Operando XRD Investigation Towards Industrially Relevant Battery Configurations Using the DANOISE Cell

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Batteries are crucial components in modern technologies, from electric vehicles to portable devices, and their long life and reliability are directly dependent on understanding the mechanisms of their failure. Operando XRD, a technique that allows real-time monitoring of structural modifications during battery operation, provides insights into the dynamic structural changes that occur during battery cycling, enabling a better understanding of the causes of material degradation, such as crystal lattice breakdown, phase formation, and stress accumulation within the electrodes.[1] For operando XRD measurements, home-made 3D printed DANOISE cell in transmission mode was used.[2]

Results cover from ex-situ XRD measurements of the graphite or NMC electrode in the DANOISE cell, without applied current, to operando XRD measurements in the half-cell, as well as measurements with coated electrode with mentioned active materials. This is done in order to get closer to the industrial scale where samples are deposited on the Cu or Al foil, respectively, and not pressed into the pellets. The aim is to identify specific structural phenomena associated with battery failure, with a focus on improving the performance and stability of future battery materials and technologies and to compare the results obtained from pellet and from coated electrode. The main accent is on the crystallographic analysis of the operando XRD data, by using a sequential refinement in TOPAS.[3]

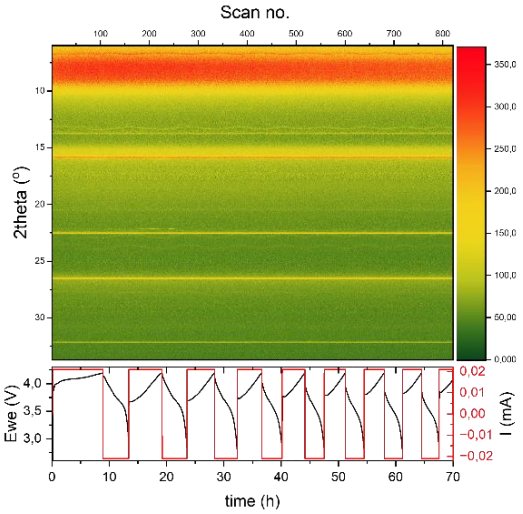


Figure 1. *Background subtracted contour plot of operando PXRD of NMC deposited on Al foil correlated to the capacity*

[1] Z. Wen et al. Front. Energy Res. (2018). 6, 66.

[2] M. Johansen et al. *Batteries &* Supercaps (2024). 7, e202400033J.

[3] G. W. Stinton and J. S. O. Evans, J. Appl. Cryst. (2007). 40, 87–95.

The authors greatly appreciate the support of the Ministry of Science, Education and Youth and the Croatian Science Foundation for funding this work. This work is funded by the European Union funds "National plan for Recovery and Resilience" under the number NPOO.C3.2.R3-I1.04.0187.