Experimental report

12/09/2019

Proposal: **7-03-174** **Council:** 10/2018

Title: Na-ion diffusion mechanism in the cathode material $Na_xFe_{0.5}Mn_{0.5}O_2$

Research area: Materials

This proposal is a new proposal

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Samples: $Na_{0.67}Fe_{0.5}Mn_{0.5}O_2$

Instrument	Requested days	Allocated days	From	To
THALES	6	6	05/07/2019	11/07/2019

Abstract:

P2-$Na_xFe_{1/2}Mn_{1/2}O_2$ has been identified as a potential cathode material for Na-ion batteries since it has comparable electrochemical performance to commercially available Li-ion cathodes and it is composed entirely of abundant elements. For x = 2/3 it has the P2-Na_xCoO_2 structure, however, the absence of superstructures is expected to lead to a different diffusion mechanism and better electrochemical performance. We aim to study the diffusion mechanism in a large powder sample of P2-$Na_xFe_{1/2}Mn_{1/2}O_2$ using quasi-elastic neutron scattering. Our previous measurements with unpolarised neutrons at ISIS indicate the presence of incoherent, magnetic and nuclear scattering. We now propose to use XYZ polarisation analysis on ThHALES to isolate the spin-incoherent scattering, for comparison with Chudley-Elliott models of jump diffusion and molecular dynamics simulations.

Na-ion diffusion mechanism in the cathode material P2-$Na_{2/3}Fe_{1/2}Mn_{1/2}O_2$

The quasi-elastic neutron scattering (QENS) was measured from a powder sample of P2-$Na_{2/3}Fe_{1/2}Mn_{1/2}O_2$ using XYZ polarisation analysis on ThALES. We were able to detect quasi-elastic energy broadening, and to separate the spin-incoherent, magnetic and nuclear components of the scattering. Figure 1 shows typical data measured at T ~ 530 K.

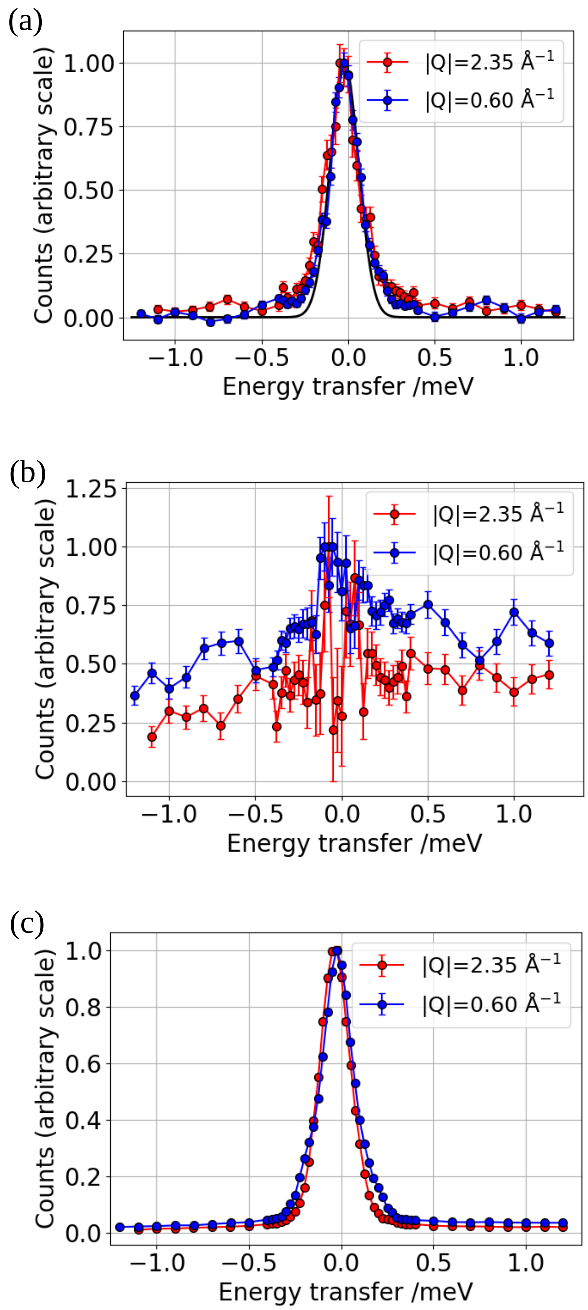

Fig. 1. QENS measured from P2-$Na_{2/3}Fe_{1/2}Mn_{1/2}O_2$ at T ~ 530 K on ThALES using XYZ polarisation analysis. (a) Spin incoherent, (b) magnetic and (c) total (unpolarised) scattering cross sections. These data demonstrate that unpolarised QENS gives the wrong Q-dependence of the energy line width due mainly to the inclusion of the magnetic QENS. Polarisation analysis is essential in order to determine the diffusion mechanism.

By isolating the spin-incoherent QENS, it is possible to determine the diffusion mechanism via a fit of the Chudley-Elliott model of jump diffusion to the energy line width as a function of *Q*. The temperature dependence of the energy line width at fixed *Q* provides an estimate of the activation energy. P2-$Na_{2/3}Fe_{1/2}Mn_{1/2}O_2$ has a different diffusion mechanism to P2-$Na_{0.8}CoO_2$ and this leads to superior electrochemical performance, see Fig. 2.

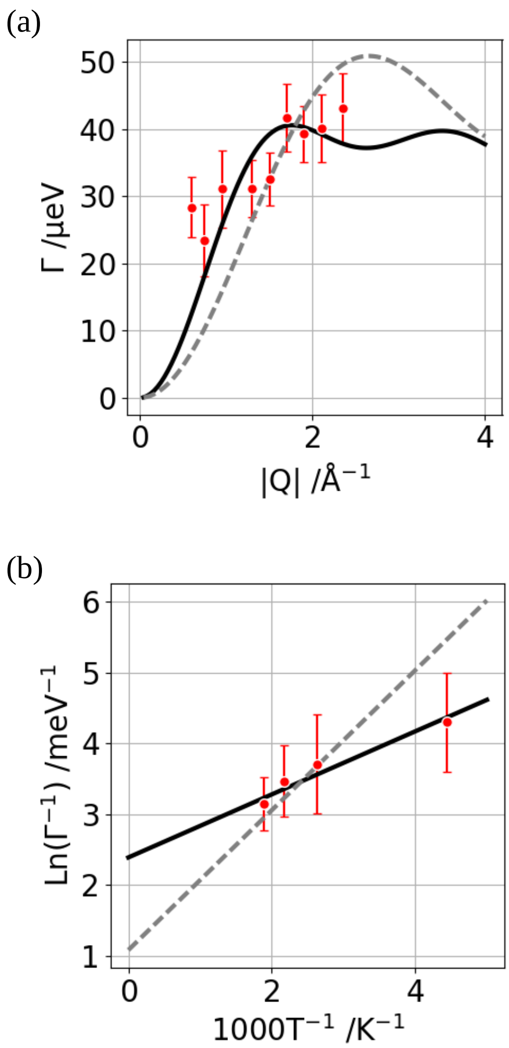

Fig. 2. The energy line widths of the spin-incoherent QENS from P2-$Na_{2/3}Fe_{1/2}Mn_{1/2}O_2$. (a) The fit of the Chudley-Elliot model of jump diffusion (solid line) shows that the diffusion mechanism is different to P2-$Na_{0.8}CoO_2$ (dashed line) (b) The fit of the activation energy (solid line) gives a value E_A ~ 38(7) meV, which is lower than P2-$Na_{0.8}CoO_2$ (dashed line).