Prognosis and Health Management of Solid-State Batteries

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Solid-state batteries (SSBs), in which the organic liquid electrolyte is substituted by solid electrolytes (SEs), have shown to be a proper substitute for lithium-ion batteries (LIBs) by replacing the organic electrolyte with solid materials. SSBs are nonlinear dynamical electrochemical systems with complex internal mechanisms. In contrast to LIBs, SSBs significantly improve component safety, electrochemical stability, energy and power density, and the durability of battery packs. However, in order to make battery packs market-ready, reliability, health state, and operational safety of the batteries should be evaluated and guaranteed. Herein, battery prognostics and health management (PHM) has emerged as a reliable engineering discipline that ensures the safety and availability of batteries. Battery PHM refers to a multifaceted advanced set of techniques that ensures the integrity and functionality of the battery systems. In particular, it follows a systematic framework to accurately predict batteries' state of charge (SOC), state of health (SOH), and remaining useful life (RUL) by estimating the products performance given the current degree of deviation and degradation and suggesting an optimal health management strategy. Due to the complex nature of electrochemical and mechanical behavior of SSBs, predicting the remaining lifetime and SOH of batteries become an extremely difficult task. However, it is essential to accurately estimate the battery status to ensure the functionality and timely maintenance of the batteries under various operating conditions.

Keywords: solid-state batteries ; prognostics and health management ; physics-based approach ; data-driven approach

1. Model-Based (Physics-Based) Approaches

1.1. Electrochemical (Mechanistic) Models

The electrochemical model mainly completes the accurate modeling of the battery by describing the electrochemical reaction process inside the battery ^[1]. However, the differential equations that are established by this model usually contain a large number of unknown parameters, which increases the complexity of this model. In addition, the input variables in the electrochemical model include a large number of internal battery parameters, such as the effective area of the electrode space, ionic conductivity of the electrolyte, average distance from the electrode to the current collector and so on. These parameters are normally difficult to obtain by measuring the external structure and cycle performance of the battery.

The electrochemical model is established based on electrochemical principles, which can reflect the relationship between the external characteristics and the internal parameters of the battery and can describe the change in the output characteristics during the charging and discharging process. The types of SE (LiPON ^{[2][3][4]}, Li₃PO₄ ^{[5][6]}, LiTFSI ^[Z], LATP ^[8], Li₆PS₅CI ^[9], and polymers ^[10]), anode (lithium metal ^{[3][4][5][11][12]} and graphene ^[13]), and cathode (LiCoO₂ ^{[3][4][12]} and TiS₂ ^{[4][11]}) in the macroscopic model can be adjusted according to the actual application. The electrochemical model can be used to analyze the charge-discharge behavior and cycle performance of the battery. In addition, the effects of contact areas and compressive pressure ^[Z], the contributions of individual overpotential and impedance, the definition of diffusion coefficient, the expansion of the electrode particles that is caused by intercalation ^[14] can also be evaluated.

Danilov et al. ^[5] proposed a mathematical model for SSBs that takes into account the insertion and de-insertion of Li⁺ at the electrolyte/electrode interface and ignores the side reactions that are occurring at the interface. Herein, the discharge curves at different current densities are in good agreement with the experimental results ^[5]. Ansah et al. ^[9] also studied the effect of structural parameters on the discharge performance and found out that increasing the thickness of the cathode and decreasing the thickness of the electrolyte were beneficial to increasing the battery capacity. However, due to the complexity of SSBs, it is difficult to validate the results. Considering that several parameters, such as the mobility number and diffusion coefficient of Li⁺, are not suitable for SSBs, Fabre et al. ^[3] then employed various electrochemical techniques such as galvanostatic intermittent titration technique (GITT) and electrochemical impedance spectroscopy

(EIS) to modify these parameters. Kodama et al. ^[15] used nonlinear stress analysis to calculate the ionic conductivity and showed that the simulation results between the diffusion coefficient and the concentration of Li⁺ are consistent with the experimental results ^[16]., Liu et al. ^[12] proposed an improved Planck–Nernst–Poisson and Frumkin–Butler–Volmer (MPNP-FBV) electrochemical model and considered the influence of electric double layer (EDL) structure and vacancies to investigate the essential phenomena at the equilibrium state in SSBs. They found that the total electrostatic potential drop at equilibrium is related to the difference in free enthalpy between different materials. In addition, the charge transfer resistance of the diffused bilayer structure is higher than that of the dense bilayer structure.

Actually, solid electrolytes (SEs) are fragile that even slight volume changes in SSBs could cause particle fracture, disconnection, and eventually pulverization ^[127]. To improve the interface contact quality and reduce the interface impedance, several methods have been proposed, including depositing buffer layers between SEs and the electrodes by pulsed laser deposition (PLD) or atomic layer deposition (ALD) ^{[127][18][19]}, grinding nanocomposites to reduce the particle size and increase surface area ^{[20][21]}, and fabricating composite cathodes ^[14]. Tian et al. ^[4] and Shao et al. ^[4] introduced a parameter to describe the contact area, which adjusts the current density in the 1-D Newman model. They found that the capacity drop was correlated with the loss of contact area, and the optimal charging performance could be obtained under medium compressive pressures (0.4–1 MPa). To illustrate the relationship between lithiation-induced stress evolution and electrode structure, Fathiannasab et al. ^[8] presented a 3D model by using a synchrotron transmission X-ray microscopy tomography system to reconstruct the morphology of the SSBs. They revealed that SE with lower stiffness can decrease stress in the microstructure, but aggravate the anisotropic displacement of AM particles can also be prevented by applying external compressive pressure. In addition, bending also has a significant effect on battery performance, as bending the SSB from anode to cathode when a force is applied can reduce the cell potential, while bending in the opposite direction induces a potential change and leads to a reduction in lithiation ability ^[22].

Becker-Steinberger et al. [23] proposed an SSB model that takes into account ion transport in crystalline metal oxide solid solutions. Specifically, the diffusion part of the electric double layer is dynamically described by the Poisson equation, while the Stern layer potential drop is modeled by the Robin boundary condition. In addition, electrochemical reactions at the electrode/electrolyte interface (EEI) are modeled with nonlinear Neumann boundary conditions. Danilov et al. [5] developed an isothermal SSB model that takes into account the incomplete dissociation of ions in the electrolyte. The model consists of two partial differential equations (PDEs) describing the diffusion process in the SE and cathode. Based on this model, Kim et al. ^[6] proposed battery management algorithms such as state estimation. However, the equation order of this method is higher, and the efficiency of the algorithm has not been determined. Deng et al. ^[24] used a combination of Padé approximation, polynomial profile approximation, and equal response coefficient assumptions to reduce the rigorous PDE model with significantly reduced computational burden and high fidelity that is suitable for online parameter estimation and condition monitoring. Despite the high accuracy of electrochemical models, these models have shortcomings such as complex model structure, difficult parameter identification, and low computational speed. In order to improve the robustness of the models, alternative approaches have been adopted with higher accuracy, such as P2D (Pseudo Two-Dimensional) model, single particle model, and the electrode average model. In addition, there are also methods such as polynomial approximation, Padé approximation, finite volume discretization, and orthogonal decomposition, which are less prevalent.

1.2. Equivalent Circuit Models

Even though electrochemical models offer efficiency for battery modeling and system state predictions, due to the difficulty in solving the coupled partial differential equations and the high demands on model parameterization and computation time, it has been attempted to propose alternative models that can obviate these challenges. SSB is highly nonlinear and time-varying during the operational time, and internal parameters such as internal resistance, state of charge (SOC), state of health (SOH), and self-discharge parameters during battery operation cannot be obtained by direct measurements. In order to analyze the relationship between the internal variation law of the battery and related parameters, establishing an equivalent model of the battery is an effective research method ^[25]. To achieve the expected high performance, practical applications of SSBs require accurate and computationally efficient models onboard management algorithms so that the SSB safety, health, and cycling performance can be optimized under a wide range of operating conditions. Equivalent circuit model (ECM) has been widely used in battery management modeling as a compromise between accuracy and feasibility. In the ECM, the power batteries' dynamic response, static characteristics, and dynamic polarization effect are described by ideal electrical components, constant voltage source, and RC network, respectively. This strategy has been successfully applied to the estimation of SOC, SOH, and SOE due to its simple model equations, convenient parameter identification, and good real-time performance. ECM is a semi-empirical model, which describes the charge and discharge

characteristics of the battery by arranging and combining electrical components such as voltage sources, resistors, inductors, and capacitors ^[26].

The system parameters of the electrical components in ECM models can be determined by combining different parameter identification methods, such as extended Kalman filtering, particle filtering, and other algorithms. At present, the development of ECMs is relatively complete, and the more frequently used models include Rint, first-order RC, second-order RC, and PNGV ^[2Z]. In theory, the multi-order models have higher accuracy than low-order models, but they have less advantages in accuracy and computational efficiency due to the large number of parameters that need to be identified and the inevitable errors in each parameter.

In the Rint model, the battery is treated as the series connections of the ohmic internal resistance and the ideal voltage source, and polarization effects are not considered. The Rint model is characterized by a simple structure and the least number of parameters. Notably, the error of the model increases with the increase of the charge and discharge rate of the battery ^[28]. The first-order RC model, also known as the Thevenin model, is composed of an ideal voltage source, an ohmic resistance, a polarization resistance, and a polarization capacitor in series. Compared with the Rint model, the first-order RC model describes the polarization effect of the battery during charging and discharging. In addition, the first-order RC model has high accuracy in terms of constant temperature and constant current charging and discharging conditions, and can realize the estimation of the state parameters of LIBs. However, the aging or temperature change of the LIB will cause the internal impedance characteristics of the battery to change from a single impedance arc to a double impedance arc, which significantly impacts the accuracy of the battery model ^[29].

Compared with the first-order RC model, the second-order RC model adds a series-connected RC network to describe the battery's electrochemical polarization and concentration polarization at different stages of the charging and discharging process. The second-order RC model is more computationally expensive than the electrochemical model and the ECM. Notably, the second-order RC model has high accuracy in describing the dynamic polarization behavior of LIBs under high-rate current, and the operating results are closer to the actual state of the battery, and therefore, are widely used in the research of single batteries ^[30].

The PNGV model is a derivative model of the first-order RC model, which can describe the battery capacity while reflecting the DC response characteristics. The primary working principle of PNGV models is that a capacitor is connected in series based on the first-order RC mode. The purpose of this model is to describe the relationship between the open circuit voltage of the battery and the accumulative charge and discharge capacity. Then, the model can realize the estimation of the available capacity of the battery, and is mostly used to assess the SOH ^[27]. The general nonlinear (GNL) model is also called the nonlinear equivalent model, which is derived from the generalization and development of the Rint model, Thevenin model, and the PNGV model. The addition of circuit components in the GNL model makes the physical meaning of each part clearer, so that the voltage change process can be better simulated.

Since the parameters in the ECM are closely related to the working state of the battery, the effectiveness of parameter identification during battery operation is crucial. The current identification methods mainly include the nonlinear least squares method, neural network algorithm, and bionic optimization algorithm ^{[31][32][33]} Among them, bionic optimization algorithms include genetic algorithm, particle swarm algorithm, simulated annealing algorithm, and so on ^[34]. The ECM method is one of the most commonly used single-cell models in modeling LIB and SSB packs. The output characteristics and accuracy of the battery pack model depend on the series-parallel sequence and modeling method of the selected single-cell model. However, the current production level and manufacturing process are difficult to ensure the consistency between individual cells. Therefore, the single-cell model cannot accurately represent the predictive model of the battery pack through simple quantitative accumulation. The ECM models generally focus on the external physical quantities such as terminal voltage and current. Moreover, ECM models do not reflect the electrochemical properties and complex variations in the microstructure of the battery. The main modeling principles of the ECM method for a single cell are: (1) The model includes the chemical reaction mechanism of the battery and adapt to different environments and working conditions; (3) the single-cell model is as simple as possible within the scope of the design requirements to simplify the calculation process and improve the usability of the model.

The physical structure of SSBs is fundamentally different from conventional liquid electrolyte-based Li-ion batteries. A suitable SSB model with high fidelity and a low computational burden is essential for most model-based management algorithms. The ECM has the advantage of being easy to implement in a wide range of applications, in particular, in circuit simulation and control system design software packages such as MATLAB/Simulink. In these packages, various numerical solvers have been included, which can be selected to solve circuit models and facilitate control system design.

However, ECMs lack mechanistic insight into electrochemical dynamics, have limited applicability for battery performance prediction under wider operating ranges and changing system dynamics, and fail to properly address battery degradation and internal safety issues. Additionally, modern applications of batteries need to be designed for increased load dynamics, higher current rates, and harsher operating environments. Herein, the functional complexity, model order, and testing effort for identifying ECM parameters must increase substantially to achieve sufficient extrapolation.

1.3. Empirical Models

Building mathematical models is an effective method to analyze and optimize the performance of batteries. Generally, mathematical models are divided into two types: one is a mechanism model that is established by theoretical analysis; the other is an empirical model, which is proposed on the basis of experiments and can simulate the performance and explain the behavior of the battery to a certain extent. The former is often used to describe the mechanism by which various factors affect battery performance, while the latter is often applied to simple simulations of the performance of single batteries in a battery pack. In addition, there are also semi-empirical models that combine mechanism and empirical models. The empirical model refers to the model description of the cell capacity decay process that can directly or indirectly reflect the change law of the state variable of the capacity decay with time, the total discharge capacity or the number of cycles through the empirical formula. In the process of estimating the SOH of lithium batteries, the empirical model usually needs to use statistics to process the data to determine the initial parameter values of the model.

The modeling and simulation of LIBs has always been a research hotspot in the field of electrochemistry. However, most existing reports have studied the numerical and empirical models of LIBs separately. Establishing an LIB degradation model is one of the important links in predicting cycle life. However, it is difficult to establish an accurate battery degradation process model that is based on the electrochemical processes inside LIBs that are under actual operating conditions. In addition, the degradation process of the battery is directly affected by various factors such as temperature, impedance, end of charged voltage (EOCV), and depth of discharge (DOD). Generally, the more parameters that are involved in the model, the higher the accuracy of the model. However, some parameters are not easy to obtain in the process of battery capacity degradation, and the model establishment is more complicated. Empirical models that are commonly used in LIBs include internal resistance model, ECM, neural network model, fuzzy algorithm model, and the genetic algorithm model. Saha et al. [35] first carried out experiments on the performance degradation of LIBs under different conditions and obtained a large amount of test data. Some scholars conducted accelerated life tests on lithium power batteries at multiple temperatures (40–70 °C) [36][37]. They proposed a completely empirical model according to the variation law of the battery's internal resistance, temperature, and SOC, and finally developed a multi-sigmoid model. Ramadass et al. [38] quantitatively studied the capacity fading of batteries through the changes of SOC, resistance, and diffusion coefficient of an SEI membrane, and proposed a semi-empirical model for battery capacity degradation. Furthermore, Ning et al. ^[39] improved a semi-empirical model that was based on the quantitative analysis of the effects of EOCV and DOD on the cycle life of batteries.

1.4. Fused Models

Fused models combine all available knowledge, information, and data sources, bringing the advantages of model-based and data-driven approaches. Specifically, fused models can combine the robustness and interpretability of model-based methods with the specificity and accuracy of data-driven methods. They incorporate different types of battery models to extract additional features from the available data. The differential equations that are established by the electrochemical models usually contain a large number of unknown parameters, and the input variables include many internal parameters of lithium batteries, which are difficult to obtain by measuring the external characteristics of lithium batteries. Therefore, electrochemical models are rarely used in practical BMS. The ECM avoids the extensive use of internal parameters of lithium batteries and reduces the difficulty of establishing the model. In order to achieve high-precision modeling, Verbrugge et al. ^{[40][41]} introduced a first-order delay in the RC model of lithium batteries, which was experimentally demonstrated to have better performance under dynamic current conditions. Plett et al. ^[42] modeled the fused model by fusing the Shepherd model, the Unnewehr general model, and the Nernst model. Liu et al. ^[42] modeled the lithium battery based on the fusion model and achieved an accurate estimation of the state of the lithium battery based on the improved fusion model.

The RUL is usually defined as the number of remaining charge and discharge cycles when the battery reaches the end of life (EOL), which is used to measure the reliability of the battery in its life span and is a description of the future state of the battery at the macro scale. However, SOH belongs to the description of the current state of the battery at the macro scale. To fully evaluate the aging degree of the battery, it is necessary to perform SOH estimation and RUL prediction simultaneously ^[43]. So far, joint estimations of SOC-SOH are now common, but predictions of RUL are usually done

separately. Since it is difficult to achieve an accurate prediction of RUL using only a single method, fusion algorithms are regarded as the main research direction. In addition, RUL is a description of the future state of the battery, and therefore, it is necessary to provide an uncertainty expression of the predicted results to improve reliability. Xing et al. ^[44] proposed a fused model method that was based on exponential and polynomial to achieve RUL prediction by using PF to update the model parameters online. These types of models are simple, but usually only provide point forecasts and perform poorly in long-term RUL forecasts. In addition, data-driven methods using machine learning are also widely used in RUL prediction. Wang et al. ^[45] established a multi-step capacity prediction model, which takes energy efficiency and average operating temperature as the input of SVM. Although machine learning algorithms can achieve accurate modeling of nonlinear systems, they have poor multi-step iterative prediction ability, and usually only single-step prediction can be performed ^[46].

1.5. Comparison of Physics-Based Approaches

Although the electrochemical model has high accuracy, it has obvious shortcomings such as complex model structure, difficult parameter identification, and low operation speed. Therefore, the electrochemical model is not suitable for the BMS of the actual vehicles. The electrochemical model mainly realizes the accurate modeling of the lithium battery by describing the electrochemical reaction process inside the battery. However, the differential equations that are established by the electrochemical model usually contain many unknown parameters, which increases the complexity of the electrochemical model. Meantime, the input variables in the electrochemical model include many internal parameters of the lithium battery, which are difficult to obtain by measuring the external characteristics of the lithium battery, such as the effective area of the electrode space, the ionic conductivity of the electrolyte, the average distance of holes from the electrode to the current collector and so on ^[47]. The ECM simulates the lithium battery by establishing a circuit, which avoids the extensive use of internal parameters of the lithium battery and reduces the difficulty of model establishment.

2. Data-Driven Approaches

2.1. Artificial Neural Network (ANN)

Artificial neural network (ANN) motivated from the biological arrangement and characteristics of the human brain is a widely used method in data-driven approaches that is based on a collection of connected neurons. Each connection transmits or receives a signal from adjoining neurons that connected to them. The model is constituted by three components: the input layer, hidden layer and the output layer and are classified into different types where the primary used methods are: feedforward neural network (FNN) and recurrent neural network (RNN). Their difference originates from the fact that in RNN, the connections between the nodes form a directed or undirected graph, while in FNN, the connections do not form a cycle. Many researchers over the recent decades have focused on employing the ANN methods to perform health diagnosis and SOC estimation of LIBs and SSBs ^[48].

2.2. Kernel Ridge Regression (KRR)

A generalized version of linear regression and ridge regression methods, KRR extends the linear regression into a nonlinear correlation between the available data and maps them into a higher-dimensional feature space. The nonlinear regression scheme is then transformed into a linear format in the feature space ^[49]. Due to the difficulty in selecting an appropriate mapping function, the kernels are applied, representing a similarity between the inputs. For this, a non-linear kernel function is applied in the input space instead of mapping the data and solving high-dimensional non-linear regression. Examples of kernel methods are Gaussian, polynomial, and Laplacian kernel. Fitting the KRR models are commonly a challenging task due to computationally intensive demand of the data which limits the application of medium-sized datasets ^[50].

2.3. Data-Driven Prognosis (DDP)

Recently, a novel data-driven method called data-driven prognosis (DDP) was proposed by Chandra et al. ^[51] that relies on in situ data measurements and estimates the system's failure based on the curvature information that is extracted from the system. This method was later on employed to analyze LIBs ^[52]. The proposed approach extracts the constitutive parameters of LIBs in the shape of curvature and analyzes the curvature information in the system based on the pairwise information of the data points. Then, it estimates the probable timeframe that the system might enter the instability stage and using a set of threshold criteria, predicts the failure of the system ^[52].

2.4. Support Vector Machine (SVM)

SVM methods align with KRR techniques in that they attempt to solve linear classification problems in a high-dimensional feature space ^[53]. The principle the SVM function under is to locate a hyperplane in the feature space and classifies the data points, and identify the plane with a maximum distance between the data points ^[54].

2.5. k-Nearest Neighbor (kNN)

A commonly employed nonlinear ML method, kNN is used to solve both classification and regression problems. It hypothesizes that similar data points are in the vicinity of feature space and classifies the new data points into a category governed by its kNNs ^[55]. This procedure is counted as the classification task. In order to perform, regression, among the kNNs, a weighted average label value is calculated. a requirement for a reasonable distance metric is a limitation of this method ^[55].

2.6. Random Forest (RF)

RF is an ML technique that is used for classification and regression problems ^[56]. It constructs an ensemble of decision trees on various domains of the data points, makes a prediction that is based on each decision tree, and calculates their mean. Higher accuracy and less overfitting is achieved by selecting a large number of decision tress. The employment of ensemble-based architecture in RF methods leads to high accurate predictions and efficiency in the results ^[56].

2.7. Bayesian Method (BM)

BMs are an optimization approach that are used to produce a probabilistic model for a target function commonly utilizing Gaussian Processes (GPs) ^{[28][31]}. GPs use stochastic procedures to describe probability distributions over the functions and assigns a probability to each of these functions. Then, the probability distribution is used to represent the most probable characterization of the data. A notable advantage of Gaussian process regression is their ability to describe the uncertainty of each prediction model. On the other hand, it might be computationally intensive and time-consuming ^[32].

3. Application of ML-Based Data-Driven Techniques in Solid-State Batteries Research

3.1. Anode Materials

Eremin et al. ^[33] integrated topological analysis with density-functional theory (DFT) modeling in addition to ridge regression in the configurational space of LiNiO₂ and LiNi_{0.8}Co_{0.15}Al_{0.05}O₂ cathode materials. They showed that the topology of Li layers, ions, and dopants substantially influence the energy balance. In a similar study, Natarajan et al. ^[34] combined ANNs with adapted cluster functions to predict the formation of Li-vacancy orderings on the spinel LiTiS_s and demonstrated that the ANN method can produce the DFT-computed convex hull with information regarding the pair cluster correlation as the input variable. In 2020, Eckhoff et al. ^{[52][58]} used an ANN method to model Li_xMn₂O₄ that utilized a Jahn–Teller distortion model to predict several properties of SSBs such as an Li diffusion barrier and phonon frequencies and oxidation. Bartel et al. ^[59] investigated seven ML methods to study the formation energy of Li transition metal oxides using chemical formula and showed that models can predict the formation energies accurately.

3.2. Cathode Materials

Similarly, several studies have been carried out to simulate the SSBs anode materials using ML-based data-driven methods. Artrith et al. ^[60] employed atomistic ANN models to evaluate the crystal structure of TiO_2 and the features if amorphous Si anodes. Based on their results, they showed that the computed average voltage was in alignment with experimental results and validated their model. Onat et al. ^[61] used an ANN method to represent the atomic interactions of amorphous Li-Si alloys and computed the Li diffusivity to compare their results with the available references. Yoo et al. ^[62] studied Si crystals as well as nanoclusters with atomic energy mapping modeled in ANN. In a study by Zuo et al. ^[63] that was conducted to compare the performance of several ML interatomic models, including ANN potential with SF representation as well as GPR potential, it was found out that all the ML potentials illustrated accurate prediction of forces, energies, and thermal properties.

3.3. Electrolyte Materials

The electrolyte in SSBs is an important component of the battery that should be accurately modeled to possess high ionic conductivity and compatibility with electrodes and mechanical stability. Lacivita et al. ^[64] devised a set of data-driven

methods to determine the N defects in Li₃PO₄. Their study focused on the potential energy surface (PES) sampling and used ANN for fast screening. According to the investigation by Li et al. ^[65] which used ANN models to evaluate Li diffusion in amorphous Li₃PO₄, it was shown that including Li diffusion transient structures in the simulations is an essential parameter to reduce the error of the barrier energies. Miwa et al. ^{[66][67]} constructed an automatic Bayesian optimization model without including any stochastic assumption. Their study presented that the promotion of Li diffusion in β -Li₂B₁₂H₁₂ is achieved by lattice expansion and predicted the conductivity of Li and activation barriers in Nb-doped LLZO. Deng et al. ^[24] proposed an electrostatic spectral analysis potential (eSNAP) and simulated the diffusion. Wang et al. ^[68] studied the Li diffusion pathways in the interphase and examined the Li ionic conductivities of Li materials on the interfaces of electrolytes using LOTF-MD methods. In a study that was conducted by Fujimura et al. ^[69], an SVM method was employed to model a diffusion-based model considering the temperature and energy formation and diffusion coefficient to study the ionic conductivity of electrolytes. Due to the importance of fast ionic conductivity and electrochemical stability, Sendek et al. ^[70] carried out a study that showed the inclusion of Cl-, Br-, and I-based solid ion conductors lead to more efficient stability and ionic conductivity.

3.4. Comparison of Data-Driven Approaches

Data-driven prognosis and health assessment of SSBs are complex procedures requiring an extensive survey in the system's domain under analysis. System characteristics, data availability, and application constraints are the primary components that need to be taken into consideration before selecting the appropriate method. With that being said, no unique technique can be identified as the most efficient approach as requirements of the users and decision-makers vary from project to project. Thus, it is recommended that the selection of the data-driven method be completely based on the specific system, working environment, and the cost of the assessment.

4. Hybrid Approaches

Even though physics-based models provide valuable insight about the internal state of SSBs, they require extensive parameter estimation of the components. Furthermore, in some systems, it is not amenable to perform off-line testing of the system to extract measurements of the cells, particularly when the model parametrization is further become challenging by the inherent cell-cell variability. To overcome these bottlenecks, hybrid models are introduced that can be used as an advanced SSB state estimation tool in battery BMS. Hybrid approaches combine physics-based methods with data-driven methods to obtain accurate predictions of the SOH of battery systems. The most commonly used hybrid approaches are series and parallel [71]. Combining a model-based model with available prior knowledge about the process and a data-driven method lead to a series approach. Similarly, in parallel methods, physics-based and data-driven approaches are simultaneously considered from the model. There have been limited research studies that focused on using hybrid methods to estimate the battery state. The bottleneck that is embedded in the vast adoption of hybrid model lies beneath the fact that high-fidelity multiphysical and multiscale models are needed so that it would be possible to train machine-learning models and ultimately create new opportunities for fusing the advantages of both modelling approaches ^[72]. The studies that are mentioned here are the most prevalent techniques that have been developed in the battery management field. A study by Song et al. ^[2], implemented a data-driven least-square support vector machine that is combined with a model-based unscented-particle filter that can be used to increase SOC and SOH of SSBs and LIBs. Lyu et al. [23] used a Thevenin model and a data-driven method to estimate the SOH of batteries. In 2021, Lin et al. [74] proposed a hybrid approach in which a continuous hidden Markov model was combined with kernel density estimation to estimate the SOH of batteries.

References

- 1. Miguel, E.; Plett, G.L.; Trimboli, M.S.; Oca, L.; Iraola, U.; Bekaert, E. Review of computational parameter estimation methods for electrochemical models. J. Energy Storage 2021, 44, 103388.
- Tian, H.; Qin, P.; Li, K.; Zhao, Z. A review of the state of health for lithium-ion batteries: Research status and suggestions. J. Clean. Prod. 2020, 261, 120813.
- Fabre, S.D.; Guy-Bouyssou, D.; Bouillon, P.; Cras, F.L.; Delacourt, C. Charge/discharge simulation of an all-solid-state thin-film battery using a one-dimensional model. J. Electrochem. Soc. 2011, 159, A104–A115.
- 4. Tian, H.K.; Qi, Y. Simulation of the effect of contact area loss in all-solid-state Li-ion batteries. J. Electrochem. Soc. 2017, 164, E3512–E3521.

- 5. Danilov, D.; Niessen, R.A.H.; Notten, P.H.L. Modeling all-solid-state Li-ion batteries. J. Electrochem. Soc. 2011, 158, A215.
- Kim, Y.; Lin, X.; Abbasalinejad, A.; Kim, S.U.; Chung, S.H. On state estimation of all solid-state batteries. Electrochim. Acta 2019, 317, 663–672.
- Shao, Y.Q.; Liu, H.L.; Shao, X.D.; Sang, L.; Chen, Z.T. An all coupled electrochemical-mechanical model for all-solidstate Li-ion batteries considering the effect of contact area loss and compressive pressure. Energy 2022, 239, 121929.
- 8. Fathiannasab, H.; Zhu, L.; Chen, Z. Chemo-mechanical modeling of stress evolution in all-solid-state lithium-ion batteries using synchrotron transmission X-ray microscopy tomography. J. Power Source 2021, 483, 229028.
- 9. Ansah, S.; Shin, N.; Lee, J.S.; Cho, H.H. A comprehensive parametric study for solid-state lithium-ion battery through finite element simulation. Electron. Mater. Lett. 2021, 17, 532–542.
- 10. Grazioli, D.; Verners, O.; Zadin, V.; Brandell, D.; Simone, A. Electrochemical-mechanical modeling of solid polymer electrolytes: Impact of mechanical stresses on Li-ion battery performance. Electrochim. Acta 2019, 296, 1122–1141.
- Doyle, M.; Fuller, T.F.; Newman, J. Modeling of galvanostatic charge and discharge of the lithium polymer insertion cell. J. Electrochem. Soc. 1993, 140, 1526–1533.
- 12. Liu, Y.; Ma, Y.B.; Jaegermann, W.; Hausbrand, R.; Xu, B.X. Interface equilibrium modeling of all-solid-state lithium-ion thin film batteries. J. Power Source 2020, 454, 227892.
- 13. Safari, M.; Delacourt, C. Mathematical modeling of lithium iron phosphate electrode: Galvanostatic charge/discharge and path dependence. J. Electrochem. Soc. 2011, 158, A63.
- 14. Bucci, G.; Swamy, T.; Chiang, Y.M.; Carter, W.C. Modeling of internal mechanical failure of all-solid-state batteries during electrochemical cycling, and implications for battery design. J. Mater. Chem. 2017, 5, 19422–19430.
- Kodama, M.; Horikawa, N.; Ohashi, A.; Hirai, S. Coupled nonlinear stress and electric field numerical simulation for allsolid-state lithium-ion batteries. J. Power Sources Adv. 2021, 8, 100049.
- 16. Kazemi, N.; Danilov, D.L.; Haverkate, L.; Dudney, N.J.; Unnikrishnan, S.; Notten, P.H. Modeling of all-solid-state thinfilm Li-ion batteries: Accuracy improvement. Solid State Ion. 2019, 334, 111–116.
- 17. Zhang, Y.; Zhao, C.; Guo, Z. Simulation of crack behavior of secondary particles in Li-ion battery electrodes during lithiation/de-lithiation cycles. Int. J. Mech. Sci. 2019, 155, 4802.
- West, W.C.; Hood, Z.D.; Adhikari, S.P.; Liang, C.; Lachgar, A.; Motoyama, M.; Iriyama, Y. Reduction of charge-transfer resistance at the solid electrolyte—Electrode interface by pulsed laser deposition of films from a crystalline Li2PO2N source. J. Power Source 2016, 312, 116–122.
- Takada, K.; Ohta, N.; Zhang, L.; Fukuda, K.; Sakaguchi, I.; Ma, R.; Osada, M.; Sasaki, T. Interfacial modification for high-power solid-state lithium batteries. Solid State Ion. 2008, 179, 1333–1337.
- 20. Nagao, M.; Hayashi, A.; Tatsumisago, M. High-capacity Li2S–nanocarbon composite electrode for all-solid-state rechargeable lithium batteries. J. Mater. Chem. 2012, 22, 10015–10020.
- Nishio, Y.; Kitaura, H.; Hayashi, A.; Tatsumisago, M. All-solid-state lithium secondary batteries using nanocomposites of NiS electrode/Li2S–P2S5 electrolyte prepared via mechanochemical reaction. J. Power Source 2009, 189, 629–632.
- Song, X.; Lu, Y.; Wang, F.; Zhao, X.; Chen, H. A coupled electro-chemo-mechanical model for all-solid-state thin film Liion batteries: The effects of bending on battery performances. J. Power Source 2020, 452, 227803.
- 23. Becker-Steinberger, K.; Funken, S.; Landstorfer, M.; Urban, K. A mathematical model for all solid-state lithium-ion batteries. ECS Trans. 2019, 25, 285–296.
- Deng, Z.; Chen, C.; Li, X.-G.; Ong, S.P. An electrostatic spectral neighbor analysis potential for lithium nitride. npj Comput. Mater. 2019, 5, 75.
- 25. He, H.; Xiong, R.; Fan, J. Evaluation of lithium-ion battery equivalent circuit models for state of charge estimation by an experimental approach. Energy 2011, 4, 582–598.
- Rajabloo, B.; Jokar, A.; Wakem, W.; Désilets, M.; Brisard, G. Lithium iron phosphate electrode semi-empirical performance mode. J. Appl. Electrochem. 2018, 48, 663–674.
- 27. Jeon, D.H.; Baek, S.M. Thermal modeling of cylindrical lithium ion battery during discharge cycle. Energy Convers. Manag. 2011, 52, 2973–2981.
- Rasmussen, C.E. Gaussian Processes in Machine Learning. In Advanced Lectures on Machine Learning: ML Summer Schools 2003; Lectures Lecture Notes in Computer Science; Springer: Berlin/Heidelberg, Germany, 2004.
- 29. Cho, S.; Jeong, H.; Han, C.; Jin, S.; Lim, J.H.; Oh, J. State-of charge estimation for lithium-ion batteries under various operating condition using an equivalent circuit model. Comput. Chem. Eng. 2012, 41, 1–9.

- 30. Zhu, W.H.; Zhu, Y.; Tatarchuk, B.J. A simplified equivalent circuit model for simulation of Pb-acid batteries at load for energy storage application. Energy Convers. Manag. 2011, 52, 2794–2799.
- 31. Snoek, J.; Larochelle, H.; Adams, R.P. Practical bayesian optimization of machine learning algorithms. arXiv 2012, arXiv:1206.2944.
- 32. Ling, C. A review of the recent progress in battery informatics. npj Comput. Mater. 2022, 8, 33.
- Eremin, R.A.; Zolotarev, P.N.; Ivanshina, O.Y.; Bobrikov, I.A. Li(Ni,Co,Al)O2 cathode delithiation: A combination of topological analysis, density functional theory, neutron diffraction, and machine learning techniques. J. Phys. Chem. C 2017, 121, 8293–28305.
- Natarajan, A.R.; Ven, A.V.D. Machine-learning the configurational energy of multicomponent crystalline solids. npj Comput. Mater. 2018, 4, 56.
- 35. Saha, B.; Goebel, K.; Poll, S.; Christophersen, J. Prognostics methods for battery health monitoring using a bayesian framework. IEEE Trans-Actions Instrum. Meas. 2009, 58, 291–297.
- Wright, R.B.; Motloch, C.G.; Belt, J.R.; Christophersen, J.P.; Ho, C.D.; Richardson, R.A.; Bloom, I.; Jones, S.A.; Battaglia, V.S.; Henriksen, G.L.; et al. Calendar and cycle-life studies of advanced technology development program gen-eration 1 lithium-ion batteries. J. Power Source 2002, 110, 445–470.
- Christophersen, J.P.; Bloom, I.; Thomas, E.V.; Gering, K.L.; Henriksen, G.L.; Battaglia, V.S.; Howell, D. Advanced Technology Development Program for Lithium-Ion Batteries: Gen 2 Performance Evaluation Final Report; U.S. Department of Energy: Washington, DC, USA, 2006.
- Ramadass, P.; Haran, B.; White, R.; Popov, B.N. Mathematical model-ing of the capacity fade of Li-ion cells. J. Power Source 2003, 123, 230–240.
- 39. Ning, G.; White, R.E.; Popov, B.N. A generalized cycle life model of rechargeable Li-ion batteries. Electrochim. Acta 2006, 51, 2012–2022.
- 40. Verbrugge, M.; Tate, E. Adaptive state of charge algorithm for nickel metal hydride batteries hysteresis phenomena. J. Power Source 2004, 126, 236–249.
- 41. Verbrugge, M.; Koch, B. Generalized recursive algorithm for adaptive multiparameter regression application to lead acid, nickel metal hydride, and lithium-ion batteries. J. Electrochem. Soc. 2006, 153, A187–A201.
- 42. Liu, C.; Liu, L. Optimal design of li-ion batteries through multi-physics modeling and multi-objective optimization. J. Electrochem. Soc. 2017, 164, E3254–E3264.
- Lipu, M.H.; Hannan, M.; Hussain, A.; Hoque, M.; Ker, P.J.; Saad, M.; Ayob, A. A review of state of health and remaining useful life estimation methods for lithium-ion battery in electric vehicles: Challenges and recommendations. J. Clean. Prod. 2018, 205, 115–133.
- 44. Xing, Y.; Ma, E.W.; Tsui, K.L.; Pecht, M. An ensemble model for predict-ing the remaining useful performance of lithiumion batteries. Microelectron. Reliab. 2013, 53, 811–820.
- Wang, S.; Zhao, L.; Su, X.; Ma, P. Prognostics of lithium-ion batteries based on flexible support vector regression. In Proceedings of the Prognostics & System Health Management Conference, Zhangjiajie, China, 24–27 August 2014; Volume 7, pp. 6492–6508.
- 46. Rezvani, M.; AbuAli, M.; Lee, S.; Lee, J.; Ni, J. A comparative analysis of techniques for electric vehicle battery prognostics and health manage-ment (PHM). SAE Pap. 2011, 191, 1–9.
- 47. Prada, E.; Di Domenico, D.; Creff, Y.; Bernard, J.; Sauvant-Moynot, V.; Huet, F. Simplified electrochemical and thermal model of LiFePO4-graphite Li-ion batteries for fast charge application. J. Electrochem. Soc. 2012, 159, A1508–A1519.
- Li, F.; Cheng, X.; Lu, L.-L.; Yin, Y.-C.; Luo, J.-D.; Lu, G.; Meng, Y.-F.; Mo, H.; Tian, T.; Yang, J.-T.; et al. Stable all-solidstate lithium metal batteries enabled by machine learning simulation designed halide electrolytes. Nano Lett. 2022, 22, 2461–2469.
- 49. Hastie, T.; Tibshirani, R.; Friedman, J.H.; Friedman, J.H. The Elements of Statistical Learning: Data Mining, Inference, and Prediction, 2nd ed.; Springer Series in Statistics; Springer: New York, NY, USA, 2009.
- Ahmad, Z.; Xie, T.; Maheshwari, C.; Grossman, J.C.; Viswanathan, V. Machine learning enabled computational screening of inorganic solid electrolytes for suppression of dendrite formation in lithium metal anodes. ACS Cent. Sci. 2018, 4, 996–1006.
- 51. Chandra, A.; Kar, O.; Wu, K.-C.; Hall, M.; Gillette, J. Prognosis of anterior cruciate ligament reconstruction: A datadriven approach. Proc. R. Soc. A Math. Phys. Eng. Sci. 2015, 471, 20140526.
- 52. Liu, L.; Kouhestani, H.S.; Chandra, A. Data-driven prognosis of the failure of lithium-ion batteries. ECS Meet. Abstr. 2021, 2021, 1864.

- Suykens, J.A.K.; Vandewalle, J. Least squares support vector machine classifiers. Neural Process. Lett. 1999, 9, 293– 300.
- 54. Liu, H.; Ma, S.; Wu, J.; Wang, Y.; Wang, X. Recent advances in screening lithium solid-state electrolytes through machine learning. Front. Energy Res. 2021, 9, 639741.
- 55. Dudani, S.A. The distance-weighted k-nearest-neighbor rule. IEEE Trans. Syst. Man Cybern. 1976, SMC-6, 325–327.
- 56. Svetnik, V.; Liaw, A.; Tong, C.; Culberson, J.C.; Sheridan, R.P.; Feuston, B.P. Random forest: A classification and regression tool for compound classification and QSAR modeling. J. Chem. Inf. Comput. Sci. 2003, 43, 1947–1958.
- 57. Eckhoff, M.; Lausch, K.N.; Blöchl, P.E.; Behler, J. Predicting oxidation and spin states by high-dimensional neural networks: Applications to lithium manganese oxide spinels. J. Chem. Phys. 2020, 153, 164107.
- 58. Eckhoff, M.; Schönewald, F.; Risch, M.; Volkert, C.A.; Blöchl, P.E.; Behler, J. Closing the gap between theory and experiment for lithium manganese oxide spinels using a high-dimensional neural network potential. Phys. Rev. B 2020, 102, 174102.
- 59. Bartel, C.J.; Trewartha, A.; Wang, Q.; Dunn, A.; Jain, A.; Ceder, G. A critical examination of compound stability predictions from machine-learned formation energies. npj Comput. Mater. 2020, 6, 97.
- 60. Artrith, N.; Urban, A.; Ceder, G. Constructing first-principles phase diagrams of amorphous lixsi using machinelearning-assisted sampling with an evolutionary algorithm. J. Chem. Phys. 2018, 148, 241711.
- 61. Onat, B.; Cubuk, E.D.; Malone, B.D.; Kaxiras, E. Implanted neural network potentials: Application to Li-Si alloys. Phys. Rev. B 2018, 97, 094106.
- 62. Yoo, D.; Lee, K.; Jeong, W.; Lee, D.; Watanabe, S.; Han, S. Atomic energy mapping of neural network potential. Phys. Rev. Mater. 2019, 3, 093802.
- Zuo, Y.; Chen, C.; Li, X.-G.; Deng, Z.; Chen, Y.; Behler, J.; Csányi, G.; Shapeev, A.V.; Thompson, A.P.; Wood, M.A.; et al. Performance and cost assessment of machine learning interatomic potentials. J. Phys. Chem. A 2020, 124, 731–745.
- 64. LaCivita, V.; Artrith, N.; Ceder, G. Structural and compositional factors that control the li-ion conductivity in LiPON electrolytes. Chem. Mater. 2018, 30, 7077–7090.
- 65. Li, W.; Ando, Y.; Minamitani, E.; Watanabe, S. Study of li atom diffusion in amorphous Li3PO4 with neural network potential. J. Chem. Phys. 2017, 147, 214106.
- 66. Miwa, K.; Ohno, H. Interatomic potential construction with self-learning and adaptive database. Phys. Rev. Mater. 2017, 1, 053801.
- 67. Miwa, K.; Asahi, R. Molecular dynamics simulations with machine learning potential for Nb-doped lithium garnet-type oxide Li7-xLa3(Zr2-xNbx)O12. Phys. Rev. Mater. 2018, 2, 105404.
- 68. Wang, C.; Aoyagi, K.; Aykol, M.; Mueller, T. Ionic conduction through reaction products at the electrolyte–electrode interface in all-solid-state Li+ batteries. ACS Appl. Mater. Interfaces 2020, 12, 55510–55519.
- Fujimura, K.; Seko, A.; Koyama, Y.; Kuwabara, A.; Kishida, I.; Shitara, K.; Fisher, C.A.J.; Moriwake, H.; Tanaka, I. Accelerated materials design of lithium superionic conductors based on first-principles calculations and machine learning algorithms. Adv. Energy Mater. 2013, 3, 980–985.
- 70. Sendek, A.D.; Cheon, G.; Pasta, M.; Reed, E.J. Quantifying the search for solid li-ion electrolyte materials by anion: A data-driven perspective. J. Phys. Chem. C 2020, 124, 8067–8079.
- 71. Xie, W.; Liu, X.; He, R.; Li, Y.; Gao, X.; Li, X.; Peng, Z.; Feng, S.; Feng, X.; Yang, S. Challenges and opportunities toward fast-charging of lithium-ion batteries. J. Energy Storage 2020, 32, 101837.
- 72. Wu, B.; Widanage, W.D.; Yang, S.; Liu, X. Battery digital twins: Perspectives on the fusion of models, data and artificial intelligence for smart battery management systems. Energy AI 2020, 1, 100016.
- 73. Lyu, Z.; Gao, R. A model-based and data-driven joint method for state-of-health estimation of lithium-ion battery in electric vehicles. Int. J. Energy Res. 2019, 43, 7956–7969.
- 74. Lin, M.; Zeng, X.; Wu, J. State of health estimation of lithium-ion battery based on an adaptive tunable hybrid radial basis function network. J. Power Source 2021, 504, 230063.