Electrochemical modeling of insertion/extraction reactions of Mg in Mg/Bi electrode

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A rechargeable magnesium cell, using magnesium metal as anode active material is expected to be a potential candidate for high energy density battery systems due to (1) a high specific capacity (3833 $mAhcm^{-3}$) owing to the two electron transfer reaction of the electrodeposition / dissolution of magnesium and (2) high cell voltage owing to the low equilibrium electrode potential of magnesium (-2.356 V vs. SHE) compared with other multivalent metal such as zinc (-0.763 V vs. SHE) or aluminum (-1.676 V vs. SHE). Recently it was reported in literature [1] that electrochemically deposited magnesium does not form dendrite as lithium in Li-ion cells under the same condition. This result suggests that magnesium metal may also have advantage as an anode active material for a high-energy secondary battery system in terms of cycle life and safety. However the rechargeable magnesium cell system has a number of challenges in terms of power density, rate capability, cycle life, calendar life, etc..

In this study, bismuth is used for magnesium insertion/extraction reactions. The physical and electrochemical properties of Mg organohaloaluminate electrolyte such as diffusion constant of Mg^{2+} ion, ionic conductivity of the electrolyte, transference number, and activation energy of the magnesium deposition/dissolution are estimated from experiments. In addition, the electronic conductivity, particle size, electrode porosity, and solid-state diffusion of magnesium into bismuth needed for the modeling studies are also estimated from experiments.

The existing porous electrode model [2] developed for Li-ion cell is extended in the proposed study to describe the behavior of the magnesium during charge-discharge reactions. This model is further modified to include structural information and experimentally evaluated parameters such as microstructure, internal resistance, electrode kinetics, thermodynamics, and diffusion of magnesium in the active particles.

This electrochemical model, modified with the estimated parameters for Mg electrolyte and Bi/Mg electrodes as input, was used to predict the electrochemical performance of the Bi/Mg anode cell as shown in Figure 1. Details of the electrochemical performance and the factors that govern the performance of the Bi/Mg cell will be discussed in the presentation.

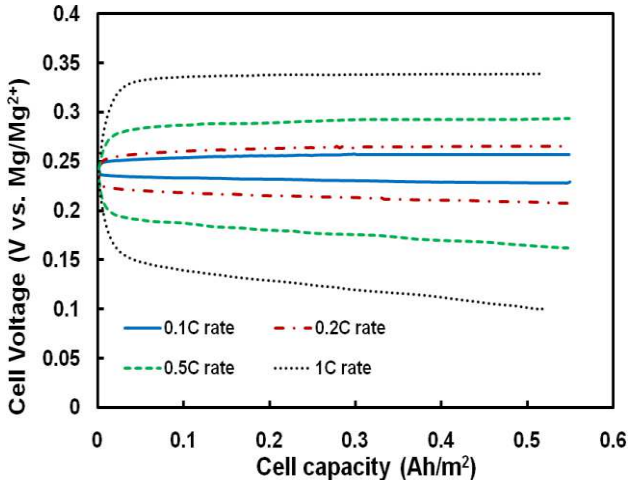

Figure 1. Electrochemical modeling of performance of the Mg insertion anode at different discharge/charge rates.

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References:

1. M. Masaki, J. Power Sour., **196** (2011) 7048-7055.

2. M. Doyle, and J. Newman, J. Electrochem. Soc.,**143** (1996) 1890-1903.