

Na diffusive behavior in Na_xCoO_2 detected by QENS

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Due to reversible deintercalation and intercalation of Na ions in a layered cobalt dioxide, NaCoO_2 , the electrochemical properties of NaCoO_2 have been heavily investigated as one of the candidates of a cathode material for Na-ion batteries [1, 2]. Following upon the muon-spin relaxation (μSR) measurements on Na_xCoO_2 [3], we have performed a QENS experiment on Na_xCoO_2 at high temperatures to determine a diffusion coefficient of Na^+ .

The powder sample of $\text{Na}_{0.5}\text{CoO}_2$ was prepared by a chemical deintercalation reaction of Na from $\text{Na}_{0.7}\text{CoO}_2$. Figure 1 shows the scattering function $[S(Q, E)]$ of $\text{Na}_{0.5}\text{CoO}_2$ obtained at 702 K on a backscattering spectrometer DNA at BL02 in MLF/J-PARC. Assuming that $S(Q, E)$ at 200 K corresponds to a resolution function, $S(Q, E)$ above 300 K were fitted by a combination of the resolution function and a single Lorentzian. One can clearly see a broad QENS spectrum in Fig. 1, which appeared above 498 K. Also, since the elastic intensity at 702 K is rather small compared with that at 200 K, Na^+ ions are found to diffuse above 498 K.

Based on the Q dependence of EISF (Fig. 2), the jump distance (d_{Na}) of Na^+ ions was estimated as 0.197 nm. Therefore, Na^+ ions are considered to jump between the nearest neighboring Na^+ sites (0.163 nm) rather than between the second nearest neighboring sites. The self-diffusion coefficient (D_{Na}) at 500 K is evaluated as $\sim 10^{-7} \text{ cm}^2/\text{s}$ from the Q dependence of the full width at half maximum (FWHM) of the QENS spectra.

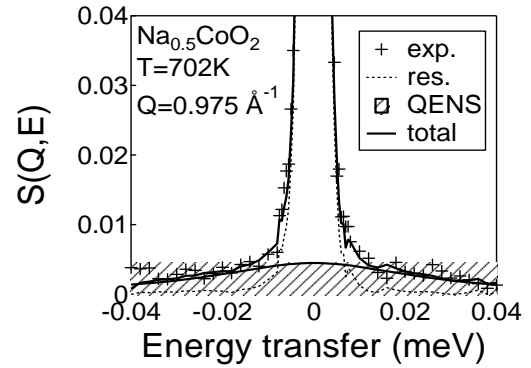


Figure 1. The scattering function of $\text{Na}_{0.5}\text{CoO}_2$ at 702 K. Fig. 1 Caption

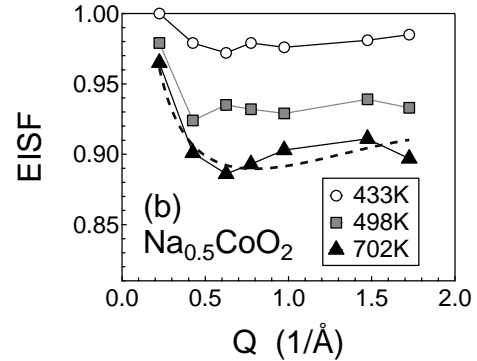


Figure 2. Q dependence of EISF. A dashed line indicates the fitting result using a jump diffusion model.

References

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