Carbonate deprotonation on Ni-rich layered cathode: Development of a new cis isomerism oligomer as an organic coverage

Fu-Ming Wang

Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taipei, 106, Taiwan
mccabe@mail.ntust.edu.tw

Ni-rich layered cathodes have a high practical capacity (>200 $mAh \cdot g^{-1}$) and tapped density (>3.6 $mg \cdot cm^{-2}$), thus attracting wide attention in large applications such as electric vehicles and energy storage. However, high surface reactivity of these cathodes promote the decomposition of carbonates solvents, which contributes to the growth of the cathode–electrolyte interphase (CEI) as well as rapid fading of the battery's capacity during long-term cycle. Carbonates are favorable for deprotonation reaction by the oxygen atom in the Ni-rich layered cathode and further in the formation of the CEI. In this study, the deprotonation mechanism of cyclic and linear carbonates on a Ni-rich layered cathode was thoroughly investigated using operando Fourier-transfer infrared spectroscopy, and the reasons for cathode fading could be confirmed in terms of the carbonate structures. In addition, a new maleimide oligomer was developed and covered on a Ni-rich layered cathode to inhibit the deprotonation of the carbonates. The maleimide oligomer acts as a cis isomerism that provides a bridge function for reacting with oxygen on the cathode surface by its cis formulation. Moreover, this bridge function will keep the carbonates away from the cathode surface for further decomposition during cycling. On the contrary, the battery performance exhibited a cycling ability at a high rate, and the new cis isomerism maleimide oligomer helped improve the rate capability. A full-cell (>3 Ah) test containing graphite as the anode with a cis formulation of the maleimide oligomer coverage was completed.

References

[1] Laurien Merinda, **Fu-Ming Wang***, Nae-Lih Wu*, Ulya Qonita, Wei-Hsiang Huang, Lester Tiong, Ching-Kai Chang, Ping-Hsuan Hsu, Chih-Wen Pao, Jeng-Lung Chen, Chi-Liang Chen, Ting-Shan Chan, "Carbonate deprotonation on Ni-rich layered cathode: Development of a new cis oligomer as an organic coverage", *J. Mater. Chem. A* **12** (2024) 28886.