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Application of Software Modeling and Simulation in Lithium-ion Battery Teaching

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Abstract: *The rapid development of lithium-ion battery industry has put forward an urgent demand for qualified and efficient practical personnel. New energy technologies/ materials include lithium-ion batteries, fuel cells, photovoltaic cells, hydrogen energy, etc. Lithium-ion battery teaching content is an important component of new energy technology/materials courses. How to introduce software simulation into lithium-ion battery classroom teaching is the focus of this paper. This paper introduces the structure diagram, working principle, concept and aging mechanism of lithium ion battery related to software simulation technology. Combining software simulation technology with classroom teaching can play a complementary role. Software simulation technology can strengthen the basic knowledge and the application scenario of lithium ion battery. Classroom teaching can provide foundation and theoretical support for software modelling.*

Keywords: *modelling, structure diagram, working principle, concept, aging mechanism*

1. Introduction

New energy is one of the important means to solve the energy crisis and environmental problems, which has achieved rapid development. In view of the rapid development of new energy technology/materials, many colleges and universities in China have set up new energy materials and devices majors, and many majors have opened new energy materials/technology. Ordos institute of technology is the first undergraduate college named “Applied Technology” approved by the Ministry of Education during the transformation and development of local colleges and universities in China. In response to the national policy of vigorously developing new energy technologies, the department of chemical engineering of ordos Institute of Technology has opened a new energy technology/materials course. Lithium-ion battery is an important part of new energy materials/technologies. The modeling and simulation of lithium-ion battery is a necessary tool to realize rapid understanding of battery and battery system, optimization of design scheme, and design of automatic control system.

These simulation tools enable the analysis of unrestricted parameters and process conditions at a relatively low cost, followed by the necessary validation of the model through experimental testing. Similarly, the modeling and simulation of lithium-ion battery is also important for the teaching of lithium-ion battery materials and technologies. In this paper, the structure diagram, working principle, concept and aging mechanism of lithium-ion battery in software modeling and simulation are integrated into the teaching of lithium-ion battery materials and technology.

2. Application of simulation modeling software in the structure diagram of lithium ion battery

The battery is constructed by winding a laminated bi-battery sheet into a spiral, which is placed in a cylinder and filled with liquid electrolyte. The battery model consists of the following parts: negative electrodes, positive porous electrodes, negative current collector, positive current collector, separator regions [1]. The geometric configuration of spiral wound cylindrical lithium-ion battery in this paper was drawn using Comsol Multiphysics software. On the right of Figure 1, from top to bottom, are positive tab, positive current collector, positive porous electrode, separator, negative porous electrode, negative current collector, negative porous electrode, separator, positive porous electrode, positive current

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collector, positive porous electrode, separator, and so on. The model helps students familiarize themselves with the construction of cylindrical lithium-ion batteries.

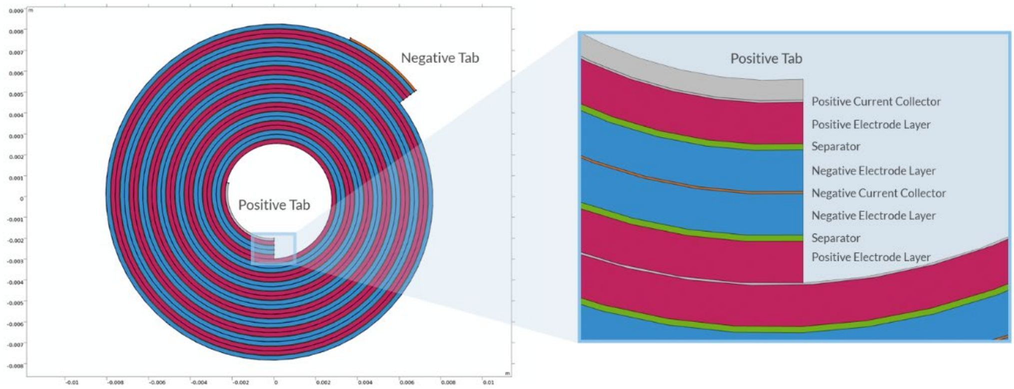

Figure 1: Modeled geometry. Spirally wound bi-battery in circular casing filled with liquid electrolyte.

3. Application of simulation modeling software in working principle of lithium ion battery

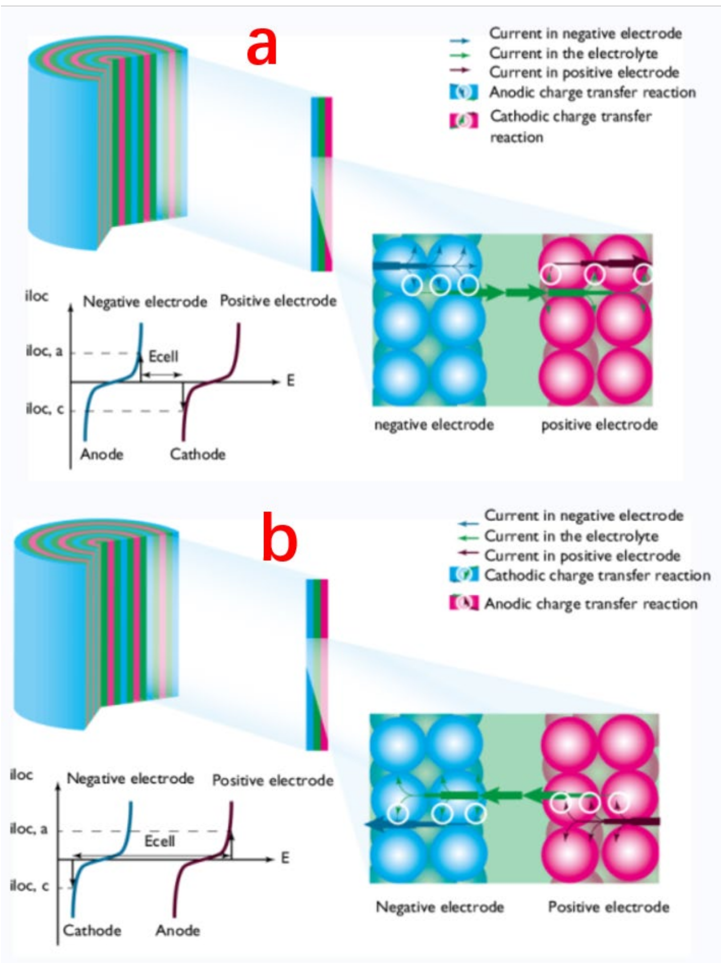

Figure 2a: Direction of the current and charge transfer current during discharge in a battery with porous electrodes.

Figure 2b: During charge, the positive electrode acts as the anode while the negative one acts as the cathode.

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A standard lithium-ion battery consists of positive porous electrodes, negative positive electrodes, and porous separators between positive porous electrodes and negative positive electrodes. During the charging and discharging process of lithium ion battery, the following processes will occur: charge transfer reaction on the surface of active electrode material, mass transfer (diffusion and migration) in electrolyte, lithium diffusion in active electrode material particles, changes in charge of active electrode material, electric conductor and double electric layers on other surfaces, contact impedance between conductive materials [2].

The charging and discharging processes are shown in Figure 2a and Figure 2b, respectively. And the schematic diagram of the charging and discharging principle of lithium ion battery is shown in Fig. 3.

Combined with Fig. 2 and Fig. 3, during the discharge process, the chemical energy is converted into electrical energy. Lithium ions are de-intercalated from the negative electrode into the positive electrode through the diaphragm, so that the positive electrode reaches a lithium-rich state. The lithium ions entering the surface of the positive electrode are re-diffused into the inside of the positive electrode, and the electrons flow from the negative current collector to the positive current collector. During the charging process, electrical energy is converted into chemical energy, and lithium ions are de-intercalated from the positive electrode to the negative electrode through the separator, so that the negative electrode reaches a lithium-rich state. Lithium ions entering the surface of the anode diffuse into the interior of the anode.

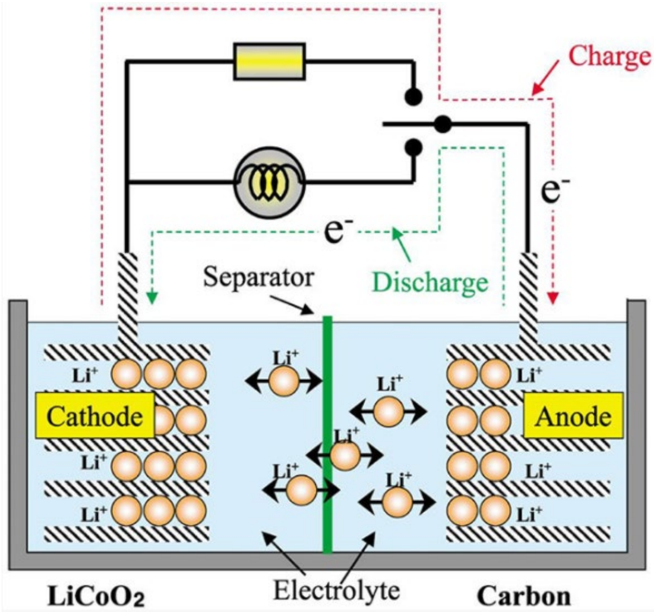

Figure 3: Charging and discharging principle diagram of lithium ion battery.

4. Application of simulation modeling software in concept teaching of lithium-ion battery

The equilibrium potential [3] is the potential when the net current at the electrode electrolyte interface is zero.

$$E_{eq} = \phi_{s,eq} - \phi_{l,eq} \tag{1}$$

Overpotential [3] is the difference between the potential at which an electrode reaction deviates from equilibrium and the equilibrium potential of the electrode reaction.

$$\eta = \phi_s - \phi_l - E_{eq} \tag{2}$$

Battery voltage [4] is the voltage at the positive current collector.

$$E_{cell} = \varphi_S \big|_{ccpos} \tag{3}$$

The voltage of each electrode is the difference between the voltage at the collector where the electrode is located and the voltage at the separator.

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$$E = \varphi_S\big|_{cc} - \varphi_L\big|_{sep} \tag{4}$$

Battery internal resistance is the ratio of the difference between open circuit voltage and battery voltage to current.

$$R = \left.\frac{E_{OCV,cell}(SOC) - E_{cell}}{-I}\right|_{t=10s} \tag{5}$$

Battery efficiency is the ratio of output energy to input energy.

$$\eta_e = \frac{W_{out}}{W_{in}} = \frac{\int_{t_{out,1}}^{t_{out,2}} (I \bullet E_{cell})dt}{\int_{t_{in,1}}^{t_{in,2}} (I \bullet E_{cell})dt} \tag{6}$$

The overall SOC of the battery is the ratio of the amount of lithium that can be recycled by the battery negative electrode to the sum of the amount of lithium that can be recycled by the battery positive and negative electrodes.

$$SOC_{cell} = \frac{\int_{\Omega_{neg}} c_{s,avg,cycl} F \varepsilon_S d\Omega}{\int_{\Omega_{neg}} c_{s,avg,cycl} F \varepsilon_S d\Omega + \int_{\Omega_{pos}} c_{s,avg,cycl} F \varepsilon_S d\Omega} \tag{7}$$

Recyclable lithium concentration is the difference between the electrode concentration and the product of minimum SOC and maximum concentration

$$C_{s,avg,cycl} = C_{s,avg,electrode} - SOC_{\min} C_{s,\max} \tag{8}$$

5. Application of software modeling inthe teaching of lithium-ion battery aging mechanism

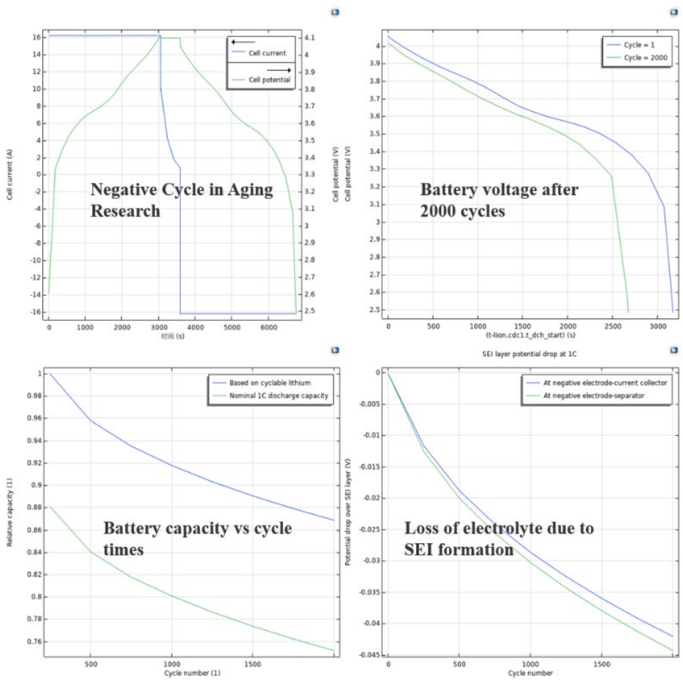

Figure 4: Formation mechanism and calculation results of SEI film [5, 6].

SEI membrane is a side reaction generated in the lithium-ion migration process of lithium ion batteries.

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It will reduce the efficiency of lithium ion batteries, and will lead to the loss of active lithium or electrolyte, reducing the porosity of porous electrodes.

The aging of lithium-ion battery means that the capacity of lithium-ion battery declines, which affects the battery life. There are many reasons for the aging mechanism of lithium ion batteries, such as SEI film generation, stress aging, lithium precipitation, gas generation, corrosion, *etc.* [5]. Formation mechanism and calculation results of SEI film are shown in Fig.4.

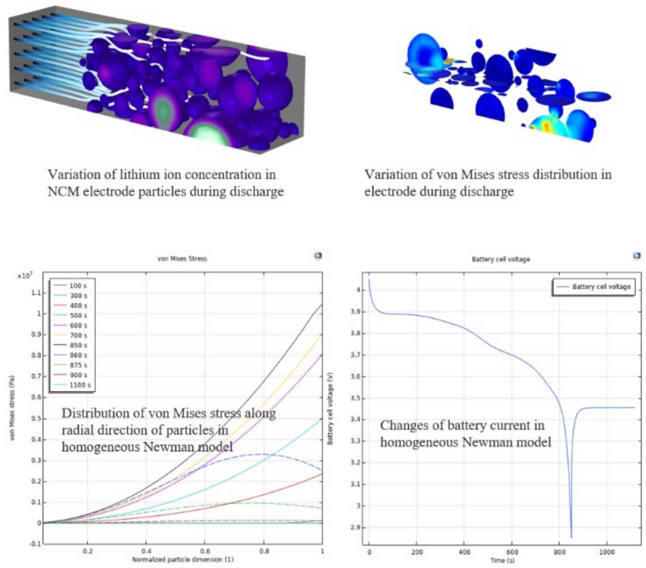

Figure 5: Mechanical aging mechanism and calculation results [7-8].

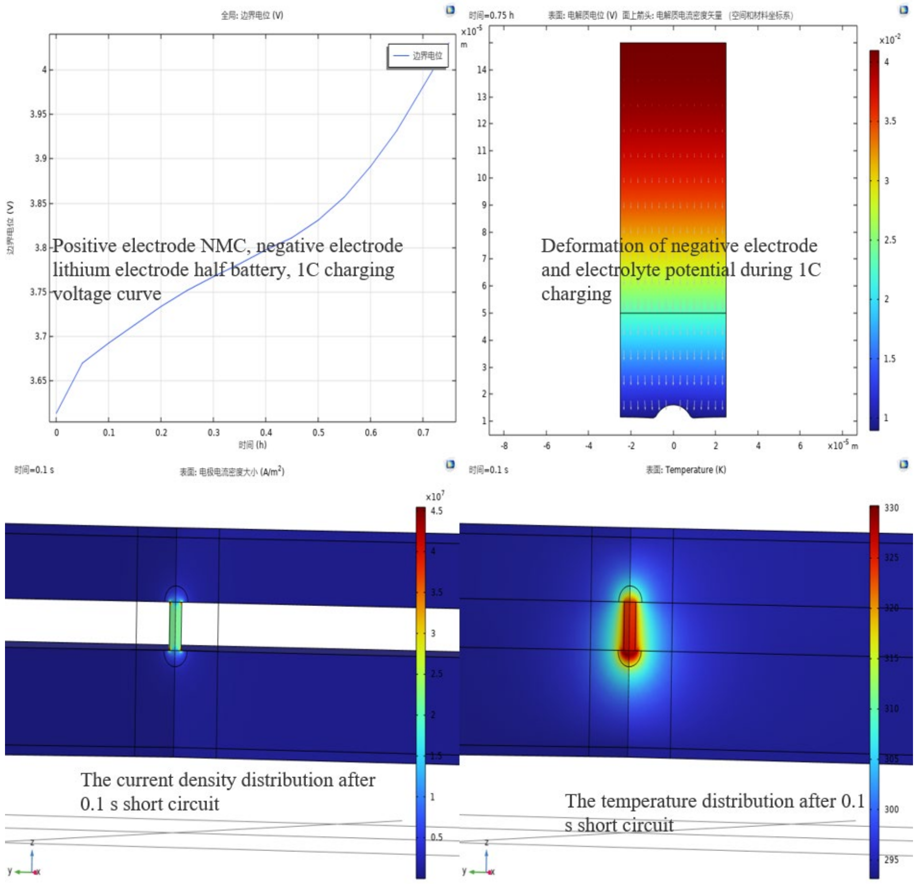

Figure 6: Lithium evolution mechanism and calculation results [9].

Figure 5 shows mechanical aging mechanism and calculation results. Lithium ions are embedded in the crystal structure of graphite particles, and the particles expand with the increase of lithium content. When lithium leaves the particle, the particle shrinks, resulting in stress and strain in the particle. Repeated expansion and contraction cycles will lead to a lot of cyclic fatigue. The neck between particles has the highest stress, which is the place where the crack finally forms.

Figure 6 shows lithium evolution mechanism and calculation results. Lithium evolution is a process in which lithium ions are reduced to lithium metal on the surface of active particles or on the collector fluid. Lithium precipitation can lead to the formation of lithium dendrites, which pierce the separator and cause internal short circuit. At first, the short circuit will produce hot spots. The dendrites with a thickness of 10μm will make the temperature reach about 55 ℃, accelerating the aging. Eventually, this can lead to battery failure. As SEI is easier to form on lithium metal, the risk of SEI formation increases with lithium precipitation.

6. Conclusions

The rapid development of new energy industry, especially lithium-ion batteries industry, has put forward an urgent demand for qualified and efficient practical personnel. Lithium-ion battery teaching content is an important component of new energy technology/materials courses. In this paper, software simulation is introduced into lithium ion battery classroom teaching. This paper focuses on the structure diagram, working principle, concept and aging mechanism of lithium ion battery related to software simulation technology. Combining software simulation technology with classroom teaching can play a complementary role. Software simulation technology can strengthen the basic knowledge and the application scenario of lithium ion battery. Classroom teaching can provide foundation and theoretical support for software modeling.

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