Modeling Battery Performance Due to Volume Change in Porous Electrodes

Due to Intercalation

by

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The demand for energy continues to increase as the economies of developing countries become more modern and show an increased need for a reliable energy infrastructure in order to meet the increased demand associated with a large and more mobile population. An increased demand puts a strain on all sectors, however it is specifically noticeable in the transportation sector where a significant portion of the fuel utilized for transportation comes from petroleum and other fossil fuels. Recently, using alternative forms of energy for transportation has become reality, and in turn, using electricity as a transportation fuel has gained significant momentum, specifically for use in battery-only rechargeable vehicles. Significant strides have been made to improve the range, cost, and fueling times of these battery-only vehicles through the improvement of the design and control of cells, and several automobile manufacturers are releasing battery powered vehicles with price points that target the general public. New materials have also been examined in order to increase the energy densities of these batteries in order to increase the range of battery powered vehicles, and decrease the volume displacement in the vehicle powertrain.

Some of the new battery electrode materials see significant expansion during cycling, which results in stress linked to capacity fade, battery failure, separator deformation, and electrolyte degradation. In order to accurately predict the behavior of complicated electrochemical devices undergoing a variety of different structural and electrochemical changes, sophisticated models that take into consideration transport processes, electrochemical phenomena, mechanical stresses, and structural deformations must be developed in order to predict the associated effects on the operation of an electrochemical system. There are many models in the literature that can predict the electrochemical performance of devices with porous electrodes under a variety of operating and design conditions, however, in many of these models, when the porosity of the porous electrode is accounted for it is assumed to be a function of current density, since the volume changes seen during the intercalation reaction can be small. However, electrodes that have been developed in recent years show battery systems that have significant volume changes during intercalation. The battery model developed here incorporates aspects of a porous electrode model that accounts for the stresses that build up in porous electrodes due to volume change in the active material. The material balances here are coupled to stress-strain relationships that are derived from rock mechanics, in which the deformation of the porous rock occurs during thermal expansion similar to the deformation of the porous electrode that occurs during intercalation. This allows for a prediction of dimensional changes and porosity changes in a porous electrode and the associated effect on battery performance.