



Non-invasive *in situ* NMR Methodology Development for Characterization of Lithium Ion Rechargeable Battery

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Electrochemical processes (i.e. inter-conversion between electric energy and chemical energy) are essential for rechargeable battery materials. Many conversions between structural phases in the electrodes are taking place during this inter-conversion, some of which become irreversible, leading to capacity decay, low energy efficiency, and a short cycle life. A non-invasive NMR methodology is being developed at the NHMFL to characterize the ion transfer mechanism in the electrodes under *in situ* conditions.

Stray-field imaging (STRAFI) utilizes the maximum field gradient in a magnet for imaging solid substances containing nuclei with very short spin-spin relaxation times, as in paramagnetic solids. As diagramed in Fig. 1, samples in the sample chamber, are placed at the strongest static field gradient. Thus, only the atoms of interest within a very thin slice along the field gradient direction can be observed. By moving the samples vertically (by a computer controlled step motor), the population of the spins along the field gradient direction is detected. Fig. 2 shows the preliminary ${}^7\text{Li}$ STRAFI profile of a fully charged $\text{Li}_x\text{V}_2\text{O}_5$ rechargeable battery cell. Both sensitivity and resolution are expected to be improved significantly with our recently engineered probe design. Higher magnetic fields (being developed at the NHMFL) and their stronger field gradient will further enhance the sensitivity and resolution.

STRAFI allows us to visualize *in situ* Li ion motion in a battery cell during the charge/discharge process, thus to understand ionic transport properties, interfacial properties, chemical reaction, electrochemical stability, and structural transformation of the electrode materials. This technique can also be used to study other layered structural materials such as fuel cells.

Facilities: NMR facility/ultra-narrow bore 19.6T NMR spectrometer.

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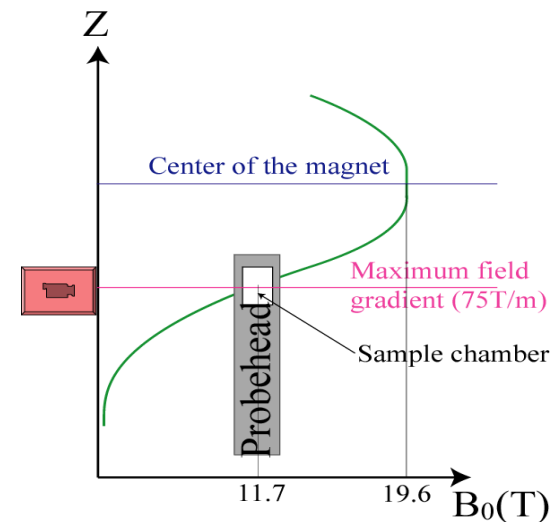


Fig. 1 Schematics of stray-field imaging (STRAFI) spectroscopy on the ultra-narrow bore 19.6T magnet.

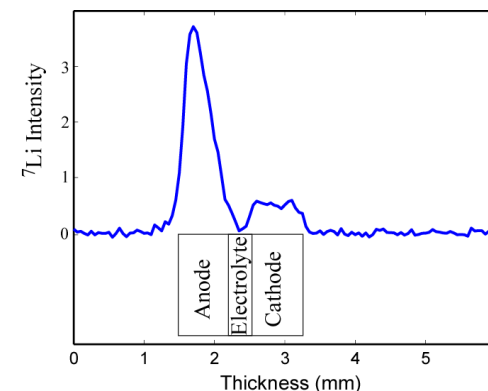


Fig. 2 Preliminary ${}^7\text{Li}$ STRAFI profile of a fully charged $\text{Li}_x\text{V}_2\text{O}_5$ rechargeable battery cell.