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Review

Lithium ion rechargeable batteries: State of the art and future needs of microscopic theoretical models and simulations

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ABSTRACT

This review deals with the recent developments and present status of the theoretical models for the simulation of the performance of lithium ion batteries. Preceded by a description of the main materials used for each of the components of a battery -anode, cathode and separator- and how material characteristics affect battery performance, a description of the main theoretical models describing the operation and performance of a battery are presented. The influence of the most relevant parameters of the models, such as boundary conditions, geometry and material characteristics are discussed. Finally, suggestions for future work are proposed.

Contents

1. Introduction

The XX and XXI centuries are characterized by rapid technological advances, in particular in the electronics, informatics and communication industries. The development of products such as computers, mobile phones, tablets and other portable devices lead to an increasing need for battery autonomy and performance [1–3]. Increasing battery performance (Fig. 1) is associated to the use of novel materials and concepts leading to increasing loading capacity, cycle life and safety [4–7]. Fig. 1 illustrates the evolution of batteries with respect to energy density.

Nowadays, large attention is being paid to the development of batteries for the automobile industry in order to reduce fossil fuel dependence and emission gases responsible for the greenhouse effect and therefore to reduce the environmental impact associated to the energies used for mobility [8–10].

The main goal of the battery industry is to obtain specific levels of battery performance for the different applications (e.g. applied

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voltage and capacity) with low production costs. In this context, intensive research is being devoted to the development of rechargeable or secondary batteries [11,12].

For many years, nickel–cadmium batteries (Ni–Cd) were the most suitable for portable communications systems and computing equipments. However, at the beginning of the 90s, lithium ion batteries increased in attention and acceptance by consumers. Nowadays, lithium ion batteries are the most widely used and still show a promising growth potential [13,14]. The pioneering work with lithium ion batteries began in 1912 and it was in the 70s that the first non-rechargeable lithium ion batteries were commercialized [15,16]. Lithium is the lightest of all metals, showing a large electrochemical potential and high energy density relative to its weight [17]. Several attempts to develop rechargeable lithium ion batteries failed due to safety problems [18,19], associated to the inherent instability of lithium metal, in particular during the charge cycle.

The lithium ion is safe provided that certain precautions are taken during battery charge and discharge cycles. The safety of the lithium-ion battery is one of the key issues for improving the performance of the battery. Thus, the interest in developing lithium-ion batteries increased and in 1991 the Sony Corporation commercialized the first lithium-ion batteries [20].

For increasing battery performance and optimizing materials and designs it is critical to have suitable theoretical models that allow battery simulation. The mathematical theoretical models for lithium-ion batteries describe the physical processes and mechanisms of the different components of the batteries and are essential for optimizing performance, design, durability and safety of lithium-ion batteries.

Mathematical models for lithium ion batteries have been developed at different scales of battery operation from the macro to the nano scales [21].

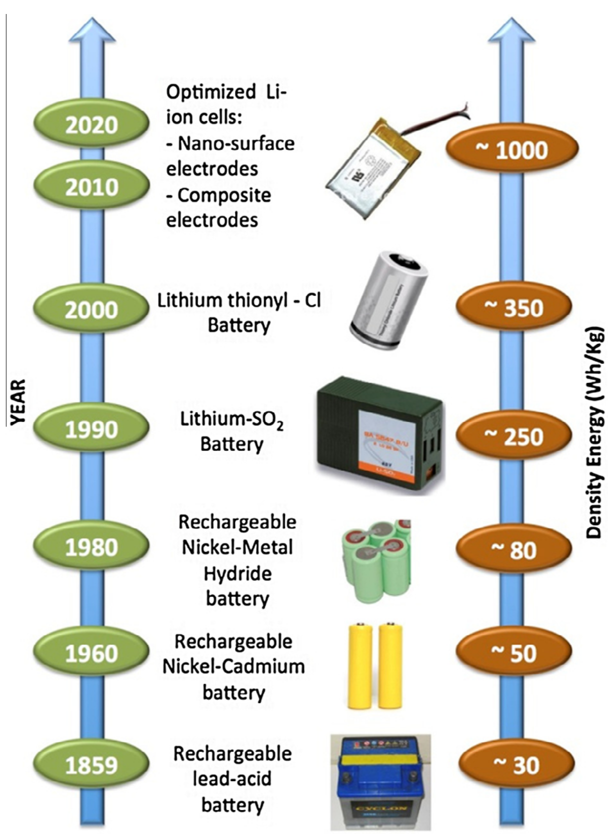

Fig. 1. Battery evolution with respect to their energy density.

The mathematical models at the micro-scale are the most widely used for research, development and battery optimization as they allow the correlation of the theoretical results with experimental transport and electrochemistry data [22].

This review is divided into the following sections: first, the advantages and disadvantages of lithium-ion batteries in relation to other types of batteries are outlined; then, the process of insertion/extraction of lithium ions and each of the main components of the battery are described; finally, the microscopic mathematical models dealing with the description of the operation of lithium ion batteries are reviewed and their results discussed; the reviews finish with some concluding remarks on the open questions and future research directions in this specific topic.

1.1. Advantages and disadvantages of lithium ion batteries

A critical assessment on the main advantages and disadvantages should be performed for each type of battery [2]. The main advantages and disadvantages of the use of lithium ion batteries when compared to other types of batteries such as Ni–Cd, Lead–Acid battery and Nickel–Metal Hydride Cells are illustrated in Table 1. By comparing lithium ion batteries with nickel–cadmium batteries (Ni–Cd), the energy density of the lithium ion batteries is approximately twice as large as the energy density of nickel–cadmium batteries [23,24]. The charging cycle, on the other hand, shows similar characteristics for nickel–cadmium and lithium-ion batteries [25,26]. Lithium-ion electrochemical cells show high voltages and in case, for example, of an electrical apparatus requiring a voltage of 3.6 V, it requires just one cell instead of a package of three cells of 1.2 V for nickel–cadmium batteries. Lithium-ion batteries show no memory effect in their charge and discharge cycles which leads to increased life time [27]. Furthermore, their self-discharge effect is lower in comparison to nickel–cadmium batteries. Despite the mentioned advantages, lithium-ion batteries also show some disadvantages. In particular, lithium-ion batteries require a protection circuit to maintain safe operation. This protection circuit limits the peak voltage of each cell during charge and prevents the cell voltage to strongly decrease during discharge [28].

The temperature of lithium-ion batteries should be also controlled in order not to exceed 100 °C. The maximum charge and discharge current in the majority of these batteries is limited between 1C and 2C [29]. Aging is also a concern for most lithium-ion batteries and deterioration is observed after one year, approximately, whether in use or not [30–32]. However, in some specific applications the durability of lithium-ion batteries can extend up to about five years [7].

In the automotive industry there are many options for electric vehicle batteries, each system offering unique features with advantages and disadvantages [37–39]. Currently, some of the most promising approaches are based on lithium-ion batteries, due to their high energy density [7]. However, lithium-ion batteries show problems with sensitivity of overload that can reduce their life cycle. Other options under consideration include fuel cells with rechargeable batteries. In any case, it should be noted that these options do not provide the same amount of energy in comparison to fossil fuels: ~40 MJ/kg for fossil fuel against 1.5–0.25 MJ/kg for fuel cells and advanced batteries, respectively [34]. Although electric vehicles are being designed and built, currently there is no energy source that matches the power and energy of the internal combustion engine [40,41]. Nevertheless, research is conducted to develop a robust system capable of achieving reasonable acceleration for the vehicle and the ability to perform long distances [42]. In this sense, fuel cells and lithium-ion batteries are suitable alternatives for application in electric vehicles due to their large improvement potential based on novel materials and optimized design [43–45].