Cell Casing Design for *in situ* Nuclear Magnetic Resonance Imaging on Electrochemical Systems

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Introduction: MRI was successfully applied to study Li^+ concentration gradients developing under an applied electric current [1]-[3]. Ion transport properties can be extracted and impact modeling of migration and diffusion processes of a battery. Essential for MRI experiments is a proper cell design in order to rely on genuine electrolyte properties. Assembly remains a critical factor, due to possible side products occurring during electrode formation or residual moisture leading to Li^+ loss.

Methods: A cell casing was developed, providing sufficient chemical resistance by using polyether ether ketone (PEEK) and perfluorocarbon rubber (FFPM) sealing. Electrical connectivity was realized with standard terminals and micro spring connector. The presented approach intended to avoid metallic lithium or artificial electrodes and the parts were constructed such that requirements for re-usability are fulfilled. 1D and 2D spin-echo and gradient-echo MRI techniques were used to image the electrolyte volume (700 µL of 1 M EC/EMC = 50/50 (v/v) with 11 x Whatman GF/B separators) of a working lithium-ion battery (LIB) with Graphite (C) as anode material and different cathodes, i.e. Lithium-Manganese-Oxide (LMO) and Lithium-Nickel-Manganese-Cobalt (NMC).

Results and discussion: The concentration gradient was generated by constant current charging and investigated by 1D spin-echo ^{7}Li MR imaging. Adequate potential ranges for the materials were applied. With a variation of an automated processing method [4] the electrolyte and ion distribution between NMC/C electrodes along *z* was analyzed. The electrolyte distribution in the axial plane was investigated by ^{1}H MRI and demonstrates gas locks or other impurities due to assembly.

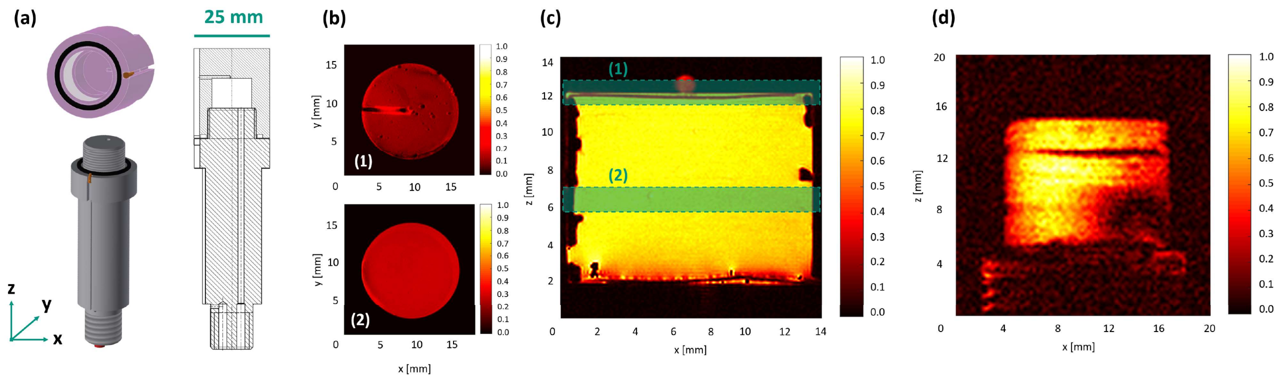

Fig.1: **(a)** Schematic drawing of the cell casing **(b)** Axial ^{1}H MR intensity images (2D MSME) of a working LMO/C battery cell revealing current collector contact by Cu-wire on top (1) and a homogeneous electrolyte distribution in separator stack (2). **(c)** Coronal slice indicating the location of the axial slices between the electrodes C on top and LMO at the bottom **(d)** ^{7}Li MRI (2D FLASH) coronal slice of the NMC/C battery cell with an artefact at the bottom right.

Conclusion: Electrochemical characterization of the cell and concentration profiles were measured within the presented design. The electrode diameter and electrolyte volume are adjustable by variation of screwable counterpart and hence readily applicable.

References:

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