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Research on preparation of layered $LiNi_{0.5}Mn_{0.5}O_2$

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Abstract: An O_2-type layered $LiNi_{0.5}Mn_{0.5}O_2$ was prepared by rapidly-quenched method, and the structural feature was studied by X-Ray Diffraction. The material synthesized at 950℃ was with a single O_2-type structure. Charge and discharge in a voltage range of 2.0-4.35V, the discharge specific capacity of material at the 1st cycle is 143.1 mAh/g in a current density of 0.5 mA/cm^2, and the plot of discharge was with two voltage plat at 3.6 V and 2.8V.

Key words: lithium ion batteries; layered structure $LiNi_{0.5}Mn_{0.5}O_2$; rapidly quenched; electrochemical performance

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1 Introduction

Lithium secondary batteries have been rapidly developed because of their well performances such as high voltage, high specific energy, high capacity and light weight since appeared at last century. It was promising to be the main power source of electric vehicles and electric tools. The more practical interest cathode materials included mainly lithium cobalt oxide, lithium nickel oxide and lithium manganese oxide *et al*. At present, lithium cobalt oxygen was the most widely used in comerical, and its shortcoming was high cost and detriment to environment. It was difficult to synthesize single phase $LiNiO_2$, and its safety performance need to be improved. Lithium manganese oxide was considered as the most developmental prospect cathode materials because of their low cost and nontoxicity. In which spinel $Li_2Mn_2O_4$ and layered $LiMnO_2$ could be used for cathodes. But specific capacity of spinel $Li_2Mn_2O_4$ was lower, about 110 mAh/g, and its cycling performance was poor. Layered $LiMnO_2$ was a promising cathode material because its theorical specific capacity could reach to 285 mAh/g.

In this study, an O_2-type layered $LiNi_{0.5}Mn_{0.5}O_2$ was prepared by rapidly-quenched method, and the structural feature and electrochemical performance were studied by X-Ray Diffraction.

2 Experimental

MnO_2, Ni_2O_3, LiOH with a mol ratio of 1 : 0.5 : 1.05 were mixed for 24 h at a ball:material of 3 : 1. It was pressed under a pressure of 5 MPa to a pellet. The pellets loaded in a crucible were heated at 950℃ (Sample A) and 850℃ (Sample B) for 24 h, rapidly quenched to room temperature. The pellets were dried in air at 180℃ for 1h, and then were grounded to power of 5-10μm. Structure of the material was analysed

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by RINT−1100 X-ray diffractometer.

Electrochemical characterization of material was measured in 2016 type coin cells[1-2]. The positive electrodes were fabricated as follow: the sample, carbon black as conducting additive, and PVDF as binder were mixed in 8 : 1 : 1 (mass fraction) ratio, which was pressed under a pressure of 30 MPa to a electrode of 15 mm in diameter, and then dried at 120℃ for 24 h. Using the positive electrodes, 2016 type coin cells were assembled in an argon glove box with lithium as the anode, Celgard 2400 membrane as the separator, and 1 M LiPF6+EC+DMC (the volume ratio of EC/DMC was 1 : 1) as the electrolyte. Charge/discharge were carried on BTS-2200 at voltage range of 2.0-4.35 V in a current density of 0.5 mA/cm^2.

3 Results

X-ray diffraction patterns of materials synthesized at different temperature were showed in Fig. 1. All

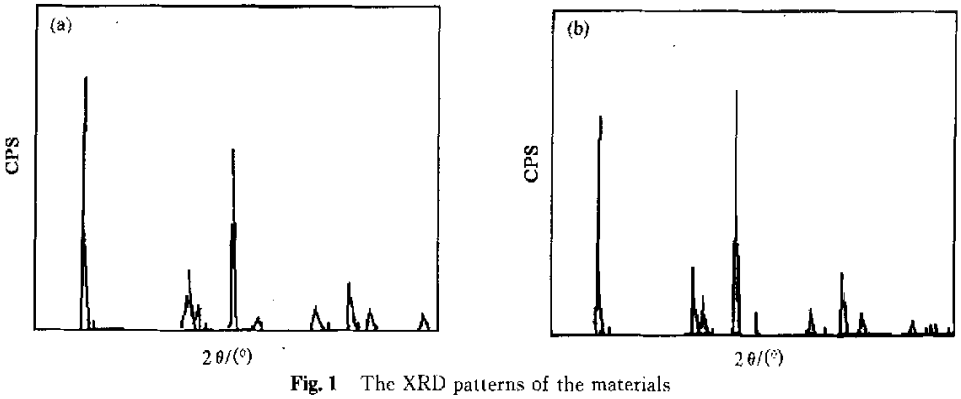

Fig. 1 The XRD patterns of the materials

(a) Sample A; (b)—Sample B

the diffraction lines of the materials could be indexed on standard JCPDS of 16-0427. The sample A synthesized at 950℃ was without other diffraction lines indicated that a single O_2 type layered structure was obtained[3] and crystal structure was perfect. Intensity of X-ray diffraction lines increased with the temperature improved. And that of diffraction lines of (002) ($2\theta = 44°$) more increased. It indicated that the atoms sites in crystalline were varied. The diffraction lines of sample B synthesized at 850℃ was wider, which indicated that stacking faults were presented[4]. A little lines of impurity was appeared at 2θ of 43.5 degree, the sites of the lines were identical to that of literary, showed that a $Li_xNi_{1-x}O$ phase was produced[5].

Lattice parameters of materials A and B were showed in Table 1. Lattice parameters of materials and crystalline volume were decreased with the temperature improved. It was because that stacking faults were presented at lower synthesis temperature and crystal structure was perfect at higher temperature.

Table 1 Lattice parameters of materials A and B

Samples	a/nm	b/nm
A	0.2845	1.4227
B	0.2867	1.4281

The electrochemical charaterization of materials were measured in 2016 type coin cells. Charge/discharge were carried at voltage range of 2.0−4.35 V, the charge/discharge curves for the 1st cycle were showed in Fig. 2. The discharge specific capacity of materials A and B were 143.6 mAh/g and 136.1 mAh/

g, respectively. The discharge curve of material A was with two plat. The specific capacity discharged at 3.6 V was 55.7 mAh/g and at 2.8 V was 87.9 mAh/g. And material B was with a plat at 3.6 V.

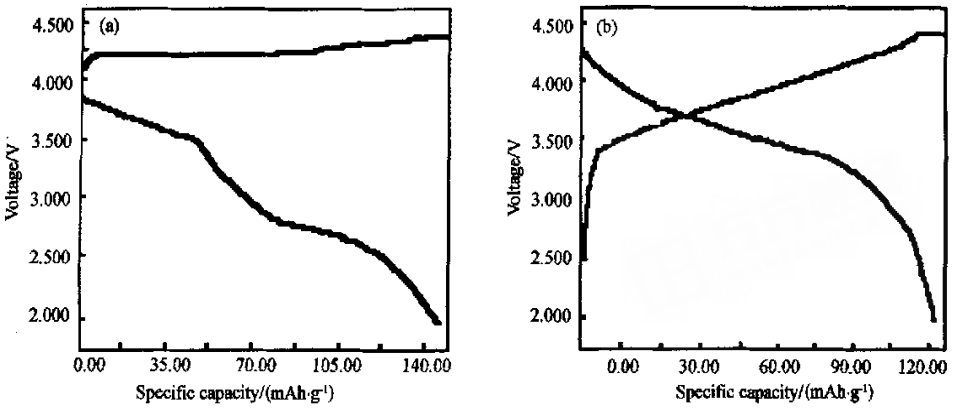

Fig. 2 Charge/discharge curves for the 1st cycle
(a)—Sample A; (b)—Sample B

4 Conclusion

(1) An O_2-type layered $LiNi_{0.5}Mn_{0.5}O_2$ was prepared by rapidly-quenched method.

(2) Charge and discharge in a voltage range of 2.0—4.35V, the discharge specific capacity of material synthesized at 950℃ at the 1st cycle is 143.1 mAh/g in a current density of 0.5 mA/cm^2, and the plot of discharge was with two voltage plat at 3.6 V and 2.8V.

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