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Life Cycle Assessment and resource analysis of all-solid-state batteries

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HIGHLIGHTS

- Laboratory scale production of an all-solid-state battery cell is assessed using Life Cycle Assessment.
- The foremost share of overall emissions results from electricity consumption on site.
- Possible improvement potential when upscaling production processes is investigated.
- LCA results prove: early research stage products are not comparable to competing technologies at commercial stage.
- Additional resource analysis shows: lanthanum, lithium and zirconium are critical materials.

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ABSTRACT

In this investigation the environmental impacts of the manufacturing processes of a new all-solid-state battery (SSB) concept in a pouch bag housing were assessed using the Life Cycle Assessment (LCA) methodology for the first time. To do so, the different production steps were investigated in detail, based on actual laboratory scale production processes. All in- and outputs regarding material and energy flows were collected and assessed. As LCA investigations of products in an early state of research and development usually result in comparatively higher results than those of mature technologies in most impact categories, potential future improvements of production processes and efficiency were considered by adding two concepts to the investigation. Apart from the laboratory production which depicts the current workflow, an idealized laboratory production and a possible industrial production were portrayed as well.

The results indicate that electricity consumption plays a big role due to a lot of high temperature production steps. It needs to be improved for future industrial production. Also enhanced battery performance can strongly influence the results. Overall the laboratory scale results indeed improve strongly when assuming a careful use of resources, which will likely be a predominant target for industrial production. These findings therefore highlight hotspots and give improvement targets for future developments. It can also be deducted, that a comparison to the results of competing technologies that have already reached a commercial stage is not recommended for early LCAs.

To round things off a resource analysis was also conducted. It identifies the usage of lanthanum, lithium and zirconium oxide as critical, especially when taking laboratory production as a base. When looking at the scale up to industrial production parameters, lanthanum and lithium remain critical, zirconium oxide not.

1. Introduction

There is a growing demand for energy storage for intermittent renewable energy such as solar and wind power, for transportation, and for a myriad of portable electronic devices [1,2]. Since its implementation in 1991 by Sony, electrical storage based on lithium ion technology has conquered the market and is found in almost every portable device, in Electric Vehicles (EV) and in battery home storage devices [3,4]. Simultaneously to an expanding market though, there is a growing demand for higher energy and power densities than current lithium ion solutions can provide [5–7]. Also, there are serious safety concerns about the blend of organic carbonate solvent and fluorine containing salts used in lithium ion batteries (LIB).

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In this publication the technological feasibility of a new type of battery, called all-solid-state batteries (SSBs) was investigated from a Life Cycle point of view. SSBs have a lot of advantages over commercially available battery chemistries regarding their potential energy density and safety aspects. Therefore their targeted applications are diverse and promising for example in the EV sector. To complement their development, a Life Cycle Assessment (LCA) is an important tool to analyze environmental effects from cradle-to-grave. Numerous LCAs for lithium ion batteries have been conducted and their advantages and disadvantages highlighted: Some of the newest investigations are for example [8–13] gives an overview of publications and their results prior to 2012. As the field of solid-state battery research is a new one and data on manufacturing steps are rare, only [14] publishes first results for a solid-state battery approach, which investigate a different manufacturing approach with different material compositions than are investigated in the LCA on hand.

Therefore the target of the LCA on hand is to analyze the specific manufacturing steps of the all-solid battery pouch manufactured at the Institute of Energy and Climate Research (IEK-1) of the Research Center Jülich (FZJ), using most promising materials like lithium lanthanum zirconate ($Li_7La_3Zr_2O_{12}$ LLZ). This investigation includes the quantification and the evaluation of all energy and material flows into and out of the system, including all emissions and waste that reaches the environment. By conducting a LCA early on in the research and development phase, possible obstacles from an environmental point of view can be identified and be taken into account in decision processes. IEK-1 is specialized in synthesis and processing of advanced technical ceramics and develops all-solid state batteries and can therefore for the first time in an LCA deliver detailed data on the different production steps and compositions.

Batteries exhibit most of their life cycle impacts during their manufacturing and possibly disposal phases. The focus of the investigation lies on the assessment of possible processing steps during battery production and theoretical properties of SSBs based on the current state of research. Use phase impacts of batteries can change results drastically depending on different factors like the batteries' application. If the all solid state battery reaches high energy densities for example, its application in the mobility sector can lead to a reduced fuel demand and therefore reduced impacts in many categories. This needs to be kept in mind and be focus of future investigations.

As detailed plans for possible recycling are not yet available, the disposal step is not part of the investigation. Showing an outlook of a future industrial scale production is a focus point. Additionally, the LCA is complemented by a resource analysis, which can identify critical materials that are used in manufacturing processes.

2. All-solid-state batteries

2.1. Lithium ion battery technology

Lithium ion technology is widely implemented in today's electrically powered devices. Nevertheless, it faces different challenges in regard to future development. The main challenge is the demand for a higher energy and a higher power density of batteries for future applications, for example in the Electric Vehicle (EV) or the Information Technology (IT) markets.

A key component for the performance of a commercially available LIB is its electrolyte. It acts as a charge-transfer medium and also contributes to cycling performance and safety aspects [15,16]. Most common electrolytes include lithium hexafluorophosphate ($LiPF_6$) dissolved in an organic solvent such as ethylene carbonate (EC), ethylmethyl carbonate (EMC), sometimes in combination with ionic liquids (ILs) and polymers [15–17]. Lithium cobalt oxide (LCO) is a common cathode material which is used for the positive electrode. For the negative electrode, typically stated as anode in a discharging battery, graphite is used in commercial batteries forming carbon intercalated lithium (LiC_6) in the charged state. For safety and manufacturing reasons the electrodes are separated by an electrolyte permeable polypropylene (PP)/polyethylene (PE) separator, because of their wet strength and chemical durability [18]. Commercially available batteries of this composition achieve theoretical energy densities of 387 Wh/kg, but in application only about 140 Wh/kg are reached [19,20]. The implementation of pure Li metal anodes instead of commonly used carbon-anodes improve the theoretical specific energy significantly to 534 Wh/kg [19,21]. On battery system level, the mass reduction of the anode (capacity matching to the cathode) and a more effective cell and battery packaging/housing will also contribute greatly to improve the specific energy.

Another point of concern regarding conventional LIB are serious safety issues about the blend of organic carbonate solvent and fluorite containing salts used in lithium ion batteries. Evaporation of the solvent above 70 °C may lead to cell rupture and possible leakage of toxic and flammable electrolyte [22,23]. At elevated temperature the solid-electrolyte interphase (SEI) breaks down and the separator may melt, which leads to a short circuit that can result in ignition of the cell [24]. In addition, the liquid electrolyte is not stable with Li metal. Li metal reacts spontaneously with all atmospheric gases, except noble gases and also with all polar aprotic solvents. Metallic lithium dendrite growth caused by high current loads of the battery system can lead to cell failure and in a worst case scenario to thermal runaway or even explosion of the battery [25,26].

A third area of improvement is the lifetime of battery systems. For vehicles for example, a lifetime of 10 years or at least 160,000 km is desirable and targeted by research [27]. Lifetime of conventional cells is correlated to the stability of the electrolyte. Degradation caused by decomposition of (liquid) electrolyte at anode or cathode eventually leads to an increase of resistance and loss of capacity [28].

2.2. Next generation cells: all-solid-state batteries

A new battery concept uses a solid-state electrolyte. Solids have a much higher intrinsic stability. Moreover, they are in general less toxic. Therefore these batteries fulfil the targeted safety requirements. Furthermore, some of the available solid electrolytes are compatible to lithium metal anodes, allowing for even higher energy and power densities and simpler fabrication. In addition, electrolyte-related degradation may be minimized, as solid electrolytes provide generally high cycling stability [28,29].

Lithium phosphorous oxynitride (LIPON) has been developed for thin film electrolytes over the last decade. It is an amorphous material with an average ionic conductivity in the order of σ_{ION} $\sim 10^{-6}$ S/cm, a relatively wide electrochemical stability window and a compatibility with lithium metal. Using physical vapor deposition techniques like sputtering, it was successfully implemented into a thin film lithium battery [30]. In order to achieve higher capacities, thicker cathodes must be implemented. These thick cathodes can only transport ions sufficiently if mixed with an electrolyte to form a mixed cathode. However, LiPON has an insufficient conductivity for this purpose.

Besides LIPON, lithium lanthanum zirconate (LLZ), an oxide ceramic, is one of the most promising candidates for SSB application and worldwide in researchers focus [31–40]. In combination with its good total ion conductivity of $\sigma_{ION} > 10^{-4}$ S/cm at room temperature, LLZ is electrochemically stable in contact with lithium metal. Furthermore its wide electrochemical stability window (up to $\sim$>7 V vs. Li/Li^+) would enable higher energy densities