MS20-01 | Combined Analysis of Structure and Strain in Engineering Materials by Neutron and Synchrotron X-Ray Diffraction, and Electron Microscopy

Korsunsky, Alexander (University of Oxford, Oxford, GBR)

Heterogeneous multi-scale nature commonly observed in advanced engineered and natural materials are the subject of active experimental and modelling research. Key ideas will be introduced for materials and tissues such as human dentine and enamel, nickel-base superalloys, and materials for Li-ion battery cathodes.

Structure and processes in battery cathodes were considered using combined techniques. Damage during cyclic charging develops from the atomic lattice scale to nano-, micro- and macro-scale. Recent results will be overviewed:

1. *Operando* X-ray absorption spectroscopy (XANES, EXAFS) of Mn, Co and Ni atomic environment evolution during (dis)charging reveals 'staged', partially reversible nature [1].
2. *Operando* synchrotron X-ray diffraction analysis of unit cell dimension and phase transformation in $Li(Mn,Co,Ni)O_2$reveals the origins of anisotropic lattice straining [2].
3. TOF-SIMS quantitative nanoscale mapping of Li distribution in mixed transition metal oxide cathodes reveals the presence of Li "hot spots" and "trapping" causing local strains and strain gradients [3].
4. Analytical solutions for Li concentration and stress in secondary spherical particles in cathodes during charging/discharging [4].
5. Progressive fragmentation of secondary active material particles in cyclic charging under lithiation-induced inter-granular strains [5].
6. Nano- to micro-scale FIB-SEM serial sectioning tomography of Li battery cathodes for visual evidence of active material fragmentation [6].

[1] Kim TH et al., 2016
[2] Song BH et al., PCCP, 2016
[3] Song BH et al., NanoEnergy 2015
[4] Korsunsky AM, Sui T, Materials & Design, 2015
[5] Sun GH et al., Extreme Mechanics Letters, 2016
[6] Song BH et al., J Mater Chem A, 2015