Symp B2

$Fd\bar{3}m$ 과 $P4_332$ 의 공간군을 가지는 $LiNi_{0.5}Mn_{1.5}O_4$ 양극 활물질에 관한 비교 연구

Comparative Study of $LiNi_{0.5}Mn_{1.5}O_4$ Cathodes Having Two Crystallographic Structures: $Fd\bar{3}m$ and $P4_332$

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$LiNi_{0.5}Mn_{1.5}O_4$ cathodes with two different structures ($Fd\bar{3}m$ and $P4_332$) were synthesized by molten salt method. Mixed precursors of LiOH, LiCl, $Ni(OH)_2$, and γ-MnOOH (2:1:3) were calcined at 900°C for 3 h. After then, the resulting powders were thoroughly washed with distilled water to remove residual lithium salt, then dried at 110°C. The obtained $LiNi_{0.5}Mn_{1.5}O_4$ powders were oxidized by annealing at 700°C for 48 h in air. Rietveld refinement of X-ray diffraction (XRD) data and selected-area electron diffraction (SAED) study confirmed that face-centered spinel ($Fd\bar{3}m$) transformed into primitive simple cubic ($P4_332$) by additional heating at 700°C. $LiNi_{0.5}Mn_{1.5}O_4$ with $Fd\bar{3}m$ structure showed better electrochemical behaviors than the cathode with $P4_332$ structure. $LiNi_{0.5}Mn_{1.5}O_4$ with $Fd\bar{3}m$ and $P4_332$ structures exhibited area specific impedance (ASI) values of *c.a.* 55 and 75 Ω-cm^2 at 20-80 % of SOC(state of charge). When the $LiNi_{0.5}Mn_{1.5}O_4$ electrodes with $Fd\bar{3}m$ and $P4_332$ structures were cycled at 3 C-rate, capacity retentions were 91 % and 84 % after 50 cycle. XRD and SAED of the electrode after 50 cycles revealed that $LiNi_{0.5}Mn_{1.5}O_4$($P4_332$) had low reversibility between fully lithiated and delithiated structures whereas $LiNi_{0.5}Mn_{1.5}O_4$($Fd\bar{3}m$) showed good reversibility at high rate. Compared with one-step phase transition of the $Fd\bar{3}m$ structure, the $P4_332$ structure had an additional intermediate phase during charge/discharge cycle, and this two-step phase transition led to deterioration of the structural reversibility at high rate.

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