Contribution ID: **50** Type: **Poster**

Probing the operation of non-graphitizable carbon and Na3V2(PO4)2F3 in Na-ion batteries by operando solid-state nuclear magnetic resonance

Wednesday, November 29, 2023 5:50 PM (2h 10m)

A possible Na-ion batteries (SIB) consists of non-graphitizable carbons for the negative electrode and Na3V2(PO4)2F3 (NVPF) for the positive electrode. (De)intercalation and (de)insertion of Na ions from/into non-graphitizable carbons and NVPF are focus of many recent studies [1]. The mentioned battery is relatively new compared to Li-ion, and the exact mechanism of its operation and degradation is not yet clear [2]. In this study, the physical and electrochemical properties of half-cell corncob derived non-graphitizable carbon prepared at 1400℃ [3] and NVPF were established via operando solid-state nuclear magnetic resonance (NMR) spectroscopy.
It is likely that various metastable, intermediate, and/or short-lived phases occur during the electrochemical reactions in the cell are not captured in the ex-situ mode. Therefore, recent research is moving towards operando measurements. In this mode, the battery is not destroyed during operation, but rather non-invasive methods are used to observe the battery in operation and thus provide information on dynamic structural changes and processes in real time. The main reasons that operando NMR method has rarely been used is that it is quite difficult to manipulate samples in a very limited space and in a very strong magnetic field. Also, the sample during the operando NMR measurement is static so the signal peaks are broader and thus the resolution of the measurement is lower compared to ex-situ NMR measurements where the magic angle spinning method can be used [4][5].
By measuring 23Na NMR spectra of non-graphitizable carbon in a half cell configuration, we obtained information about sodium intercalation in the active material, leading to a shift of the NMR peak during the sodiation process, the formation of a solid electrolyte interphase (SEI) on the electrode surface in the form of Na2CO3 and the potential formation of plating and metal sodium dendrites. Additionally, we were also able to observe changes in the chemical environment of the NVPF material during sodiation in half-cell configuration.

This research received financial support from CERIC-ERIC and the Slovenian Research and Innovation Agency (ARIS) under research program P2-0423 and project N2-0266.

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Session Classification: Happy Hour and Poster Session