Nuclear Magnetic Resonance for the characterization of battery materials

E.Salager,[1] V.Sarou-Kanian,[1] R.J.Messinger,[2] T.V.Huynh,[1] L.Croguennec,[3] M.Ménétrier,[3] A.Boulineau,[4] M.Duttine,[3] D.Carlier,[3] J.M.Ateba Mba,[3] C.Masquelier,[5] J.M.Tarascon,[5] M.Deschamps[1]

1- Orléans University, UPR 3079 CNRS CEMHTI, Orléans, FRANCE
2- CUNY Energy Institute, City College of New York, New York, USA
3- ICMCB, CNRS UPR 9048, Bordeaux University, 33600 Pessac, France
4- CEA, LITEN, F-38054 Grenoble, France
5- LRCS, CNRS UMR 7314, Université Picardie Jules Verne, F-80039 Amiens, France

Nuclear Magnetic Resonance spectroscopy is especially useful for the characterization of the chemical nature of the environments of ^{7}Li spins. In materials like $LiVPO_4F$, the structure seems well ordered, as seen by XRD or TEM, however, ^{7}Li NMR spectroscopy shows that 10-20 % of the lithium content is in a different environment than the crystallographic site. Dipolar correlation experiments show that these lithium atoms are within a nanometer of the main site, and therefore are defects within the structure.

On the other hand, pulsed field gradients can also provide the positions of ^{7}Li spins in space. This feature is the key to the success of MRI of working batteries. Moreover, the spectra of the cathodes and anodes in a working battery can be separated in situ by PFG-NMR, and the power of spectroscopic imaging is demonstrated in a $LiCoO_2/Li_4Ti_5O_{12}$ battery. In favorable cases, the lithiation front can be observed in thick electrodes with a 100 μm resolution, highlighting the limitation in lithium transport in electrodes with porosity issues.