Supplementary Information

Lithium-ion batteries: direct solid sampling for characterisation of black mass recyclates using graphite furnace atomic absorption spectrometry

Maria Dommaschk,* Tim Sieber, and Jörg Acker

Brandenburg University of Technology Cottbus-Senftenberg, Department of Physical Chemistry, 01968 Senftenberg, Germany. E-mail: Maria.Dommaschk@b-tu.de



Supplementary Figure S 1. Time- and wavelength-resolved absorption spectra for about 0.4 mg of solid NMC standard in the vicinity of the **(a)** Li line at 323.2657 nm **(b)** Ni line at 294.3912 nm **(c)** Mn line at 321.6945 nm and **(d)** Co line at 308.6792 nm using the optimised temperature programme for solid analysis with HR-CS GF AAS.



Supplementary Figure S 2. Analytical contents (n = 5) for lithium, nickel, manganese and cobalt in NMC/graphite solid dilutions with the successive dilution factors 100/10 and 32/32 (dilution factor 1/dilution factor 2) in mg g⁻¹. The solid samples were dissolved wet-chemically and analysed with ICP-OES. The measurement uncertainty corresponds to 1σ .



Supplementary Figure S 3. 111NMC/Graphite material (dilution factor 1000): SEM micrograph (a) Magnification 264X, (b) EDX element mapping for nickel indicated by yellow color.

Supplementary Table S 1 Calculated stoichiometric ratios of NMC (mean \pm standard deviation, n = 3) for the determination of Li, Ni, Mn and Co (mg g⁻¹)) in the certified reference material "BAM-S014 Li-NMC 111 Cathode Material" and in various recyclates of cathode coatings.

		Stoichiometric factors			
Sample		Li	Ni	Mn	Со
CRM	Found	1.25 ± 0.49	0.32 ± 0.10	0.34 ± 0.10	0.34 ± 0.10
BAM-S014	ICP-OES	1.11 ± 0.01	0.33 ± 0.01	0.33 ± 0.10	0.34 ± 0.01
Li-NMC 111	Certified	1.09 ± 0.21	0.34 ± 0.06	0.33 ± 0.06	0.33 ± 0.07
Recyclate 1	Found	0.91 ± 0.37	0.41 ± 0.13	0.31 ± 0.09	0.28 ± 0.10
	ICP-OES	0.95 ± 0.01	0.41 ± 0.01	0.29 ± 0.00	0.30 ± 0.00
Recyclate 2	Found	0.55 ± 0.21	0.39 ± 0.12	0.31 ± 0.10	0.30 ± 0.10
	ICP-OES	0.63 ± 0.01	0.41 ± 0.01	0.29 ± 0.01	0.30 ± 0.01
Recyclate 3	Found	0.78 ± 0.08	0.39 ± 0.12	0.28 ± 0.02	0.33 ± 0.03
	ICP-OES	0.84 ± 0.01	0.41 ± 0.01	0.29 ± 0.00	0.30 ± 0.00
Recyclate 4	Found	0.85 ± 0.38	0.57 ± 0.21	0.23 ± 0.08	0.20 ± 0.09
	ICP-OES	1.09 ± 0.05	0.61 ± 0.02	0.21 ± 0.01	0.19 ± 0.01