

研究论文

层状锰酸锂衍生物的阳离子价态与锂电池的电化学性能研究

唐爱东, 黄可龙*

(中南大学化学化工学院功能材料化学研究所 长沙 410083)

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摘要 采用溶胶-凝胶法, 通过锂盐、镍盐、钴盐与锰盐生成锂镍钴锰氧化化合物的前驱体, 随后采用高温固相法合成了 $\text{Li}(\text{Mn}_{1/3}\text{Co}_{1/3}\text{Ni}_{1/3})\text{O}_2$. 借助于X射线光电子能谱(XPS)、X射线衍射(XRD)、循环伏安(CV)及充放电测试等现代测试手段研究了材料的晶型结构、离子价态及电化学性能. 前驱体经950 °C煅烧可获得晶体结构完整、晶胞参数为 $a=0.2864$ nm, $c=1.4235$ nm的六方层状 $\text{Li}(\text{Mn}_{1/3}\text{Co}_{1/3}\text{Ni}_{1/3})\text{O}_2$ 化合物; XPS结果表明 $\text{Li}(\text{Mn}_{1/3}\text{Co}_{1/3}\text{Ni}_{1/3})\text{O}_2$ 化合物表面上的Mn, Ni和Co分别以 Mn^{4+} , Ni^{2+} 和 Co^{3+} 存在; 材料的高温放电比容量比室温要高, 在55 °C下, 在2.5~4.6 V电压范围内, 电流密度为28 mA/g时材料首次放电容量195 mAh/g, 循环10次后容量保持在170 mAh/g; 循环伏安曲线上3.7 V和4.4 V的氧化还原过程对应于 $\text{Ni}^{2+/4+}$ 和 $\text{Co}^{3+/4+}$ 氧化还原电对的反应.

关键词 [Li\(Mn_{1/3}Co_{1/3}Ni_{1/3}\)O₂](#) [高温固相合成](#) [晶体结构](#) [表面分析](#) [电化学性能](#)

分类号

Cationic Ion Value State of Layered Lithium Manganate Derivative and Electrochemical Properties of Lithium Battery

TANG Ai-Dong, HUANG Ke-Long*

(Institute of Functional Material Chemistry, School of Chemistry and Chemical Engineering, Central South University, Changsha 410083)

Abstract The cathode material for lithium batteries $\text{Li}(\text{Mn}_{1/3}\text{Co}_{1/3}\text{Ni}_{1/3})\text{O}_2$ has been synthesized by sol-gel technique followed by high temperature solid state reaction. The crystalline structure, ionic value and electrochemical properties of the material were investigated via X-ray photoelectron spectra, X-ray diffraction, cyclic voltammetry and charge-discharge cycling. The hexagonal lattice parameters of the compound by calcining the precursor at 950 °C are: $a = 0.2864$ nm, $c = 1.4235$ nm. XPS studies indicate that the oxidation states of manganese, nickel and cobalt in the $\text{Li}(\text{Mn}_{1/3}\text{Co}_{1/3}\text{Ni}_{1/3})\text{O}_2$ surface region are largely 4+, 2+ and 3+ respectively with small content of Ni^{2+} ion. Initial discharge capacity of 195 mAh/g at 55 °C was obtained in the range 2.5~4.6 V and at a specific current of 28 mA/g and under the same conditions 170 mAh/g was retained at the end of the 10th cycles. From the voltage profile and cyclic voltammetry, the redox processes occurring at ~3.7 and ~4.4 V were assigned to the $\text{Ni}^{2+/4+}$ and $\text{Co}^{3+/4+}$ couples, respectively.

Key words [Li\(Mn_{1/3}Co_{1/3}Ni_{1/3}\)O₂](#) [high temperature solid state reaction](#) [crystal structure](#) [surface analysis](#) [electrochemical property](#)

DOI:

通讯作者 黄可龙 huangkelong@yahoo.com.cn

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