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Assessment of cathode active materials from the perspective of integrating environmental impact with electrochemical performance

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ABSTRACT

A method was brought forward for assessing cathode active materials from a perspective that accounts for the environmental impact and the electrochemical performance. Then the integrated performance, referred to as the “final environmental impact”, was quantified into a dimensionless score, EI_c (see Eq. (2)). Subsequently, four types of cathode active materials— $LiFePO_4/C$, $LiFe_{0.98}Mn_{0.02}PO_4/C$, $LiFe_{0.98}Ti_{0.02}PO_4/C$, and $FeF_3(H_2O)_3/C$— were assessed. The results were: (1) the EIc sequence was LiFePO4/C (1.76E-02Pt) > $LiFe_{0.98}Ti_{0.02}PO_4/C$ (1.74E-02 Pt) > $LiFe_{0.98}Ti_{0.02}PO_4/C$ (1.66E-02Pt) >$FeF_3(H_2O)_3/C$ (4.98E-03 Pt), which meant $FeF_3(H_2O)_3/C$ was the optimal material and had the minimal final environmental impact. (2) With regard to the eleven impact categories, the category respiratory effects exerted by inorganics made up the largest percentage of the EIc for the four materials. (3) In the aspects of EIm (EI (Eco-indicator) value of a 1 kg cathode active material), average specific discharge capacity, and cycle life, the sub-optimal materials' sequence of theoretical potential for optimization was as follows: $LiFe_{0.98}Ti_{0.02}PO_4/C$ > $LiFe_{0.98}Mn_{0.02}PO_4/C$ > $LiFePO_4/C$. This meant that the final environmental impact of $LiFePO_4/C$ was the most difficult to reduce, and the impact of $LiFe_{0.98}Ti_{0.02}PO_4/C$ could not be reduced very easily. (4) To reduce the final environmental impact, the following concrete measures were recommended: (a) the optimization of the synthesis processes for smaller particle diameters; (b) the adoption of other surface-coating agents, utilizing (other) dopants; (c) the substitution of the energy-efficient instruments for the energy-intensive instruments; (d) the optimization of the synthesis processes to contain fewer electricity-intensive steps.

1. Introduction

In recent decades, Li-ion batteries have been studied intensely to meet the ever-increasing demand for high-performing, economical, and safe power storage for portable electronics and electric vehicles (Armand and Tarascon, 2008; Kraytsberg and Ein-Eli, 2012). Because commercial anode materials can meet the demand of high capacity for Li-ion batteries, the present focus of the research is mainly on the development of cathode materials (Goodenough and Kim, 2010). Different types of cathode materials have been synthesized, and trials have been performed on their structures and modifications from the aspects of chemistry and morphology to pursue high specific capacity, long cycle life, and safety (Chen et al., 2013; Scrosati and Garche, 2010; Wu et al., 2013; Xu et al., 2012).

As a type of green battery, Li-ion batteries have a relatively low value of environmental impact when compared with conventional batteries (Matheys et al., 2009; Yu et al., 2012). However, with the amount of waste Li-ion batteries increases year by year, and the environmental problems caused by them become increasingly evident (Dewulf et al., 2010; Zou et al., 2013), especially considering that China is behind in the technology and management of recycling and disposing of waste batteries.

Abbreviations: BIT, Beijing Institution of Technology; C, carbon; C_r, Required capacity; ISO, International Organization for Standardization; LCA, Life Cycle Assessment; LCI, Life Cycle Inventory; EI, Eco-indicator; EI_m, EI value of 1 kg cathode active material; EI_c, EI value of each cathode active material under a certain C_r and cycle number.

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LCA (Life Cycle Assessment) defined by ISO 14040 and ISO 14044 is becoming an increasingly common method to aid in decision-making processes(ISO, 2006a, b). LCAs conducted across a variety of fields - such as the production of chemicals, the minimization of environmental impact of thermodynamic cycles, the design of railway bridge and the comparison of PLA and PET bottles - help designers and managers search for more environmentally friendly alternatives and to evaluate their decisions from an environmental perspective(Brunet et al., 2012; Cespi et al., 2014; Du and Karoumi, 2013; Pérez-López et al., 2014; Papong et al., 2014). Some LCA studies have been conducted on secondary batteries. Yu et al. evaluated two types of secondary batteries –Li-ion battery and Ni–MH battery – by using LCA. The results showed that between the two selected batteries, the environmental impact of the Li-ion battery was lower than that of the Ni–MH battery, especially with respect to resource consumption (Yu et al., 2012). Two Li-ion batteries, which were both based on lithium iron phosphate but used different solvents during cell manufacturing, were studied by Zackrisson et al. through the means of LCA. The study showed that it was environmentally preferable to use water as a solvent instead of N-methyl-2-pyrrolidone, NMP, in the slurry for casting the cathode and anode of lithium-ion batteries (Zackrisson et al., 2010). A detailed life cycle inventory of a Li-ion battery and a rough LCA of BEV-based mobility were compiled by Notter et al.; the study indicated that the major contributor to the environmental burden caused by the battery was the supply of copper and aluminum for the production of the anode and the cathode and for the required cables or the battery management system (Notter et al., 2010).

However, a product has multiple properties, of which the environmental impact is just one. In general, the purpose of LCA work is to assist people to better understand and address the environmental impacts associated with products. However, if a product with a lower environmental impact has a bad result in other major properties (like the electrochemical performance of Li-ion batteries), it may not be an acceptable alternative for the designer or manager. Thus, when an LCA is conducted for a certain product to assess its environmental impact, the other major properties concerned should be assessed as well. For instance, some researchers took the cost of the product into consideration when conducting an LCA (Lindahl et al., 2014; Vercalsteren et al., 2010).

To make the R&D of cathode materials more environmentally friendly, this study presented a method to assess cathode active materials from the perspective of integrating environmental impact with the electrochemical performance. In the method, the integrated performance was quantified into a dimensionless score through the Eco-indicator 99 system (Goedkoop et al., 2000; Goedkoop and Spriensma, 2000) and some specific formulas. The idea being emphasized in this method was that under a certain required capacity, the material with high electrochemical performance would meet the required capacity with less mass, which was responsible for the environmental friendliness to some extent. Following this method, four types of cathode active material synthesized at the Beijing Key Laboratory of Environmental Science and Engineering at BIT were assessed, and their scores were calculated to determine which type was optimal and to perform other related analyses.

2. Method

2.1. Eco-indicator 99 and Europe EI 99H/A

ISO 14040 and ISO 14044 have defined an outline of the procedures required to perform an LCA, rather than a detailed methodology. The scope, system boundary and level of detail of an LCA depend on the subject and intended use of the study (Cucurachi et al., 2012; Glew and Lovett, 2014).

A damage-oriented and endpoint method, Eco-indicator 99, was used in this study to perform the LCA. In the Eco-indicator 99 system, eleven damage models are established to link three damage categories—“damage to resources”, “damage to ecosystem quality” and “damage to human health”—with the inventory result. In Goedkoop and Spriensma (2000), the different procedures and (intermediate) results of Eco-indicator 99 system are shown in Fig. 1. It can be observed that a clear distinction is made between the intermediate results (gray boxes) and the procedures (white boxes) to go from one intermediate result to the other.

The EI (Eco-indicator) value obtained after the procedure “Normalization and Weighting” can be regarded as a dimensionless figure, though the unit of measurement is referred to as an “Eco-indicator point (Pt)”. Its scale is chosen in such a way that a value of 1 Pt represents one thousandth of the annual environmental load of one average European inhabitant (Goedkoop et al., 2000). With EI values, eleven impact categories can be compared with their respective EI values.

The Eco-indicator 99 system is integrated into the LCA software, Simapro (non-OECD Faculty version 7.2.4 with Ecoinvent V2 database), and “Europe EI 99H/A” (Goedkoop and Spriensma, 2000) was chosen to conduct the LCA in this study. “H” refers to the hierarchist damage model and normalization, which is a balanced time perspective. “A” refers to the average weighting set—resources = 20%, ecosystem quality = 40%, and human health = 40%.Based on the “Europe EI 99H/A” method, Fig. 2 shows the contribution that the eleven impact categories make to the total European damage.

2.2. Functional units

In this study, raw materials were prepared and cathode active material was obtained after several synthesis procedures. Next, the cathode active material was assembled with other components (anode, electrolyte, shell, etc.) to obtain a complete Li-ion battery.

The common structure of the four types of batteries is shown below in Fig. 2.As is shown in Fig. 2, the battery consists of shell (steel), cathode, electrolyte, separator and anode (Li). The cathode active material with binder is applied as surface coating on Al-foil

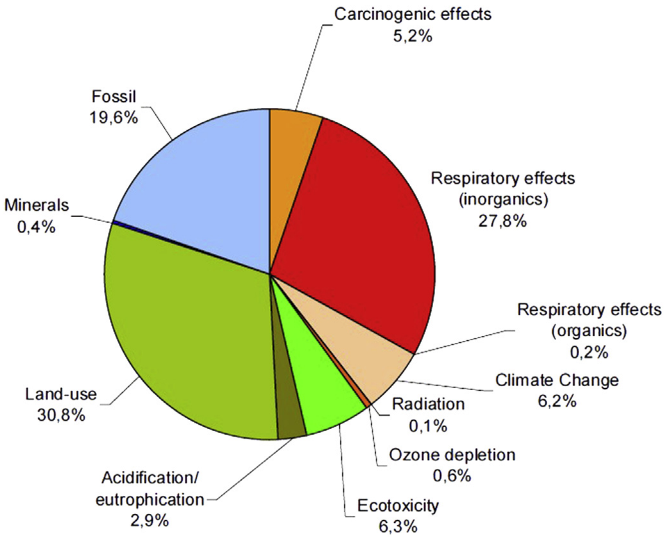

Fig. 1. Relative contribution of the impact categories to the European damage according to the “Europe EI 99H/A” method, Source: (Goedkoop and Spriensma, 2000).