Modelling of Lithium Cells using Multi-Gene Genetic Programming

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Abstract
The effect of some electro-physical parameters on the open circuit cell voltage of a Lithium-ion cell composed of $LiFePO_4$ as cathode and $Li_4Ti_5O_{12}$ as anode electrodes were investigated. The electrodes were prepared using local material (starch) as carbon source and domestic microwave oven. The electro-physical parameters studied include the current, capacity, specific capacity and energy. A mathematical model describing the influences of the aforementioned parameters was then generated using an evolutionary optimization and artificial intelligence technique called the Multi Gene Genetic Programming (MGGP).

Keywords: *Lithium-ion cells; cell voltage; charge current; capacity; specific capacity; energy; Multi gene genetic programming*

Introduction

Lithium-ion batteries are very valuable energy storage devices which have found applications in various fields such as electronic devices, electric and hybrid electric vehicles as well as renewable power resources. Cell voltages of Lithium-ion cells range from 1.5 to 3.7V, with primary applications as power sources for mobile phones, digital camera, laptop computers and many other portable electronic devices [1]. Lithium ion batteries are seen to be the best option for effective electrical energy storage as it offers high energy density, high operating voltage, ideal for use in electric vehicles [2, 3]. It has also been said to have long cycle life, and abuse tolerant properties [4, 5].

Goodenough proposed the use of $LiFePO_4$ as an alternative cathode material due to its low cost and environmental compatibility [6]. However, studies have shown that cells designed based on $LiFePO_4$ technology have not shown the ability to deliver high specific capacity at high discharge rates [7]. The rate capabilities of $LiFePO_4$ are limited by its intrinsically poor electronic conductivity which is in the range 10^{-9} Scm^{-1} to 10^{-10} Scm^{-1} and low rate of Li^+ transport within the micrometer-sized particles [8]. Improving energy efficiency and life span of Li-ion batteries has thus become the main focus of battery design.

Multi gene genetic programming (MGGP) is an artificial intelligence evolutionary computing optimization and modeling technique, derived from genetic programming and is widely used by academic researchers and industry. Genetic programming is a capable AI technology that allows computers program themselves leading to the automated synthesis of code and discovery of novel models. MGGP was invented by [9] and has been applied to fields such as mathematical modeling of chemical compounds, solar insolation predictions and modeling [10], and Educational Data Mining (EDM) [11]. Thus, it offers very good promises as a future computational intelligence technique for the discovery of novel models and expressions.

In this paper, we present some experimental details in our attempt to synthesize a composition of Lithium-ion cell and also the derivation of suitable model for the cell voltage performance analysis of the developed Lithium-ion cell using the MGGP approach.

Experimental Details

A combined technique of carbon-coating and microwave assisted hydrothermal method was used to produce electro-active $LiFePO_4$/C and $Li_4Ti_5O_{12}$/C material, at room temperature and without the use of inert (Ar.) gas, using home-made starch as the carbon source. The procedure is illustrated in figure 1.

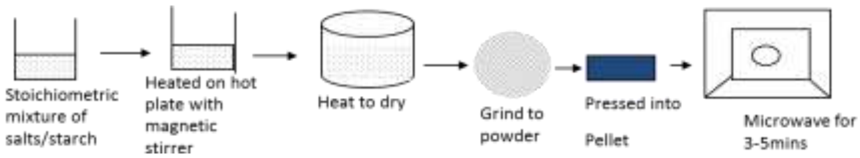

Figure 1 schematic representation of synthesis of electrode materials

Electrode preparation

A slurry of the active materials was prepared. Polyvinylidene fluoride (PVDF) binder was thoroughly dissolved in dimethyl formadime using magnetic stirrer.

Table 1: Electrode Composition

Electrode	Active Material	Activated Carbon	Binder	Dimethyl Formadime	Composite
	Mg	Mg	Mg	Mg	Mg
Cathode ($LiFePO_4$)	1.602 (80%)	0.202 (10%)	0.202 (10%)	Enough to form uniform slurry	2.006 (100%)
Anode ($Li_4Ti_5O_{12}$)	4.00 (80%)	0.500 (10%)	0.500 (10%)	Enough to form uniform slurry	5.000 (100%)

A mixture of the active material with activated carbon was made and added into the binder/dimethyl fornadime slurry. The total mixture was stirred vigorously under magnetic stirring until a uniform slurry was obtained. The slurry was uniformly coated on aluminum and copper foils current collectors for cathode and anode electrodes respectively using doctor blade technique, and dried in a vacuum oven. Electrode composition is reported in table 1.

Cell Fabrication

Battery assembling (coin cell) was performed as follows, cathode or anode electrode foil, and separator are placed in a coin cell case in the following sequence: electrode foil (cathode), separator and anode with few drops of the electrolyte added to the assemble, followed by spacer. The cell was covered with the negative cell case and sealed using coin cell crimping machine with a pressure of 650 psi.

Electrochemical Characterization

Electrochemical measurements were conducted using an eight channel battery analyzer Neware BTS 3000. The cells were cycled using the CC-CV (Constant Current-Constant Voltage) charging regime, and at a current rate of C/30, C/25, C/20, and C/10 rates. The cut-off discharge and charge voltages were set to 0.5 V and 3.6 V respectively. Electrochemical measurements (data) of the assembled coin cell were modeled and optimized using Multi-Gene Genetic Programming techniques. The result of the generated model was used to compare that of the measured value.

Results and Discussions

The experimental data generated by the electrochemical measurements are given in table 2.

Table 2: Sample of the experimental cell data

Current (mA)	**Cap (mAh)**	**CmpCap ($mAhg^{-1}$)**	**Energy (KWh)**	**Cell Voltage (mV)**
1.021	0	0	0	112.8
1.021	0.001	1.418	0	112.8
1.021	0.003	2.836	0	113.1
1.021	0.004	4.253	0	113.1
1.02	0.006	5.671	0.001	113.1
1.021	0.007	7.089	0.001	113.1
1.021	0.009	8.507	0.001	113.4
1.02	0.01	9.924	0.001	113.4
1.021	0.011	11.342	0.001	113.1
1.021	0	0	0	112.8

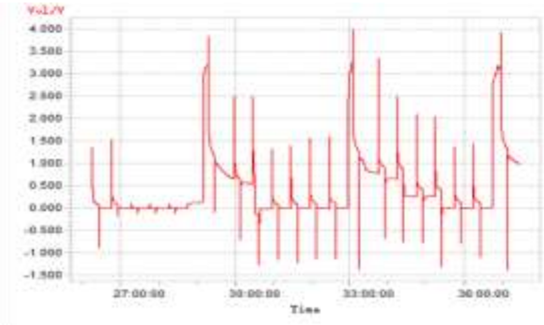

Fig 2. Voltage of the LiFePO4/ Li4Ti5O12 Cell

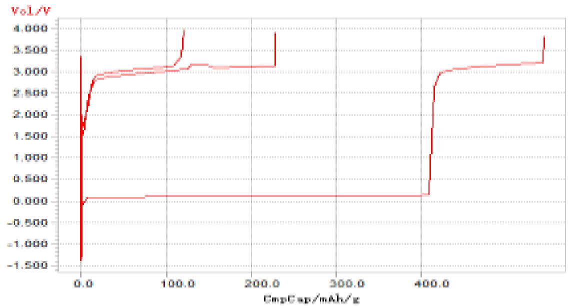

Fig 3. Charge profile of the LiFePO4/ Li4Ti5O12 Cell

The resulting voltage and charge profiles are plotted and shown in figure 2. and 3. respectively. Figure 2 shows the response of the cell voltage with time in seconds while Figure 3 shows the response of the cell voltage with the cell specific capacity. The results show that for a constant current charge of 1.02 mA, there is a steady increase of voltage with a corresponding increase in the cell capacity. The charge/discharge cycling behavior is typically of LiFePO4/Li4Ti5O12 cell which exhibited a flat charge/discharge voltage profile of about 0.1 V and 3 V at a current rate of C/30 and C/20 rates respectively, which is shown in figure 3.

Modeling and implementation of MGGP

The data obtained from the experimental processes (table 1) are regenerated by the MGGP program in MATLAB to evolve a solution model. The following MGGP model expression for the cell voltage were found to have the best fitness value after 1000 simulation generations, and is given as:

$$Y = 101.4-57.27. *x_4-.1100. *x_4. *x_3+527.2. *tanh(x_2)-.1100. *tanh(x_2).*x_3 +3084.*tanh(x_4.\hat{}2.*x_1 1.*x_2.*x_4.\hat{}2)...+.1294e^5.*tanh(4961.*x_4.\hat{}3)- .1019e^5.*tanh(799.8.*x_2.*x_4.\hat{}2); \quad (1)$$

For the MGGP mathematical modeling, the following conventions were used for the input electro-physical parameters as:

X_1 = Charge current (mA)
X_2 = Capacity (mAh)
X_3 = Specific capacity (mAh/g)
X_4 = Energy (mW)
Y = Cell voltage (mV)

The fitness function achieved an R^2 error of 0.99218 and adjusted R^2 of 0.9921 as shown in figure 4. In particular, the R^2 and adjusted R^2 are very close to unity which indicates that the developed model satisfactorily represents the cell output.

Figure 5 illustrates the fitness of the best individual of the population as a function of the generation number and also shows the convergence of the GP evolutionary cycle. The figure indicates that 1000 generations was able to achieve convergence.

Using the generated model (Eq.1) and its associated input electro-physical parameters, the predicted cell voltage is compared with the actual voltages through line plots, with very close agreement between the two plots (Figure 6).

Conclusion

Experimental studies which was carried out at ambient temperature without the use of inert gas for the synthesis of samples of LiFePO4 and Li4Ti5O12 electrode nano-materials have been conducted. The synthesized electrodes were used to fabricate a coin cell battery. Simulations using Multi Gene Genetic Programming were performed to obtain a mathematical relation describing the cell voltage in terms of some associated electro-physical parameters. The results were compared with actual values and are very promising. Li-ion batteries exhibit a non-linearity function; hence, MGGP is an important tool which can accurately model the behavior of Li-ion batteries.

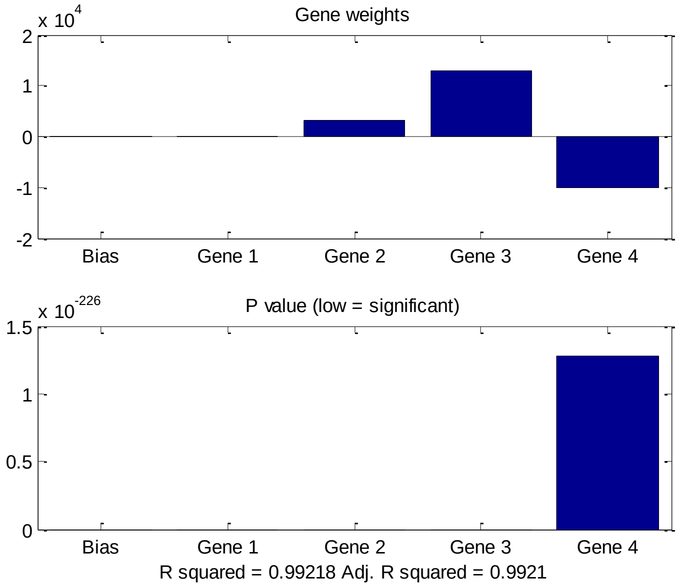

Figure 4: Reported statistical properties (R^2 and Adj. R^2) by the MGGP programme

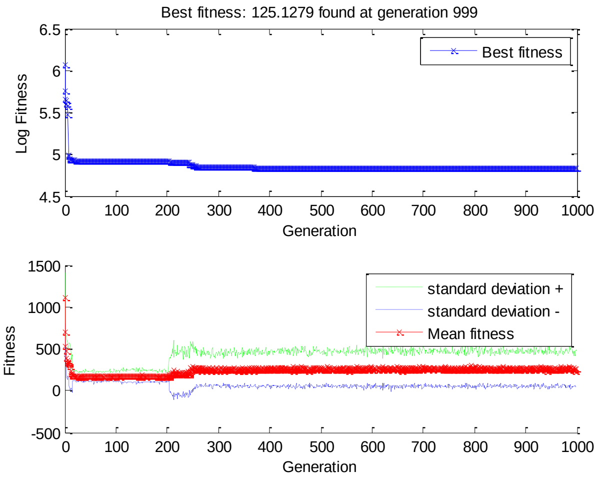

Figure 5: Best fitness found by the MGGP Programme compared after 1000 generations

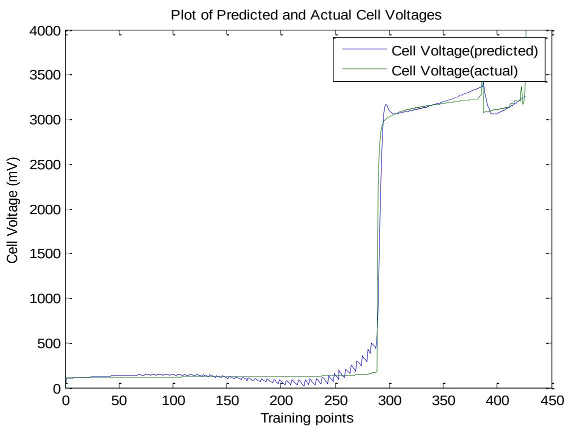

Fig. 6. Cell voltages of the model with actual values

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