Powder Diffraction

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TECHNICAL ARTICLE

Order and disorder in NMC layered materials: a FAULTS simulation analysis

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The program FAULTS has been used to simulate the X-ray powder diffraction (XRD), neutron powder diffraction (NPD), and electron diffraction (ED) patterns of several structural models for $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$, including different types of ordering of the transition metal (TM) cations in the TM slabs, different amounts of Li^+/Ni^{II+} cation mixing and different amounts of stacking faults. The results demonstrate the relevance of the structural information provided by NPD and ED data as compared with XRD to characterize the microstructure of NMC ($LiNi_{1-y-z}Mn_yCo_zO_2$) compounds. © *2017 International Centre for Diffraction Data.* [doi:10.1017/S0885715617000033]

Key words: X-ray powder diffraction, neutron powder diffraction, electron diffraction, diffuse scattering, stacking faults, layered materials, FAULTS, DIFFaX, battery materials, layered oxide

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The XRD, NPD, and SADP simulations were performed with the version July 2016 of the FAULTS program. The structures were drawn and examined with the help of the visualization programs *FullProf Studio* (Rodríguez-Carvajal and Chapon, 2004) and VESTA (Momma and Izumi, 2011). The XRD and NPD patterns were plotted using the GUI program WinPLOTR (Rodríguez-Carvajal and Roisnel, 1998; Roisnel and Rodríquez-Carvajal, 2001) included in the *FullProf Suite* (Rodríguez-Carvajal, 1993a, 1993b). The SADP patterns were drawn with the image processing program ImageJ (Rasband, 1997; Abramoff *et al.*, 2004; Schneider *et al.*, 2012).

FAULTS DOWNLOAD

The FAULTS program (Casas-Cabanas *et al.*, 2006, 2015, 2016) can be obtained either as part of the *FullProf Suite* at http://www.ill.eu/sites/fullprof, or as a separate program by downloading the compressed file at http://www.cicenergigune.com/faults. The source code is also available in the CrysFML repository at http://forge.epn-campus.eu/projects/crysfml/repository/ (Rodríguez-Carvajal and Gonzalez-Platas, 2003a, 2003b).