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Developing new varieties of electrochemical cells for operando neutron diffraction investigations of lithium ion battery materials

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While the interest and frequency of performing operando neutron diffraction experiments for lithium ion batteries has increased significantly over the past few years, it is still not nearly as popular as operando X-ray diffraction. A major contributor to this is the high difficulty of constructing an electrochemical cell which balances both electrochemical performance, quality of the obtained diffraction pattern and cost of construction. Up until now most work has been performed on, often complex, custom cells built to target a specific feature such as fast cycling at the cost of data quality or data quality with high material loading [1-3].

A significant amount of work has been performed within our group on developing multiple varieties of electrochemical cells for operando neutron diffraction. Given the nature of neutron diffraction it is extremely difficult to develop a single cell to suit all objectives and materials. To this end we have designed two vastly different operando cells; a large wound 18650-like cell and a smaller, cheaper coin cell design. The 18650-like wound cell can contain up to 4 g of active material, is able to be cycled at faster rates and provides a diffraction pattern which is of high enough quality to extract accurate structural parameters. It does, however, require expensive deuterated electrolyte and specialised equipment. Alternatively, the coin cell design is cheap, does not require deuterated electrolyte, can provide good quality diffraction and reasonable electrochemical cycling rates. It is anticipated that the coin cell design will make neutron diffraction accessible to more research groups and also presents a viable cell design for operando neutron diffraction studies of sodium ion cells. Using LiFePO_4 , $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{Li}_{0.18}\text{Sr}_{0.66}\text{Ti}_{0.5}\text{Nb}_{0.5}\text{O}_3$ as case study materials this contribution will focus on the operando neutron diffraction results obtained from both cells, thus exploring the core strengths and potential of each design.

[1] N. Sharma, X. Guo, G. Du, Z. Guo, J. Wang, Z. Wang, and V. K. Peterson. J. Am. Chem. Soc. 134 (2012), 7867

[2] M. Roberts, J. J. Biendicho, S. Hull, P. Beran, T. Gustafsson, G. Svensson and K. Edström. J. Power Sources 226 (2013), 249.

[3] M. Bianchini, J.B. Leriche, J.L. Laborier, L. Gendrin, E. Suard, L. Croguennec, C. Masquelier, J. Electrochem. Soc., 160 (2013) A2176.

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