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Data mining for quality prediction of battery in manufacturing process: Cathode coating process

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ABSTRACT
A data mining approach is proposed for evaluating the effects of battery production factors in cathode coating stage on both battery capacity and internal resistance for the first time. Specifically, an effective neural network model is built based on real data form designed experiments for obtaining reference cathode coating for coin cells. The purpose is to analyze and predict how the battery quality in both charge and discharge scenarios changes with respect to the key factors of coating including its weight and thickness. The results highlight the correlation between mentioned factors and battery quality indices, which could guide manufacturer to identify efficient ways for producing high-quality batteries.

Keywords: Battery manufacturing, Data mining, Capacity, Modelling

1. INTRODUCTION

Environmental challenges such as global warming as well as limited sources of fossil fuels has increased the demand for green energy and transportation technologies. Lithium-ion (Li-ion) battery is one of the most promising technologies not only for mobility electrification but many other applications. This has increased the overall demand for it in recent years. However, the performance of Li-ion battery such as energy or power density, capacity, lifetime, internal resistance and thermal conductivity are strongly affected by numerous factors in the battery production process. To optimize battery quality and consequently production costs, it is crucial to fully understand the correlation between production factors and battery parameters.

Unfortunately, battery production is a long and complicated chain involving numerous intermediate processes and strong-coupled influencing factors [1]. As the whole battery production chain contains a number of chemical, mechanical and electrical operations, the analysis of correlation between intermediate production factors and battery parameters are still mainly dependent on the trial and error [2], which is extremely laborious and time-consuming. In light of this, in order to achieve smarter battery production, efforts are urgently needed to develop efficient data analysis and modelling solutions to better understand intermediate production factors and predict their effects on the performance of final battery products.

With the rapid development of artificial intelligence technologies, data mining strategies have become popular in the field of battery management [3, 4]. A good deal of works have been designed for estimating battery states [5, 6], predicting battery lifetime [7, 8], performance improvements [9, 10], achieving efficient energy management [11, 12]. Overall, through designing proper data mining models, it is expected that more efficient management of Li-ion batteries can be achieved. However, these researches primarily focuses on developing produced battery performance but relatively little has been done on techniques for manufacturing their internal components. It should be noted that the battery production plays a more direct role in determining the battery quality, which also needs to be well managed.

To date, just a few reports have been found on using advanced data mining solutions to improve the battery production [13]. For instance, based on the cross-industry standard process (CRISP), Schnell et al. [14] designed a linear and a neural network model to identify the process dependencies and predict several battery

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properties such as capacity. Turetskyy et al. [15] utilized the decision tree techniques to analyze feature importance and forecast the maximum capacity of battery products. Based upon the statistical analyses of fluctuations in battery production, the influence of these fluctuations on manufactured battery capacity is evaluated in [16]. Despite the aforementioned works on the data-driven modelling of battery production, most researches simply apply conventional methodologies to predict the properties of battery production. Little has been done so far through using data mining to in-depth analyze the effects of production factors within the key manufacturing stage such as coating on the quality of final battery products. It should be noted that battery coating is extremely important for determining battery electrode qualities. The reliable sensitivity analysis of the battery properties with respect to coating specifications could benefit battery manufacturer to optimize the coating stage and further identify the cheaper and more efficient ways of produce high-quality batteries.

Given the aforementioned considerations, a data mining approach is presented in this article to predict the battery properties taking into account its different influencing factors. Battery production process is consisted of different stages such as mixing, coating, drying, calendaring, cutting, assembly, housing and forming. Here the focus is on the effect of cathode coating significant factors on final battery product. Several main objectives of this article can be summarized as: i) To understand the effect of coating process factors (coating weight and it's thickness) on battery capacity and internal resistance. ii) To predict battery capacity and internal resistance via a model. Iii) To analyses the sensitivity of the battery properties with respect to coating specifications. All this efforts can help the manufacturer to produce more efficient and qualified batteries and to reduce production costs by offering a systematic procedure for data acquisition, data handling and processing.

2. COATING PROCESS EXPERIMENTAL DETAILS

2.1 Design of experiments

A design of experiments (DoE) approach is used to reduce the total amount of experiments required for the identification of the main influencing factors of the coating process and study their effect on coating weight and thickness. In this supersaturated DoEs the minimum number of factors is considered to be five involving two settings for each [17]. Factors and their settings were chosen based on recommendations from the literature [18, 19] and experts.

The five main factors for the study include comma bar gap (80-140 µm), coating ratio (110-150 %), web speed (0.5-1.5 m/min), air speed (5-15 m/s) and drying temperature (85-110 °C). Drying is designed to takes place in an oven consisting three sections with independent temperature settings. Nevertheless, to keep the number of factors limited, only the upper section temperature was varied. Similarly, the air speed setting was kept the same for all sections as dictated by the DoE. The final design matrix was comprised of twelve number of experimental runs at different conditions. Two initial test experiments were performed to identify whether coating defects may appear at the extreme factor settings. Electrode formulation, mixing protocol and web tension were kept constant for all experiments.

2.2 Coating process

The cathode formulation was: 96% active material (NMC 622), 2% conducting carbon black (C65) and 2% binder (PVDF). First the dry components were mixed together, then solvent (NMP) was added to create a thick mixture with 77% solid content at the kneading stage. Next, the mixture was diluted with further addition of solvent to a final solid content of 67%. Fig 1 shows the coating in different stages.

(a)

(c) (b)

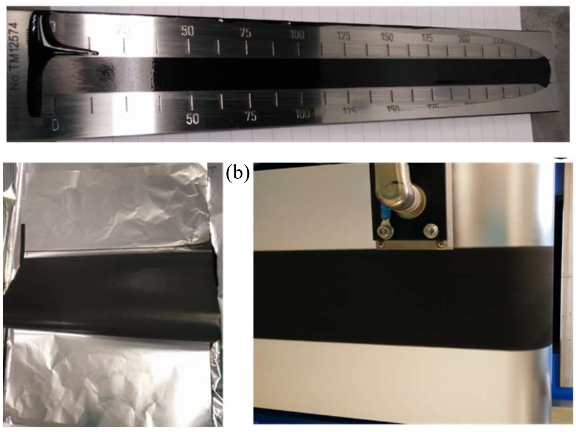

Fig 1 Intermediary products from different manufacturing stages: a) slurry tested on Hegman (fineness of grind) gauge indicating good quality and absence of large agglomerates; b) electrode after coating and drying; c) section of calendared electrode

The slurry was coated on 15µm thick Aluminum foil using a coating machine with reverse roll comma-bar and 3-zone temperature dryer.

Among the five main factors mentioned before, the comma-bar height and the coating ratio were affecting the coating weight the most. The latter is the ratio of the bumper roll and line speed compared to the backing roll and reflects the transfer ratio of the slurry onto the foil.

After coating, the electrode was dried overnight in a vacuum furnace, during drying, the solvent was evaporated under controlled temperature, air speed and line speed conditions. Then the coating was calendared to a target porosity of 30%. Electrode discs were obtained by die-cutting and then dried again before assembly. Half-cells (2032 coin cells) were made by stacking electrode, separator and Li disc, adding electrolyte and crimping the cell case. The cathode half-cell went through a formation cycle at C/20, 5 conditioning cycles at C/5, then testing at different C rates using Maccor^{TM} battery testing equipment. The internal resistance (areal specific impedance) of the cell was calculated at 50% state of charge [20].

3. DATA MINING AND MODELLING

Here a neural network is designed to predict the battery properties given its coating weight and thickness. Before training the network the data were pre-processed. In pre-processing the data were first cleaned of outliers and then improved by imputing outliers with the mean value of all records of the same batch. The pre-processed data were then divided into three sets of training (70%), validation (15%) and test (15%). Then a neural was trained with the hyper-parameters optimized based on the root mean square error (RMSE).

The network, Fig 2, consists two input neurons for weight (g/m^2), and thickness (µm), 1 hidden layer with 5 neurons and an output layer with three neurons, for capacity, which is measured at constant rate in mAh, and internal resistance of cell which is measured at 50% State of charge in (mΩ/m^2). For this network, *w* represents the neuron weight and *b* shows its bias. For hidden layer the transfer function is sigmoid and for output it is linear.

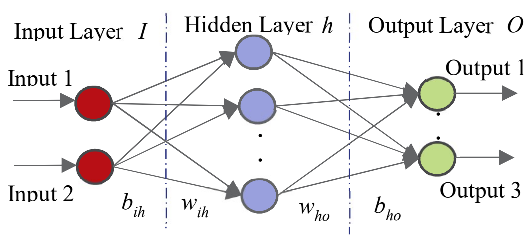

Fig 2 neural network for modelling battery quality

The following figures of Fig 3 and Fig 4 show the relationship between the cathode coating weight and thickness with its capacity and resistance. The figures clearly demonstrate the correlation between battery specifications and its coating parameters.

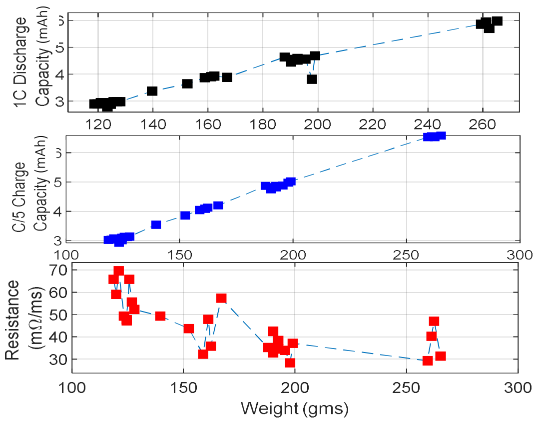

Fig 3 Correlation between cell (a) capacity and (b) charge capacity, (c) resistance with cathode coating weight

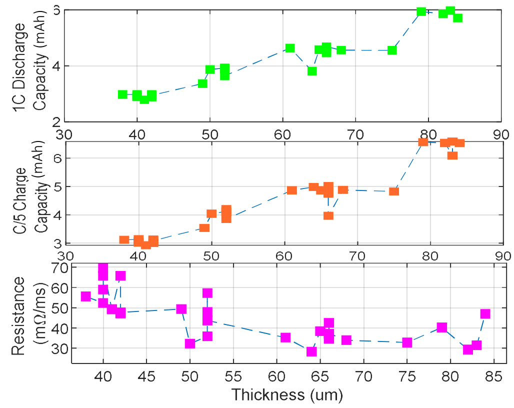

Fig 4 Correlation between cell (a) discharge capacity and (b) charge capacity, (c) resistance with cathode coating thickness

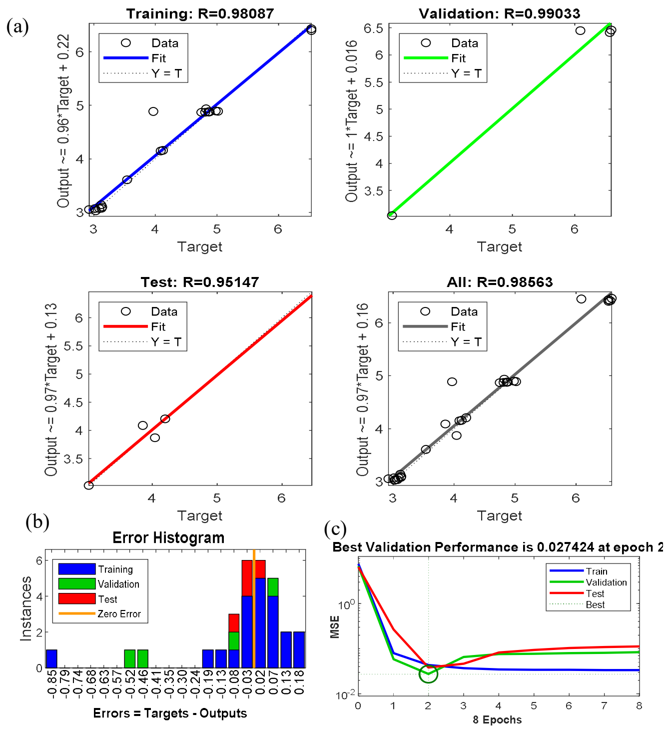

Fig 5 (a) correlation between experimental cell charge capacity (Targets) and modelled capacity (Output) (b) Histogram of prediction error, (c) Prediction performance based on RMSE

4. RESULTS AND DISCUSSIONS

The reliability of the developed model for quality prediction of cell is assessed in this section via the data of 27 cells with same cathode material. The training has terminated based on the minimum value of its performance index for validation data.

Fig 5 shows the correlation between measured data for prediction of C/5 charge capacity. The model has an error histogram distributed around zero. The model implies a R^2 of 0.9627 for 100 runs. This values show the high prediction capability of the model for capacity data. The RMSE in this case is 0.0399 mAh, which is considered to be less than 0.18% of the average capacity of samples.

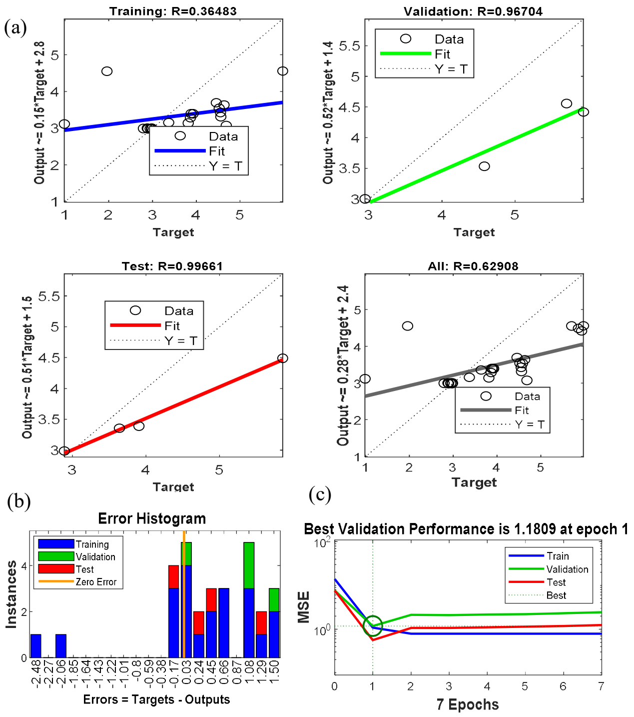

Fig 6 (a) correlation between experimental cell discharge capacity (Targets) and modelled capacity (Output), (b) Histogram of prediction error, (c) Prediction performance based on RMSE

Fig 6 show the correlation between measured discharge capacity at 1C and the two inputs of coating weight and thickness.

The average RMSE in this case is 0.8274 mAh for 100 runs, which is considered to be less than 1% of the average capacity of the samples, R^2 value is 0.7480.

Fig 7 is the performance of model for prediction of battery internal resistance. The average of RMSE for 100 runs for resistance prediction is 13.5531 mΩ/m^2, which is considered to be about 30% of the average resistance of the samples. This range of error is justifiable due to the intense change in battery resistance with its thickness and weight (Fig 3 and Fig 4). R^2 value here is 0.7486.

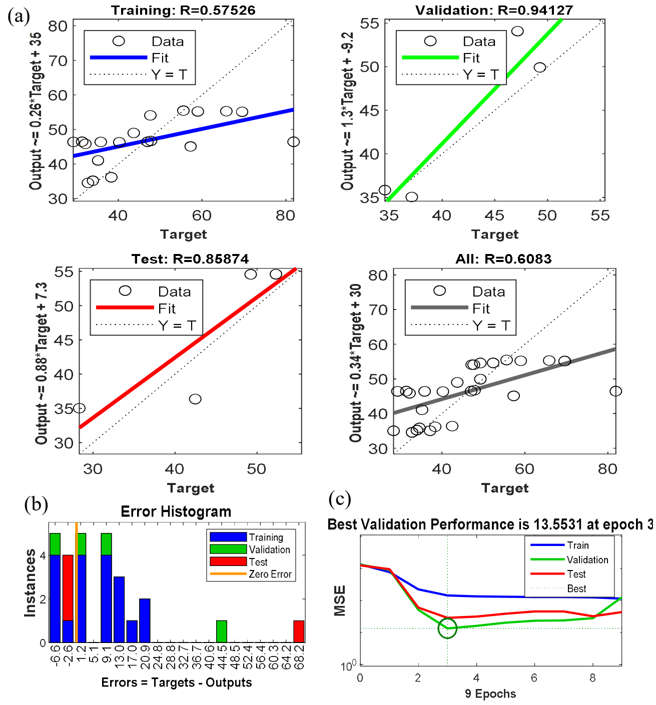

Fig 7 (a) correlation between experimental cell resistance at 50% SoC (Targets) and modelled resistance (Output), (b) Histogram of prediction error, (c) Prediction performance based on RMSE

For all three case of charge capacity, discharge capacity as well as the internal resistance at 50% SoC for cells, the prediction accuracy is showing a R^2 more than 0.6 that is considered to be acceptable [21].

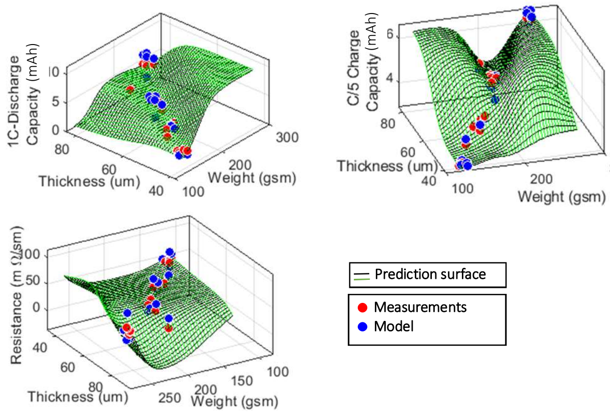

Fig 8 Prediction surface of battery capacity and resistance

Fig 8 represents the prediction surface as well as the prediction points compared to the measurements of resistance

5. CONCLUSIONS

The general trend of the data for cells shows that cells with higher weight (g/m^2) have a larger capacity both for charge and discharge (at C/5-rate). The increment rate in capacity is almost the same for charge and discharge cases. Thickness of the cathode coating has also an obvious effect on the cell capacity. According to the data at Fig 3 and Fig 4, thicker coatings end up with higher capacity cells. The results for internal resistance of the cell is showing a different type of correlation compared to capacity. An increase in weight and thickness reduces the internal resistance of the cell. In future works it is necessary to consider the effect of other influential factors such as porosity and also extend the quality factors to other indices such as cell lifetime.

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