Mathematical Modeling of Ni/H₂ and Li-Ion Batteries

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Analysis of Battery Systems
Capacity loss on cycling
Hysteresis between charge and discharge
Self-discharge rates (i.e. oxygen-evolution kinetics)
Diffusion coefficients of protons
Experimental characterization of Nickel Hydroxide
Impregnation of porous electrodes
Deposition rates of thin films
Electrochemical Deposition of Nickel Hydroxide

Modeling Effort
Modeling Effort

- Experimental Verification of Integrated Systems Model
- Integrated Power System Models for Satellites
- Experimental Verification of the Li-Ion Battery Model
- Mathematical Modeling of Li-Ion Batteries
- Experimental Verification of the Ni/H² Battery Model
- Mathematical Modeling of Ni/H² Batteries
Schematic of Ni/H₂ Battery
Proton Diffusion Coefficient
Utilization of the NIOOH
Utilization of the NIOOH
Potato Intercalation/Extraction
Boundary and Scanning Curves During
Potential (mV) vs. Ag/AgCl

The History-Dependent Path of the Ni Electrode
Potential (V) vs Ag/AgCl

Internal Hysteresis Loops in The Ni Electrode
Potential (mV) vs. Ag/AgCl
Nickel Hydroxide

Crystal Structures for
\[
\frac{\text{total number of \( \text{Ni} \) lattice sites}}{\text{number of interlamellar protons}} = 2 - z
\]

\[
\frac{\text{total number of \( \text{Ni} \) lattice sites}}{\text{number of water molecules}} = X
\]

\[
\frac{\text{number of \( \text{Ni} \) vacancies not occupied by \( K^+ \)}}{\text{number of \( H^+ \)}} = u
\]

\[
\frac{\text{number of \( \text{Ni} \) vacancies occupied by \( K^+ \)}}{\text{number of \( \text{Ni} \) vacancies}} = X
\]

![Diagram of Nickel Hydroxide Electrode]

Nickel Hydroxide Electrode

Detect Representation of the
\[
\begin{align*}
\left[\frac{(1x-I)}{(1\lambda - 1x)^1u - 1\lambda - 2} - \frac{(\zeta x - I)}{2(\zeta x - 1x)^2u - \zeta x - 2}\right] = \gamma \\
\left[\frac{(1x-I)}{1\lambda} - \frac{(\zeta x - I)}{\zeta \lambda}\right] = \zeta \gamma \\
\frac{\zeta x - I}{I - (\zeta x - 1x)^2u} - \frac{(1x-I)}{(1\lambda - 1x)^1u} = \varepsilon \gamma \\
\left[\frac{(\zeta x - I)}{\varepsilon - (\zeta x - 1x)^2u} - \frac{(1x-I)}{2 - (1\lambda - 1x)^1u}\right] = 1\gamma
\end{align*}
\]

\[
\begin{align*}
-\Theta^\gamma + \Theta^\gamma \cdot \Theta^\gamma + \Theta^\gamma \cdot \Theta^\gamma \\
\begin{bmatrix}
\frac{\zeta x - I}{1} & \frac{\zeta x - I}{1} & \frac{(\zeta x - I)}{\zeta \lambda} \\
\frac{\zeta x - I}{\zeta \lambda - \zeta x} & \frac{(\zeta x - I)}{\zeta \lambda} & \Theta^\gamma \cdot \Theta^\gamma \\
\Theta^\gamma \cdot \Theta^\gamma & \Theta^\gamma \cdot \Theta^\gamma & \Theta^\gamma \cdot \Theta^\gamma \\
\end{bmatrix}
\end{align*}
\]

Nickel Hydroxide Redox Reaction
As described by the Defect Model

Redox Reactions In the Nickel Electrode
Simulated Charge/Discharge of a Ni-H₂ Cell

Concentration of KOH (M)

Voltage (V)

Time (h)

2x-3y cycle

x=0.25

2x-3y cycle

x=0.11

No defects
Cell Potential with T/W Data
Comparison of Model Predicted
Cell Temperature With TRV Data

Comparison of Model Predicted
Cell Pressure with TRW Data
Comparison of Model Predicted
LI-Ion Cell with 1.25 M Initial Salt Concentration

Experimental and Simulated Discharge Curves for a
Li-Ion Cell with 0.5 M Initial Salt Concentration

Experimental & Simulated Discharge Curves for a
Lithium Cell with 0.25 M Initial Salt Concentration
Experimental & Simulated Discharge Curves for a
Investigate the optimal design of hybrid power systems for use in mobile systems.

Project Objectives
And at a detail level

VTB supports analysis at the system level
The VTB is a highly interactive environment for collaborative design and virtual prototyping of advanced power systems.
amplifying user knowledge at every step
stovepipe work threadling (by capturing and
distributed team work (and eliminates
V TB facilitates interdisciplinary and
Collaborators

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