Contribution ID: **439** Type: **Poster**

Neutron and X-ray diffraction investigations of the two-phase state of the cathode material LixNi0.8Co0.15Al0.05O2 during the first charge

LixNi0.8Co0.15Al0.05O2 (NCA) is one of the most common cathode materials used in the Li-ion batteries production. This material does not reveal any structural phase transitions in the voltage range recommended for operation (2.5-4.33 V). However, the NCA material separates into two rhombohedral phases during the first charge. This phase-separated state disappears completely during the first discharge and it is never observed in the following charge-discharge cycles. It is possible that abnormal phase-separated structural behavior of NCA cathode material during the first charge cycle depends on the preparation condition, e.g., on a level of electrode compaction (calendering) or amount of additives.

In the present work, structural state of NCA electrodes was studied in electrochemical cells developed for operando/in situ neutron and X-ray diffraction experiments. To investigate the calendering and binder amount impact on the structural evolution of the NCA, we have performed the neutron and X-ray diffraction experiments on the NCA cathodes prepared with different compaction degree and different amount of polyvinylidene fluoride (binder).

It was established that stronger compaction of the electrodes partially suppresses the phase separation of the cathode material: reduces a state of charge (SOC) range where two phases coexist, and decreases the difference between structural parameters of the phases. X-ray photoelectron spectroscopy has revealed a presence of Li2CO3 film at the surface of the NCA material in the amount that is unlikely to affect the NCA behavior during the first charge.

Summary

The observed correlations made it possible to suggest that factors, such as the morphology and the amount of binder, affect the phase separation of the NCA material. This observation could be expanded to layered cathode materials with similar microstructures.

Authors express their gratitude to A.V. Ivanichev and A.V. Ushakov for useful discussions and advices on contents of this contribution and to Olga Kristavchuk for help with experiments. Neutron diffraction experiments were performed at the HRFD diffractometer at the IBR-2 neutron pulsed source (FLNP JINR) and supported by Russian Science Foundation through the project No.14-12-00896. I.A. Bobrikov and O.Yu. Ivanshina would like to thank Russian Science Foundation for financial support of the data analysis through the project No. 15-13-10006.

Primary author: Dr BOBRIKOV, Ivan (Joint Institute for Nuclear Research/Saratov State University)

Co-authors: Prof. BALAGUROV, Anatoly (Joint Institute for Nuclear Research/Lomonosov Moscow State University); Dr KORNIEIEVA, Katerina (Joint Institute for Nuclear Research); Dr SAMOYLOVA, Natalia (Joint Institute for Nuclear Research/Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University); Dr IVANSHINA, Olga (Joint Institute for Nuclear Research/Saratov State University); Dr VASIN, Roman (Joint Institute for Nuclear Research); Mrs SUMNIKOV, Sergey (Joint Institute for Nuclear Research/Lomonosov Moscow State University)

Presenter: Dr IVANSHINA, Olga (Joint Institute for Nuclear Research/Saratov State University)

Track Classification: Condensed Matter Physics