental data. We also studied the effect of porosity and thickness of separator on the performance of lithium-ion battery using this model. Numerical results indicate that low rate of lithium ion transport causes lithium depleted zone in the porous cathode regions as the porosity decreases or the length of the separator increases. The lithium depleted region is responsible for lower specific capacity in lithium-ion cells. The model presented in this study can be used for design of optimal ionic liquid electrolytes for lithium-ion and lithium-air batteries.

Keyword: Li Battery / Ionic Liquid / Ternary System

Download English Version:

<https://daneshyari.com/en/article/6610865>

Download Persian Version:

<https://daneshyari.com/article/6610865>

[Daneshyari.com](https://daneshyari.com)