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Neutron & X-ray diffraction studies of graphite anodes conducted at MLZ

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Current state of the art lithium ion batteries typically use graphite as an anode material. Understanding the dynamical processes during lithiation and delithiation is crucial for comprehending performance and degradation. Especially due to the detrimental effects of fast charging or charging at low temperatures. Many aging processes, like lithium plating, depend intrinsically on the lithiation properties. Lithium plating enhances cell aging and imposes a security issue in commercial cells [1]. Detailed understanding of the material properties and the dynamic lithiation processes in commercial type cells is necessary to avoid security issues and performance deterioration due to occurrence of Li plating or phase inhomogeneity. In our studies of graphite/NMC cells with operando neutron diffraction we found that intermittent Li plating and phase inhomogeneity in graphite anodes can be observed even under unexpectedly mild conditions, although the effects are often hidden due to the fast relaxation processes at room temperature [1]. Within the ExZellTUM II project (funded by BMBF, grant no. 03XP0081), we recently studied the temperature and current density dependence and the lithiation dynamics with neutron diffraction [2]. By combining neutrons with post-mortem x-ray diffraction [3] the lithiation process in large batteries can be better understood.

[1] Zinth et al., JPS, (2014), 271, 152.

[2] Wilhelm, et al., JES, (2018), 165, A1846.

[3] Wilhelm, et al., JPS, (2017), 365, 327.

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