MS40 Operando and in situ crystallographic studies

MS40-01
Operando X-ray diffraction studies of NASICON-type positive electrodes for Na-ion batteries
S. Park 1, J.N. Chotard 2, A. Iadecola 3, D. Carlier 4, F. Fauth 5, L. Croguennec 4, C. Masquelier 2

1Tiamat Energy - Amiens (France), 2LRCS - UPJV - Amiens (France), 3SOLEIL Synchrotron - Saint-Aubin (France), 4ICMCB Bordeaux - Pessac (France), 5ALBA Synchrotron - Cerdanyola del Vallès (Spain)

Abstract
Polyanionic materials (phosphates in particular) are of special interest as positive electrodes for Li-ion or Na-ion batteries since they offer competitive electro-chemical performances compared to sodiated or lithiated transition metal oxides [1,2]. They are based upon stable 3D frameworks, which provide long-term structural stability and demonstrate a unique variety of atomic arrangements in their crystal structures. Recent electrochemical and structural investigations of vanadium-based phosphate compounds (LiVPO4O-LiVPO4F, Na3V2(PO4)2F5, Na3V2(PO4)3, …..) revealed promising perspectives [3-5].

The NASICON structural family with its large panel of compositions, Na(x)MM'(PO4)3 (0 < x ≤ 4 ; M,M' = Ti, Fe, V, Cr, Mn) is among the most widely investigated due to its specific three-dimensional framework structure, stable long-term cycling ability and high Na+ mobility [1-2, 5-6]. Among them, the vanadium phosphate Na3V2(PO4)3 [7] is of particular interest. We will present several new structures that we determined, from pristine powders or for intermediate compositions spotted by operando X-Ray diffraction.

Recently, we succeeded in synthesizing Fe-substituted Na4FeV(PO4)3 that allows the reversible extraction of close to 3 Na+ (for two transition metals) and we will report on its crystal structure and on that of Na3FeV(PO4)3 for which new Na+ order-disorder phenomena have been spotted [8, 9]. Even more recently, we reported on the existence of an intriguing definite phase of composition Na2V2(PO4)3 through computational methods [10] and operando X-ray diffraction and X-ray absorption spectroscopy during battery operation [11].

References