MAGNETIC RESONANCE FOR BATTERY RESEARCH AND DEVELOPMENT

Exploring Coin Cell Battery Technology with Operando/ In-Situ Solid-State NMR Spectroscopy

Lithium Intercalation into Graphite

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Innovation with Integrity

Rechargeable batteries are at the heart of the global energy transition, enabling sustainable solutions for mobility and stationary energy storage. As demand for high-performance, cost-effective, and environmentally friendly battery systems continues to grow, researchers and manufacturers are turning to advanced analytical tools to accelerate innovation and ensure quality. Among these, operando/in-situ solid-state Nuclear Magnetic Resonance (NMR) spectroscopy stands out as a powerful technique for real-time, non-destructive investigation of battery materials.

Coin cells, widely used in battery research due to their compact design and ease of assembly, play a crucial role in early-stage material screening and electrochemical performance evaluation. Their standardized format makes them ideal for reproducible testing and scalable insights. However, probing the internal chemical and structural dynamics of coin cells during operation has traditionally been challenging.

Bruker's advanced operando/in-situ solid-state NMR probe technology, developed in collaboration with ePROBE, now enables direct analysis of coin cells under working conditions (Figure 1). These probes are compatible with both off-the-shelf (stainless steel) and custom made (titanium) coin cell casings as well as pouch cells, allowing researchers to perform NMR experiments while

Figure 1: Single-channel coin cell operando/ in-situ NMR probe.

simultaneously charging and discharging the cell (Figure 2). Equipped with up to three highly-shielded current collector ports, the system supports a wide range of battery chemistries including Li- and Na-ion technologies.

By leveraging nuclei such as ^{7}Li, ^{23}Na, ^{13}C, ^{31}P, ^{1}H, and ^{19}F, operando/in-situ NMR provides molecular-level insights into reaction mechanisms, phase transitions, and ion mobility within coin cell components. This capability is essential for understanding performance-limiting factors and guiding the design of next-generation materials.

For operando solid-state NMR studies, a stainless-steel coin cell containing $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622), graphite, and $LiPF_6$, which was dissolved in ethylene carbonate and dimethyl carbonate, was prepared. During the cycling of the NMC622 | $LiPF_6$ | graphite CR2025 coin cell in the voltage range between 4.3 V and 2.5 V, distinct Li species could be monitored using the coin cell NMR probe (Figure 3). The spectra reveal contributions from the electrolyte (~127 ppm), Li intercalated into graphite (~168 ppm), and metallic Li (200–600 ppm). The obtained results indicate that Li ions are reversibly intercalated into the graphite electrode during the charge–discharge processes.

Recent studies[1-3] have demonstrated the value of operando/in-situ NMR in unraveling complex electrochemical processes in battery systems. With Bruker's customizable setup - including the AVANCE NEO console, specialized probes, and eCAT software - researchers can now extend these insights to coin and pouch cell configurations, bridging the gap between lab-scale innovation and industrial application.

Conclusions

In summary, integrating coin cell technology with operando/in-situ solid-state NMR opens new avenues for battery research, enabling precise, real-time characterization of materials in a format that aligns with practical testing workflows. This synergy supports faster development cycles, deeper understanding, and more reliable performance in the pursuit of sustainable energy solutions.

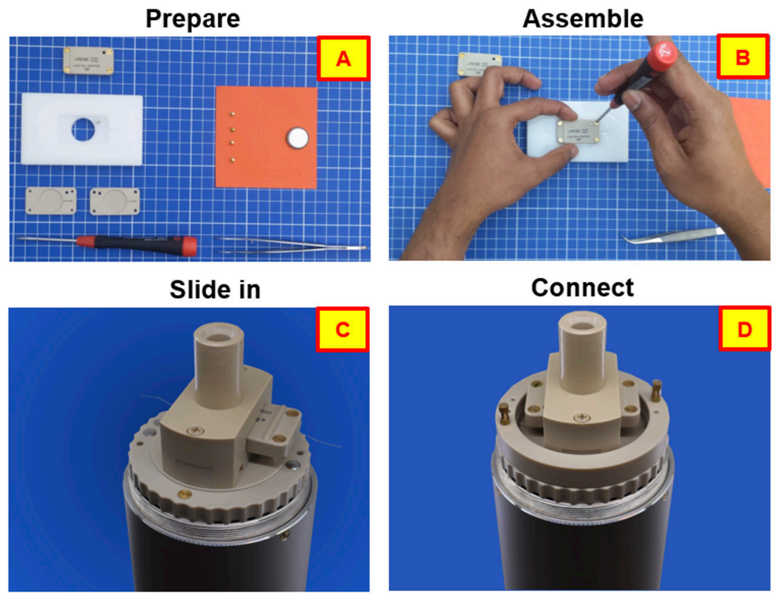

Figure 2: Coin cell holder assembly and insertion into the probe.

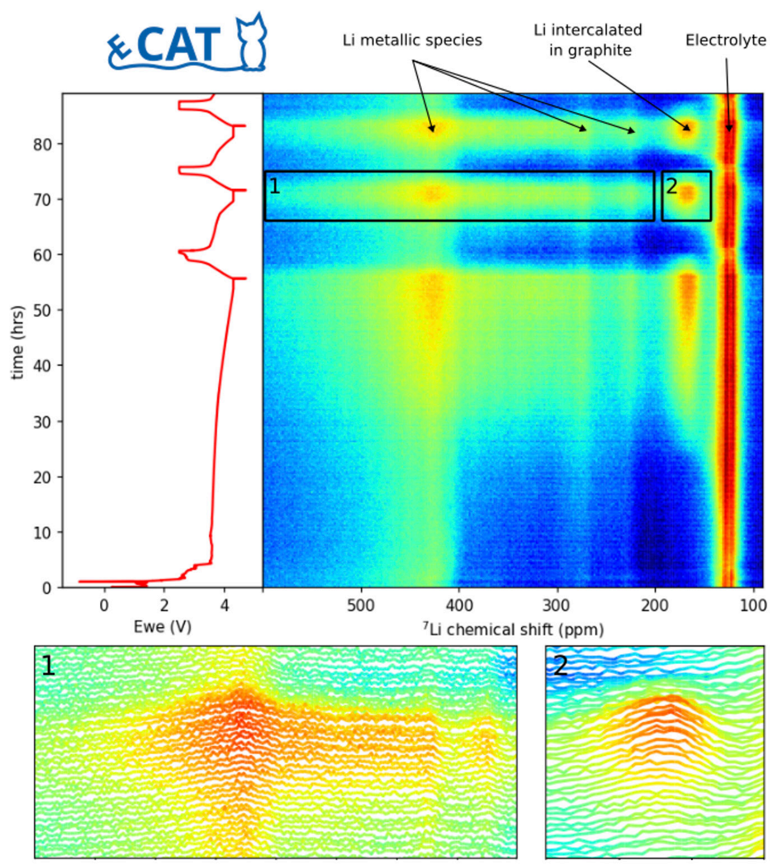

Figure 3: ^{7}Li operando NMR data of an NMC622/graphite stainless steel coin cell processed with eCAT. We gratefully acknowledge Sylvio Indris et al. at KIT (Germany) for the coin cell preparation and fruitful discussions.

References

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