Phase Transformation of $LiNi_{0.75}Co_{0.25}O_2$

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In this article, we studied the phase transformation of a cathode material, $LiNi_{0.75}Co_{0.25}O_2$, which was prepared by sol-gel pretreatment and solid-phase formation. The precursors of dry gels were first examined by thermogravimetric analysis (TGA) and differential thermal analysis (DTA), and characteristic temperatures of 350°C, 400°C, 450°C, 550°C, 600°C, 650°C, and 725°C were selected based upon the TGA and DTA results. Two series of experiments were performed. One is in-situ and the other is ex-situ. For the series of in-situ experiments, the precursors were raised in a heating chamber of XRD in such a way that at each selected temperature, the temperature was kept constant for 2h, after the sample was analyzed by in-situ XRD, the samples were heated up again to the next selected temperature, and so on. For the series of ex-situ experiments, the precursors were first heated up to each of the selected temperatures and kept constant in the oven for 2h, and then were analyzed by XRD and SEM at room temperature.

It was found that at the temperature below 600°C, the samples have a cubic structure, implying that the nickel metal in the material is present as Ni^{2+}. In this case, the material obtained can not provide the proper spatial structure for the insertion of lithium. The hexangular layer structure started to form when the temperature reaches or becomes higher than 600°C. The structure is better defined with the increase of temperature. The material is characteristic of R-3m spatial structure at 725°C. The preliminary calculation results using VASP® confirmed with the experimental observations.

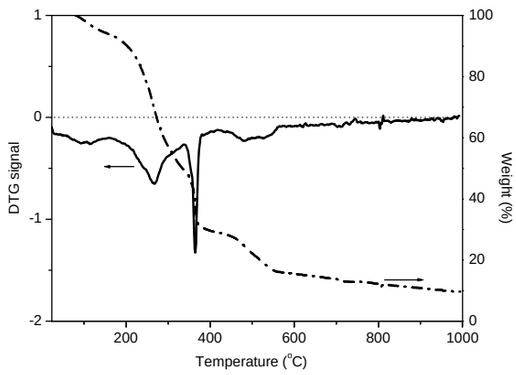

Figure 1. TG-DTG curves obtained from the dry gels of $LiNi_{0.75}Co_{0.25}O_2$ precursors

Acknowledgements

This work was financially supported by the National Key Fundamental Research Project and the Natural Science Foundation of China under the Grant Number 20073036.