

BFB12

리튬이차전지용 정극활물질 $\text{Li}_{1-x}\text{NiO}_2$ 의 열적 특성에 관한 연구
Thermal behavior and the decomposition mechanism of $\text{Li}_{1-x}\text{NiO}_2$

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Thermal behavior of electrochemically delithiated $\text{Li}_{1-x}\text{NiO}_2$ ($R\bar{3}m$ or $C2/m$) up to 400°C was studied by thermogravimetry (TG), differential scanning calorimetry (DSC), high temperature x-ray diffraction (XRD) and x-ray absorption (XAS) measurements and its thermal decomposition mechanism was proposed.

Delithiated $\text{Li}_{1-x}\text{NiO}_2$ was thermally decomposed to a spinel phase ($Fd\bar{3}m$) at around 220°C . For $x \leq 0.5$, $\text{Li}_{1-x}\text{NiO}_2$ was decomposed to LiNiO_2 and LiNi_2O_4 spinel and the fraction of the spinel in the decomposed product increased almost linearly with x . For $x > 0.5$, $\text{Li}_{1-x}\text{NiO}_2$ was converted into the spinel and this reaction was accompanied by oxygen evolution. On further heating, delithiated $\text{Li}_{1-x}\text{NiO}_2$ of all compositions turned into a rock salt phase ($Fm\bar{3}m$) with NiO structure. The temperature for the decomposition of $\text{Li}_{1-x}\text{NiO}_2$ to a spinel was independent on x , however, the temperature for the decomposition to a rock salt phase decreased with x . The thermal behavior of $\text{Li}_{1-x}\text{NiO}_2$ could be interpreted as an overlap of the exothermic rearrangement of nickel and lithium cations to form a spinel or a rock salt phase and the endothermic oxygen evolution reaction.