High Resolution Resonant Inelastic X-Ray Scattering Revealed Oxygen Redox Machenism in Li-rich Layered Oxide Cathode

Po-Cheng Ouyang(歐陽伯承)[1], Kuan-Lin Chu(朱冠霖)[1], Shi-Kai Jiang(蔣仕凱)[1], Di-Jing Huang(黃迪靖)[3]*, Wei-Nien Su(蘇威年)[2], Bing-Joe Hwang(黃炳照)[1,3]*

[1]Department of Chemical Engineering, National Taiwan University of Science and Technology.
[2]Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei 10607, Taiwan
[3]National Synchrotron Radiation Research Center (NSRRC), Hsinchu 30076, Taiwan

Abstract

Nowadays, the lack of energy has led to increasing demand for battery energy density, and the pursuit of higher energy density has become a trend. For this reason, in order to obtain higher energy density, the use of high energy density cathode materials plays an important role. Lithium-rich materials are a potential candidate which have an extremely high capacity at the first cycle and the reversible capacity is around 275 mAh/g. However, in the first cycle, lithium-rich materials are different from other kinds of cathode material, it provides the additional capacity during the initial charging process. Many groups indicate the additional capacity is due to the oxygen anion redox at high voltage in the first cycle. At the same time, it can be found through X-ray diffraction that the unique superlattice structure in Li-rich material disappears. However, until now the whole oxygen anion redox mechanism is still not clear in the Li-rich cathode, this reaction mechanism is a breakthrough for the future development of new excess metal cathodes. The high-resolution resonant inelastic x-ray scattering (RIXS) is a great tool to understand the oxygen vibration mode, energy loss, and electronic valence state. Herein, we introduce the RIXS techniques to study the oxygen K-edge phenomena in lithium-rich materials at high voltage (4.8V). Under the oxygen anion-redox behavior and try to perform more cycles to understand the reversibility of the anion redox reaction. In addition, we found that the energy loss of the first cycle is different from other cycles, it means the oxygen vibration mode is different from other cycles. In the future, we hope this kind of technique can further study on the mechanism of oxygen redox.

Keywords: Li-rich cathode; Oxygen redox; RIXS

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