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Battery Systems Engineering

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To our parents

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Preface

Energy storage is a critical and growing need in the drive to increase the efficiency and effectiveness of power systems. In the quest for higher fuel efficiency, energy storage is becoming increasingly important in ground transportation. Hybrid electric vehicles (HEVs) that recover the energy otherwise dissipated during braking are commanding a growing share of the passenger car, truck, and bus markets. Electric vehicles and plug-in HEVs charge using low-cost energy from the grid. Renewable energy sources such as wind and solar require energy storage to buffer power production deficits. Home energy storage can reduce costs by taking grid power during low-demand periods (e.g., at night) and reducing grid power during high-demand periods.

There are many ways to store energy (e.g., flywheels, ultra-capacitors, and compressed air) but batteries are the best choice for most applications. Batteries can be scaled from small (cell phone), to medium (HEVs), to large (grid) applications. They are highly efficient and have high energy-to-weight ratios. There are safe and recyclable designs. Cost and battery life, however, are concerns that prevent more widespread application of batteries for energy storage applications. Researchers are continually inventing lower cost and longer life battery chemistries. Efficient and life-extending battery management systems, designed using the techniques described in this book, can also address these concerns.

The dynamic environment of many energy storage applications requires battery management systems that are more advanced than would be required for a typical battery-powered device (e.g., laptop or cell phone). Simple battery-powered devices only require charging at periodic intervals and then draw low current, slowly discharging the pack until it is time to recharge again. HEVs, on the other hand, require fast and high-current energy storage associated with dynamic acceleration and braking of the vehicle. This rapid charge–discharge cycling of the battery pack requires sophisticated battery management systems to regulate the current in and out of the pack in real time. An effective battery management system sets the current limits low enough to maximize the battery life and ensure safety but high enough to maximize power output.

Battery systems engineering sits at the crossroads of chemistry, dynamic modeling, and systems/controls engineering, requiring a multidisciplinary approach. Battery chemists/engineers understand the electrochemistry and materials issues required to design batteries but may not have the background to address the complex mathematical modeling and control systems design required for efficient battery management algorithms. Mathematical modelers may be able to develop accurate models of battery cells but these models are often not easily adopted for systems engineering owing to the complexity of the underlying partial differential equations. Systems engineers have the controls and dynamics background to analyze, design, and simulate the system response but may not understand the underlying chemistry or modeling.

This book aims to develop the multidisciplinary area of battery systems engineering by providing the background, models, solution techniques, and systems theory that are necessary for the development of advanced battery management systems. Systems engineers in chemical, mechanical, electrical, or aerospace engineering who are interested in learning more about advanced battery systems will benefit from this text. Chemists, material scientists, and mathematical modelers can also benefit by learning how their expertise affects battery management. The book could be used in an advanced undergraduate technical elective course or for graduate-level courses in engineering.

We would like thank our students, post-doctoral scholars, and research associates for their help in the preparation of this book. In particular, Kandler Smith, Yancheng Zhang, Ying Shi, Githin Prasad, and Zheng Shen have made significant contributions to the text and deserve our thanks. Students who took the first two offerings of the course *Battery Systems Engineering* at Penn State have also provided comments and corrected typos, including Kelsey Hatzell, Ed Simoncek, Ryan Weichel, and Tanvir Tanim. Chao-Yang gratefully acknowledges his wife, May M. Lin, and daughters, Helen and Emily, for their constant love, support, and strength. I am likewise grateful for the love, support, and encouragement of my wife Jeanne, daughter Katelin, and sons Kevin and Matthew.

Christopher D. Rahn
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1

Introduction

High energy costs drive the development of power systems with increased efficiency and effectiveness. One way to increase performance is to store energy that cannot be used at the time of its production. Batteries are being used in hybrid vehicles and renewable energy applications for this purpose. These applications can require dynamic cycling of the battery that can lead to poor performance and premature aging if not controlled by a sophisticated battery management system (BMS). BMSs that are based on accurate system models hold great promise for extending the life and increasing the performance of energy storage systems. This chapter motivates the need for model-based battery system engineering and introduces the electrochemistry and design of battery cells and packs.

1.1 Energy Storage Applications

Energy storage is vitally important to many applications, ranging from small-scale portable electronics to large-scale renewable energy sources. Portable electronic devices that use batteries include video/audio players, medical equipment, power tools, meters and data loggers, and remote sensors [1]. In these applications, batteries free the user from power cords and enable portable use. The batteries in these devices are discharged over time and then recharged periodically. Energy storage can also be used in large-scale applications to reduce oil, gas, and coal consumption. Hybrid vehicles for ground transportation and renewable (e.g., wind and solar) energy sources make use of batteries to store energy that cannot be used at the time of its production. The charge and discharge cycles in these applications are more frequent and dictated by the variable power supply and demand.

To increase the fuel efficiency of ground vehicles, batteries are being used to supplement and sometimes replace the power provided by liquid fuel. Figure 1.1 shows four pioneering vehicles that use batteries to increase fuel efficiency and performance. The Toyota Prius in Figure 1.1a is a hybrid electric vehicle (HEV). It uses a nickel–metal hydride (Ni–MH) battery pack manufactured by Panasonic. The Nissan Leaf and Tesla Roadster in Figure 1.1b and d, respectively, are electric vehicles (EVs). The Leaf uses a laminated lithium-ion (Li-ion) battery pack developed by Nissan–NEC and the Tesla uses a specially built pack with thousands of

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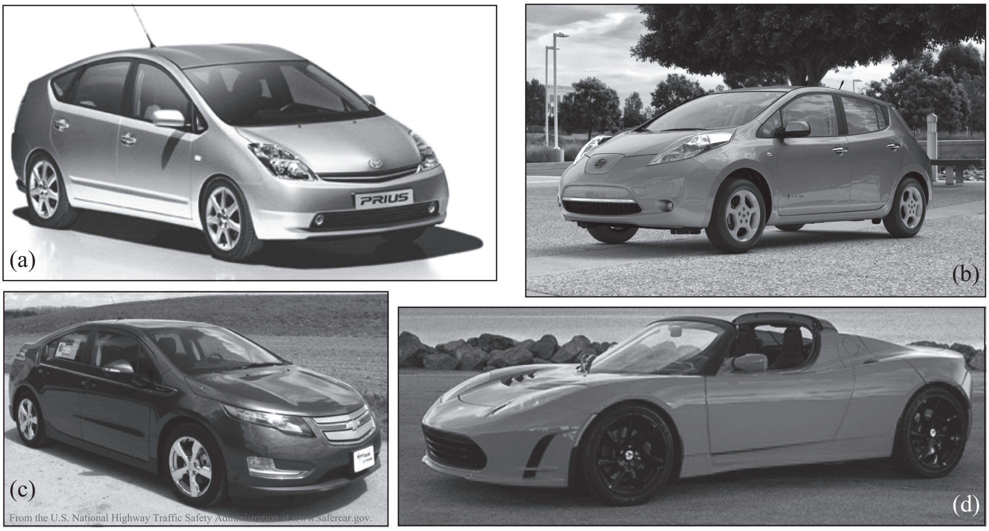

Figure 1.1 Pioneering hybrid vehicles: (a) Toyota Prius (© Toyota). (b) Nissan Leaf (© 2012, Nissan. Nissan, Nissan model names and the Nissan logo are registered trademarks of Nissan). (c) Chevrolet Volt (photo taken by US National Highway Traffic Safety Administration). (d) Tesla Roadster (© Tesla Motors, Inc.)

18650 (18 mm diameter and 65 mm long) Li-ion cells. The Chevy Volt in Figure 1.1c is a plug-in HEV (PHEV) or extended-range electric vehicle (EREV) that has a Li–polymer battery pack supplied by LG-Chem.

HEVs are commanding a growing share of the passenger car, truck, and bus markets. Hybrid powertrains consist of an internal combustion engine (ICE), powertrain, electric motor, and batteries. HEVs conserve energy because they have the ability to:

1. **Eliminate engine idling.** The engine stops when the vehicle is stationary.
2. **Recover and store energy.** The electric motor is used as a generator to brake the vehicle. The regenerated energy is stored in the batteries.
3. **Boost power.** The electric motor and engine work together to increase torque during acceleration.
4. **Operate efficiently.** The engine can be run at its most efficient speed and the electric motor can provide power during off-peak operation.

HEVs vary in cost and complexity from simple retrofits to complete redesigns of existing ICE vehicles. Micro hybrids use a higher power starter/alternator to provide the advantages of eliminating engine idling. Soft hybrids add some regenerative braking and low-speed movement under electric power. Mild hybrids insert an electric motor/generator into the drive axle to provide all of the benefits of hybrid operation. The parallel drive train often used in mild hybrids allows the electric motor/generator to run the vehicle and boost power at low speeds. Full hybrids often use a series/parallel drive train that has all of the benefits of the parallel drive train. They can be used to decouple the motor speed from the vehicle speed so that the motor can run more often at peak efficiency. Full hybrids are the most efficient and complicated HEVs, with the batteries carrying a larger percentage of the load, continually being charged and discharged.

The battery packs in PHEVs charge directly from the electric grid and run the vehicle for a distance in pure electric mode with zero gas consumption and emissions. The vehicle also has an ICE that can be used to extend the electric-only range or increase the speed above the electric-only limit. After the batteries have been depleted to a specified level, the vehicle operates in full hybrid mode until it can be fully recharged from the grid. The Chevrolet Volt PHEV uses a variation on the series drivetrain where the engine drives a generator and is not mechanically connected to the drive wheels. A series drivetrain cannot use the engine and electric motor simultaneously to provide a power boost for quick acceleration.

EVs are zero-emission vehicles that charge from the grid. Batteries provide all of the power and energy for the drive motor. The key consideration in the design of an EV is the weight and cost of the battery pack. Lighter weight batteries typically cost more. The batteries are charged and then slowly discharged during operation, with regenerative braking providing intermittent recharge pulses.

The charging infrastructure required for EVs is a major challenge to the widespread adoption of this technology. Chargers at home or work can take hours to charge the battery for an EV or PHEV without too much inconvenience to the driver. If an EV is on the road and needs a quick charge, however, the infrastructure for fast (5 min) charging should be widely available. The charging power for a 5 min charge is 12 times the power that the pack can provide for 1 h. Long-range (300 mi) EVs require roughly a 75 kWh pack, so a 5 min charge would require 0.9 MW from the grid. As more and more EVs with longer and longer ranges replace gas-powered vehicles, the power grid infrastructure will need to drastically increase to accommodate the increased demand.

Passenger cars make up the bulk of the HEV market, but trucks and buses have also been converted to HEVs and EVs. Figure 1.2 shows, for example, an all-electric switchyard locomotive developed by Norfolk Southern. The locomotive is charged during the night and then is used for an 8 h shift, moving freight cars around the yard to form trains. Over 1000 lead–acid (Pb–acid) batteries are used to power the electric traction motors.

Renewable energy sources such as wind and solar and smart-grid technology require energy storage to buffer power production deficits. Wind and solar energy sources do not produce energy at a continuous rate. Energy produced in excess of demand can be stored in large-scale battery farms to be used at a later time. Home energy storage can reduce costs by taking grid power during low-demand periods (e.g., at night) and reducing grid power during high-demand periods. A smart grid regulates the power delivered to individual homes so that household energy storage can bridge the power gaps.

1.2 The Role of Batteries

There are many ways to store energy (e.g., flywheels, ultra-capacitors, and compressed air), but batteries are the best choice for most applications. Batteries can be scaled from small (cell phone), to medium (HEVs), to large (grid) applications. They are highly efficient and have high energy-to-weight ratios. They are safe and often recyclable. Cost and battery life, however, are concerns that prevent more widespread application of batteries for energy

Figure 1.2 Norfolk Southern Electric switchyard locomotive, NS999 (photo courtesy of Norfolk Southern Corp.)

storage applications. Researchers are continually inventing lower cost and longer life battery chemistries. As batteries become integral parts of high-volume products, economies of scale will reduce costs. A life-extending BMS, designed using the techniques described in this book, ensures that the battery pack is being used in a most efficient and cost-effective manner.

1.3 Battery Systems Engineering

Battery systems engineering sits at the crossroads of chemistry, dynamic modeling, and systems engineering. Battery chemists/engineers understand the electrochemistry and materials issues required to design batteries but may not have the background to address the complex mathematical modeling and control systems design associated with efficient battery management algorithms. Mathematical modelers can develop accurate models of battery cells but these models are often not easily adopted for systems engineering. Systems engineers have the controls and dynamics background to analyze, design, and simulate the system response but may not understand the underlying chemistry or models.

One of the main objectives of this book is to bring batteries into the realm of systems engineering. From a systems engineering perspective, battery packs are multi-input, multi-output systems. The primary input, current, is prescribed by the supply and demand from the powered device. The primary output is the battery voltage. Other outputs include temperature,

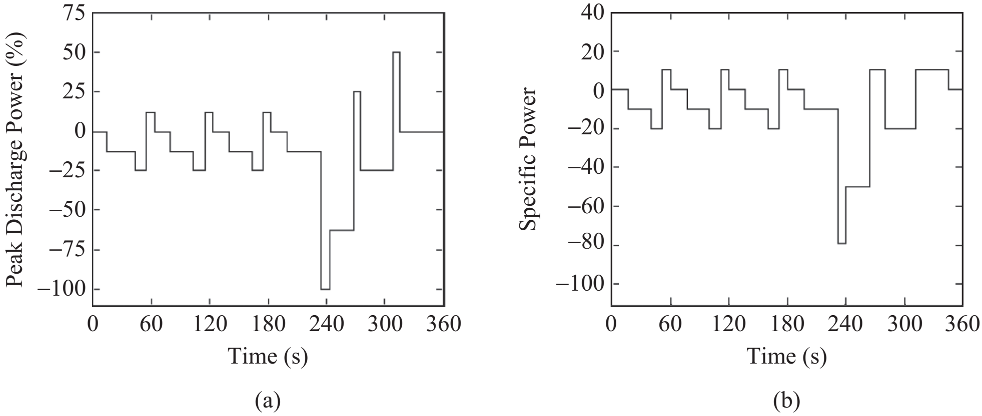

Figure 1.3 Battery cycling profiles for HEVs: (a) dynamic stress test (DST) and (b) simplified federal urban driving schedule (SFUDS)

individual battery or cell voltages, and ionic concentration distributions within a given cell. Systems engineers need cell, battery, and pack models in standard (e.g., state variable and transfer function) forms that can be used to predict, estimate, and control these outputs.

The dynamic environment of many energy storage applications requires advanced BMSs. BMSs are often concerned with charging protocols because applications require fully charging the pack at periodic intervals. The battery-powered device (e.g., laptop) then draws low current, slowly discharging the pack until it is time to recharge again. An HEV, on the other hand, requires fast and high-current energy storage associated with dynamic acceleration and braking of the vehicle. Figure 1.3 shows, for example, two HEV battery cycling profiles. The power into and out of the battery pack changes quickly over the 6 min cycles. This rapid charge–discharge cycling of the battery pack requires sophisticated BMSs to regulate the current in and out of the pack in real time. An effective BMS sets the current limits low enough to maximize the battery life and ensure safety but high enough to maximize power output.

Figure 1.4 shows a schematic diagram of the electromechanical system of an HEV. The battery system consists of cells grouped into modules that make up the battery pack, the BMS, and the thermal management system. The power electronics interface the battery system to the motor/generator that is mechanically coupled to an ICE through a transmission. The power electronics typically include high-power switching circuits, inverters, DC–DC converters, and chargers. The transmission either connects both the motor/generator and the engine to the wheels (parallel configuration), only the motor/generator to the wheels (series configuration), or some combination of the two (hybrid configuration).

While there are significant challenges in the development of new battery chemistries, power electronics, and motor/generators for HEV/PHEV/EV application, the focus of this book is on the dynamics of commercially available cells/packs and the development of estimation/control software that runs on-board the vehicle. The dynamic models can be used to simulate and optimize the system response. The software is based on the developed models and predicts and controls the battery-pack response to optimize performance and long pack life. Batteries

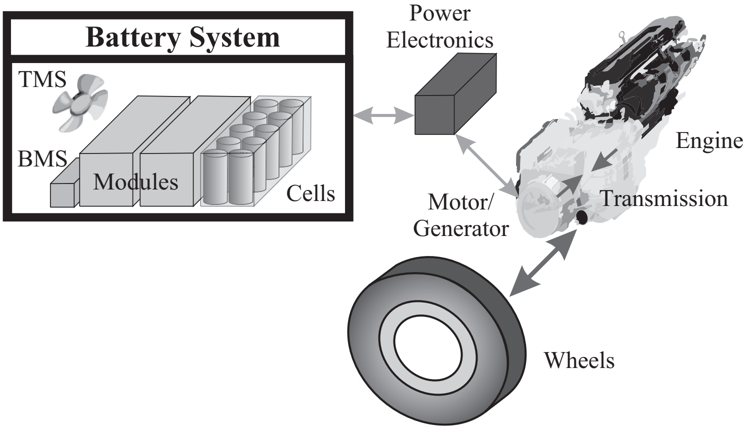

Figure 1.4 PHEV electromechanical system schematic

are the highest cost item in HEV, PHEV, and EV powertrains, so their optimal utilization is paramount to the development of affordable vehicles.

1.4 A Model-Based Approach

Batteries can be designed using empirical or model-based approaches. In an empirical approach, cells are built and tested for performance. Based on the results of the tests, the batteries are redesigned and tested again. This is a time-consuming and expensive process. In a model-based approach, a model is used to predict performance based on the battery design. This process is termed computer-aided engineering (CAE) because the battery can be designed and optimized relatively quickly on a computer. Model-based design ensures that the batteries developed have the highest possible performance, making them competitive in the marketplace.

A model-based approach builds upon a fundamental physics-based model that predicts the battery response. The model starts with the electrochemical and physical partial differential equations (PDEs) that govern the flow of ions through a battery cell. The model requires knowledge of geometric parameters (e.g., lengths, areas) that can be independently measured, physical constants (e.g., Faraday constant), and parameters that may not be independently measurable and/or known (e.g., diffusion coefficients). Given a time-varying battery input current, the model predicts the battery time response, including output voltage. The best models have parameters that are all measured independently and performance that closely matches experiments. The unknown parameters in a model provide extra knobs for the modeler to adjust to get good agreement with the experimental data. The process of model validation includes testing the model under a variety of inputs and minimizing the error between the model-predicted and experimental responses. Once the model has been validated, the input parameters can be varied according to different battery designs and the performance predicted. Thus, the battery can be optimized for maximal performance.

BMSs can also be designed using empirical or model-based approaches. Almost all BMSs rely on battery models, but the sophistication varies considerably. At the lowest level, heuristic models that roughly predict the observed performance are used. More advanced empirical models that fit equivalent circuits to the measured response over a specified frequency bandwidth have been applied extensively. The most advanced BMSs, however, are based on fundamental models of the batteries. These models are more difficult to derive and simplify for real-time applications, but they are based on the underlying physics and electrochemistry of the battery. The relationships between the response and system parameters are known. Fundamental model-based controllers have a built-in understanding of the underlying processes, allowing them to be more efficient, accurate, and safe.

1.5 Electrochemical Fundamentals

Figure 1.5 shows a schematic diagram of a battery cell. It consists of positive and negative electrodes immersed in an electrolyte solution. The electrodes can be solid material or porous to allow the electrolyte to infiltrate through. The separator prevents electrons from flowing but allows positive and negative ions to migrate between the two electrodes through the electrolyte. The positive and negative current collectors provide a pathway for electrons to flow through an external circuit. During discharge, the negative electrode is the anode and the positive electrode is the cathode. Positive ions move from the anode to the cathode through the electrolyte and separator. Negative ions move in the opposite direction. The anode builds up negative charge and the cathode builds up positive charge, creating the cell voltage $V(t)$. Negatively charged electrons flow through an external load from the anode to the cathode, creating a current in the opposite direction. The sign convention for positive current is in the opposite direction of the

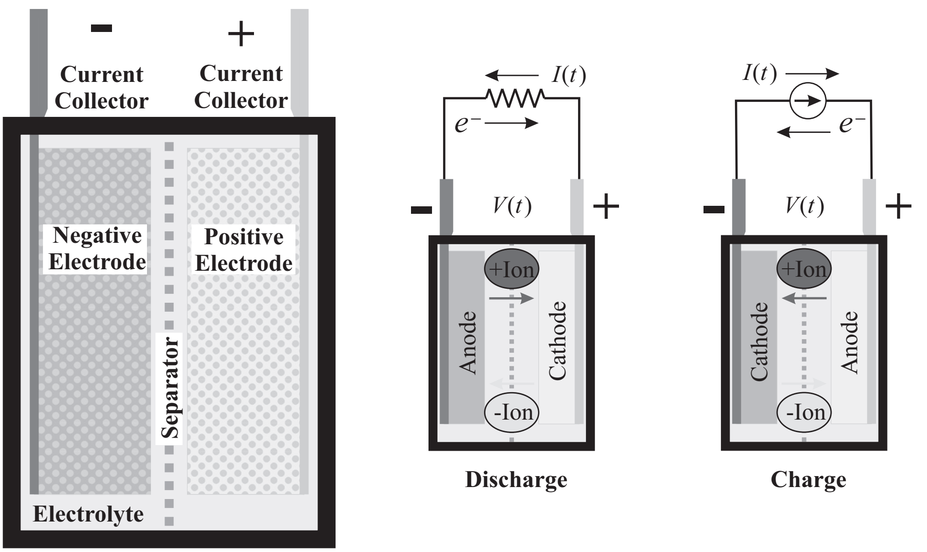

Figure 1.5 Simple cell under discharge and charge

electron flow. During charge, the process is reversed and electrons are forced into the cathode (now the negative electrode).

During charging, the negative electrode material dissolves in the electrolyte solution to form a positive ion and an electron in what is called an oxidation reaction. The positive electrode consumes electrons by depositing positive ions from the electrolyte in what is called a reduction reaction. The reactions are reversible in secondary (or rechargeable) batteries so that discharging the batteries returns the electrodes to their pre-charged states. The ions move through the electrolyte under diffusion and migration. Diffusion results from the existence of a concentration gradient in the electrolyte. Over time, if there is no ion production, the ions in the electrolyte diffuse evenly throughout the cell. Migration results from the presence of the electric field generated by the positive and negative electrodes. The positive ions migrate toward the negative electrode and the negative ions migrate toward the positive electrode. The movement of ions through the electrolyte and electrons through the external circuit enable the storage and release of energy.

1.6 Battery Design

Batteries come in all shapes and sizes, but the most common form factors are either prismatic (generally a rectangular prism) or cylindrical. Figure 1.6 shows Pb–acid and Ni–MH batteries and battery packs from Panasonic. The valve-regulated lead–acid (VRLA) batteries are prismatic and the Ni–MH batteries are manufactured in both cylindrical and prismatic form factors. The HEV battery pack shown in Figure 1.6(c) is made from many prismatic Ni–MH batteries.

VRLA batteries are typical of what one sees in ICE vehicles for starting, lighting, and ignition. Pb–acid cells produce around 2 V, so the batteries consist of several cells in series to produce the desired voltage of, for example, 6 V (three cells) or 12 V (six cells). A fully charged 12 V VRLA battery, however, can produce almost 15 V and be discharged to 8–10 V. The battery consists of lead plates and separators immersed in a diluted sulfuric acid electrolyte. Alternating plates of Pb and PbO_2 form the negative and positive electrodes, respectively. The current (and power) of the battery is proportional to the plate area. The battery case has a vent that opens if the internal pressure builds up to a sufficiently high level due to extreme overcharge conditions.

Figure 1.6 Panasonic batteries: (a) VRLA, (b) Ni–MH, and (c) Ni–MH pack (© Panasonic)

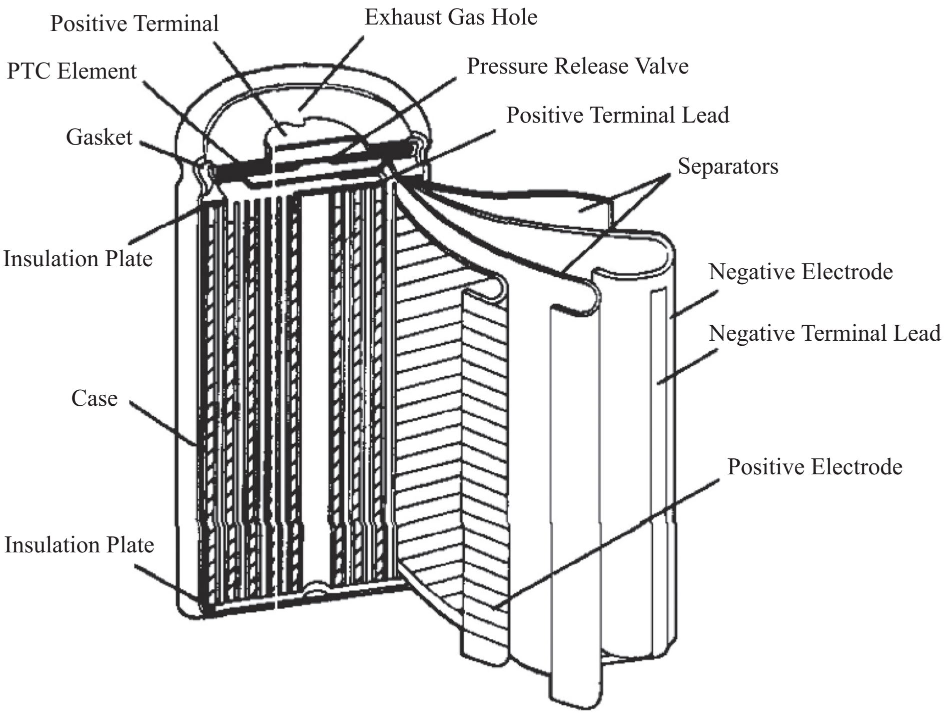

Figure 1.7 Panasonic Li-ion cylindrical cell design (© Panasonic)

The design of a Panasonic Li-ion cylindrical cell is shown in Figure 1.7. The battery is fabricated from four layers of material that are rolled up to form a cylinder. The layers are the positive electrode, separator, negative electrode, and then a second separator. The second separator layer keeps the positive and negative electrodes apart in the rolled configuration. Leads connect the positive electrode to the top terminal and the negative electrode to the bottom terminal. Li-ion batteries have a nominal voltage of over 3 V. To form higher voltage batteries, the cylindrical cells are stacked in series and sealed together. Higher current can be obtained by increasing the electrode area, resulting in a larger diameter or longer length cell.

The sealed prismatic Ni–MH cells shown in Figure 1.6b also have the same layered structure as cylindrical cells, but the layers are not rolled up. These layers can be stacked to increase the battery voltage from the nominal Ni–MH cell voltage of around 1 V. Prismatic cells are often easier to integrate into HEV packs like the one shown in Figure 1.6c. Packs connect individual batteries in series and parallel to raise the voltage and current to the desired values, respectively.

1.7 Objectives of this Book

The main objective of this book is to provide the framework for battery systems engineering as a viable field of study. The importance of batteries in energy consumption and production is growing. Batteries are often the most expensive and least well understood parts of these complex systems. This book targets design engineers who are not sufficiently familiar with batteries to be able to analyze, integrate, and optimize them as part of a more complicated system. We intend to provide a self-contained, fundamental approach to the modeling, analysis, and design of battery systems that places them within the same framework of mechanical, electrical, fluid, thermal, and computer models that engineers use to design complex mechatronic systems like HEVs and renewable energy plants.

To achieve this objective, we first develop battery models that can be understood and used by systems engineers with limited electrochemistry backgrounds. These models are well known for the Pb–acid, Ni–MH, and Li-ion chemistries discussed in Chapter 2. New battery chemistries that are developed in the future will undoubtedly use the same building blocks of conservation laws and reaction kinetics that provide the governing equations presented in Chapter 3. The focus is not on electrochemistry and the derivation of the governing equations, but on how to convert these distributed parameter models to standard forms that are commonly used by systems engineers. In Chapter 4 we study methods of spatially discretizing the underlying PDEs to reduce them to ordinary differential equations with one independent variable: time. These state-variable models are well known to systems engineers and form the basis of mechatronic systems analysis, design, and control. These models are then simulated in Chapter 5 to predict the charge–discharge, cycle, and frequency response. In Chapter 6, complete models of Pb–acid, Ni–MH, and Li-ion cells are presented and simulated using the techniques developed in Chapters 2–5.

Second, we use these models to calculate the battery system response, estimate the internal states and parameters, and develop advanced BMSs. Systems design relies on analysis and simulation to estimate and optimize performance. The models developed in this book provide systems engineers with the tools to integrate batteries with the rest of the mechatronic system. State of charge (SOC) and state of health (SOH) estimators developed in Chapter 7 provide real-time measurements of the energy stored in the batteries and the total capacity of the batteries, respectively. Rather than using heuristic or empirical approaches, we can use the models developed to hard-wire the battery dynamics in the estimators developed, improving the accuracy and robustness of SOC and SOH estimation. Finally, the model-based BMSs discussed in Chapter 8 promise to deliver safe, efficient, and cost-effective battery systems for a variety of energy storage applications.

2

Electrochemistry

In this chapter we discuss the electrochemistry of three leading battery types: Pb–acid, Ni–MH, and Li-ion. For each battery type, the anode and cathode reactions are discussed, potential side reactions are introduced, and aging mechanisms are described. Finally, the performance of the battery chemistries is compared, including energy and power mass and volume densities, cost, and cycle life.

2.1 Lead–Acid

Pb–acid batteries are a relatively old technology that maintain 40–45% of the battery market, mainly due to their extensive use as starting, lighting, and ignition (SLI) batteries in automobiles, trucks, and buses [2]. They are also attractive for HEV and energy storage applications owing to their relatively high round-trip efficiencies of 75–80%. VRLA batteries are modern Pb–acid designs that immobilize the electrolyte using either highly porous and absorbent mats or a fumed silica gelling agent. Figure 2.1 shows an Enersys VRLA battery that uses adsorbed glass mat (AGM) plate separators to immobilize the electrolyte and allow ionic but not electrical conduction.

Figure 2.2 shows a schematic diagram of a VRLA battery cell composed of a positive electrode and a negative electrode with a separator in between that acts as an electronic insulator. All three components are porous and wholly or partially filled with an electrolyte (either liquid or solid). The electrolyte is an electronic insulator but a good conductor of the ionic species inside the cell. A gas phase may also be present in the cell if it is overcharged or overdischarged. The formation of gas phase is a side reaction that is not desirable and can lead to unsafe conditions and/or reduced battery life.

Reversible electrochemical reactions at the two electrodes allow the battery to be charged and discharged. The positive electrode is coated with lead oxide (PbO_2) and the negative electrode is made from Pb. Sulfuric acid (H_2SO_4) diluted with water (H_2O) acts as the electrolyte. The sulfuric acid dissociates into positive hydrogen ions (H^+) and negative ions (HSO_4^-) in water. At the negative electrode, Pb reacts with an HSO_4^- ion to produce lead sulfate ($PbSO_4$), an

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Figure 2.1 Enersys VRLA group 31 battery (reproduced by permission of EnerSys)

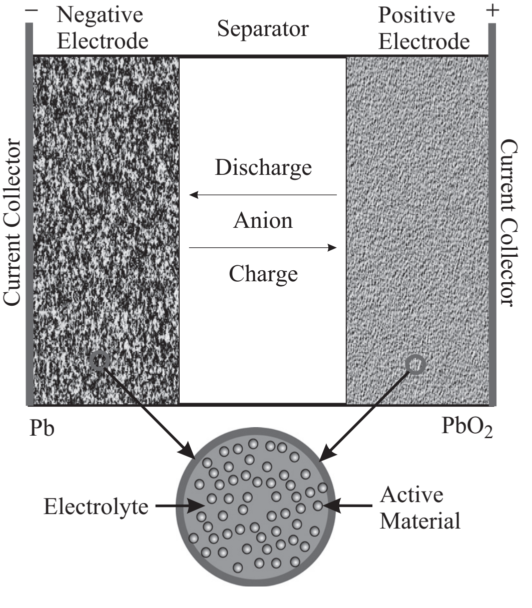

Figure 2.2 Schematic diagram of a Pb–acid cell