Ti-Substituted Layered O3 NaCr$_{1-x}$Ti$_x$O$_2$ as High-Rate-Capability Cathode Materials for Sodium Ion Batteries

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Rechargeable Na ion batteries have attracted increasing attention for large-scale energy storage applications, due to the natural abundance and low cost of sodium resources. A series of layered NaMO$_2$ (M=Ni, Co, Mn, Fe, V and Cr) materials have been extensively investigated as cathode active materials. Among them, O3-type NaCrO$_2$ has been considered as one of the most perspective cathode materials for Na-ion batteries. Based on Cr$^{3+/4+}$ redox activity, NaCrO$_2$ can reversibly (de)intercalate 0.48 mol Na ions per formula unit corresponding to a capacity of 120 mAh/g between 2-3.6 V and shows a flat operating voltage at 3.0 V vs Na.[1] However, NaCrO$_2$ electrode suffers from fast capacity fading and a disappointing rate capability.[2] The overall performance in the previous work on NaCrO$_2$ is not very satisfied.

In this study, Ti-substituted layered O3-type NaCr$_{1-x}$Ti$_x$O$_2$ (0≤x≤0.1) was synthesized through a solid state reaction. XRD data in Figure 1a clearly indicates that titanium doping does not change the structure of NaCrO$_2$ and Ti$^{3+}$ ions were successfully inlaid into the Cr-ion layer to enlarge the d-spacing of the crystal. The cycling and rate performances of the cathode material are significantly improved after Ti substitution, as shown in Figure 1b and c.

From these results, we discuss the factors affecting the structure and electrochemical performance for O3-type NaCr$_{1-x}$Ti$_x$O$_2$ layered structure as positive electrode materials of rechargeable Na batteries for more details.