Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

NiP_3: A very promising negative electrode for Li- and Na-ion batteries.

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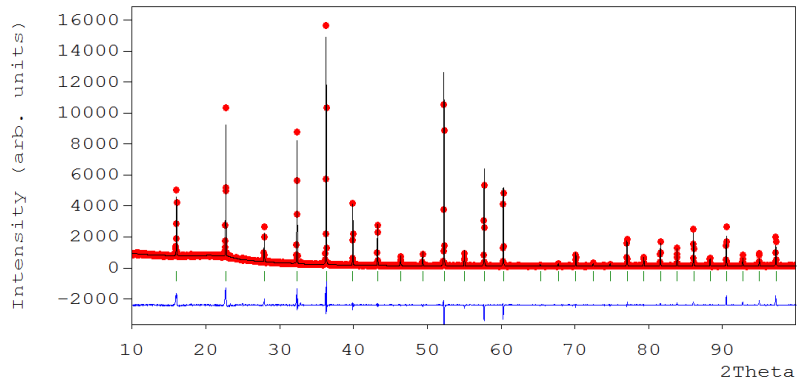
1) NiP_3 Rietweld refinement supporting information:

The XRD data of the polycrystalline NiP_3 has been recorded in a glass capillary on the XPERTPro Panalytical two circles powder diffractometer in the Debye-Sherrer configuration and equipped with a Cu K_{alpha} radiation. Single phase nature of NiP_3 has been confirmed by indexing the whole diffraction pattern and a whole-pattern decomposition (Lebail fitting) with constant scale factor and a pseudo-Voigt function profil was then applied using Fox software **(ref 1)**. Rietweld refinement technique using Fullproff **(ref 2)** was conducted in order to verify the purity and secure a detailed structural analysis of NiP_3. The presence of a very small amount of NiP_2 could have been identified, but owing to the very small quantity of this impurity present, the NiP_2 phase was not added in the Rietweld refinement process. The scale factor, zero point of detector, background parameters and lattice constants were refined in the first round, then peak shape and asymmetry parameters were added. Fractional coordinates of NiP_3 extracted from an X-Ray single crystal diffraction phase analysis were introduced and refined with an overall Debye-Waller for Ni and P atoms. Quality of the data was good enough to turn overall temperature factors into individual thermal isotropic parameters and refine the occupancy factors as well. Finally, instrumental or physical aberration corrections were added to the least squares refinement by using parameters sycos and sysin. Results of refinement are depicted below as supplementary information.

Rietweld refinement pattern and the corresponding refinement for NiP_3:



Cubic system, Space group I -3 m

a = b = c = 7.81776(4)Å; Vol: 477.800(4)$Å^3$

$B_{isoNi/P}$ Ni1 = 0.56(8)$Å^3$; P1 = 0.22(7)$Å^3$

Ni_{occ} = 1.009; P_{occ} = 2.969

Refinement parameters:

Rp(%) = 35.9; Rwp(%) = 25.9; Re(%) = 12.3

Chie2 = 4.44 ; Gof = 1.49

References:

1 J. Appl. Cryst. 35 (2002), 734-743, V. Favre-Nicolin and R. Cermy, Fox, 'Free objects for crystallography': a modular approach to ab initio structure determination from powder diffraction.

2 Fullprof 2000 version July 2001, Juan Rodrigues-Carvajal, Laboratoire Leon Brillouin (CEA-CNRS), 91191 Gif sur Yvette Cedex, France.