The Oxide/Electrolyte Interface Formation in Li-ion batteries

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The development of durable and high capacity lithium-ion batteries requires an understanding of the electrolyte decomposition and the formation of electrode/electrolyte interface layer. The EEI layer formation of negative electrodes such as lithium and graphite, also referred as Solid Electrolyte Interphase, is comprehensively studied [1,2], whereas the electrolyte decomposition and formation of the EEI layer at the positive electrodes are still unknown [3,4]. Especially, at high potentials, the role of oxide lattice oxygen becomes critical, leading to the evolution of oxygen from the oxide lattice or the formation of highly reactive species like surface peroxide and superoxide, which can modify the nature of the EEI layer.

By using X-ray Photoelectron Spectroscopy (XPS) on different $LiMO_2$ electrodes ($LiCoO_2$ and NMC electrodes with different Ni content) and different electrolytes (LP57 electrolyte with and without 1% diphenyl carbonate additive), we show how the nature of the EEI layer depends on the chemistry of the oxide and on the applied potential. We highlight the importance of using model electrodes containing only the active material, without conductive agents and polymeric binders that can modify the EEI layers on the electrode. The analysis of the XPS results points to a strong dependency of the surface reactivity on different electrode and electrolyte composition.

References:

[1] E. Peled, J. Electrochem. Soc. 126 (1979) 2047-2051.

[2] D. Aurbach, M.D. Levi, K. Gamulski, B. Markovsky, G. Salitra, E. Levi, U. Heider, L. Heider, R. Oesten, J. Power Sources 81-82 (1999) 472-479.

[3] K. Xu, Chem. Rev. 114 (2014) 11503-11618 .

[4] M. Gauthier, T. J. Carney, A. Grimaud, L. Giordano, N. Pour, H.-H. Chang, D. P. Fenning, S. F. Lux, O. Paschos, C. Bauer, F. Maglia, S. Lupart, P. Lamp, Y. Shao-Horn, J. Phys. Chem. Lett. 6 (2015) 4653–4672.