

Supplementary Information for “Interlaboratory comparison of XRF analysis on thin films, including alloys, oxides, multilayers, and a lithium-ion battery material”

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SI-1 Tabulated X-ray edge and line energies

For convenience, we have compiled a list of the relevant X-ray edge and line energies for the elements included in the interlaboratory comparison. Values are taken from the *xraylib*¹. For the transition metals listed, while the $K\beta$ line of an element with atomic number Z has sufficient energy to excite the K edge of all elements with $Z' \leq Z - 1$, only for $Z' \leq Z - 2$ does the more intense $K\alpha$ line contribute.

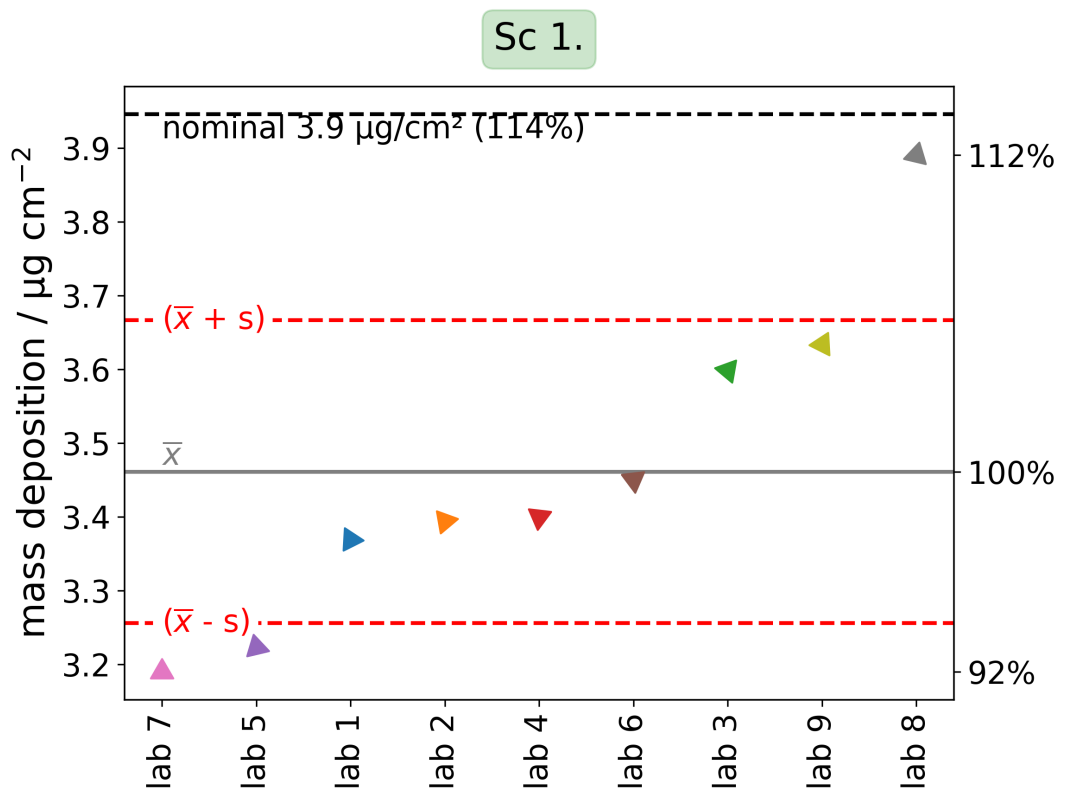
Z	Element	K edge / keV	$K\alpha$ line / keV	$K\beta$ line / keV
13	Al	1.56	1.49	1.55
21	Sc	4.49	4.09	4.46
22	Ti	4.97	4.51	4.93
24	Cr	5.99	5.41	5.95
25	Mn	6.54	5.90	6.49
27	Co	7.71	6.93	7.65
28	Ni	8.33	7.47	8.27
29	Cu	8.98	8.04	8.91

¹Tom Schoonjans et. al., *The xraylib library for X-ray-matter interactions. Recent developments*, Spectrochimica Acta Part B 66 (2011) 776-784

SI-2 Results of interlaboratory comparison

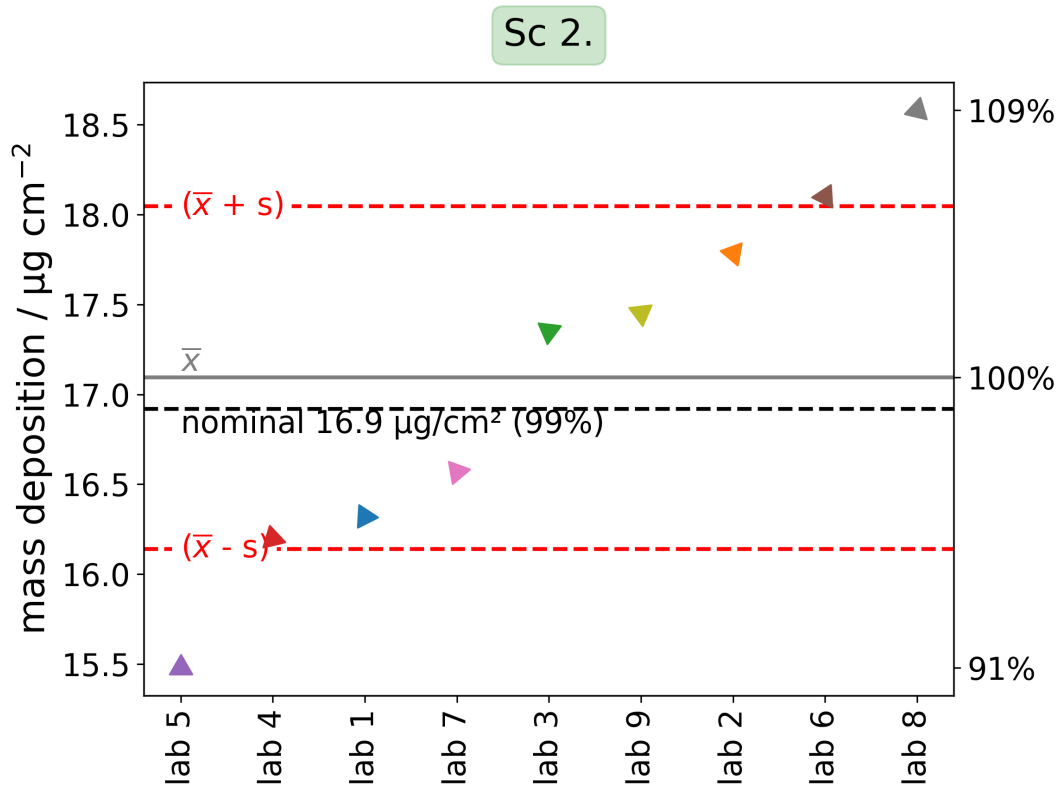
All individual results of the interlaboratory comparison are given below. Only two obvious outliers were removed (one for each TiO_2 sample). Almost all participants returned results for all samples. Two of the 17 samples were not measured by one participant: the LIB material sample (sample 17, type 5) and the Al_2O_3 sample (sample 8, type 2). First, subsections SI-2.1 to SI-2.8 on the following pages show the sorted data for the single-result samples (types 1 to 2). Second, the figures in subsections SI-2.9 to SI-2.17 show the multielemental results and compare three elements at a time (see page 13 and the following). The lab names are anonymized, yet consistent for all samples (lab 1 is always lab 1, etc.). In addition to the individual results, we also list the mean \bar{x} , the standard deviation s and the relative standard deviation $s_r = \frac{s}{\bar{x}}$.

SI-2.1 Results for sample #1 “Sc 1.”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



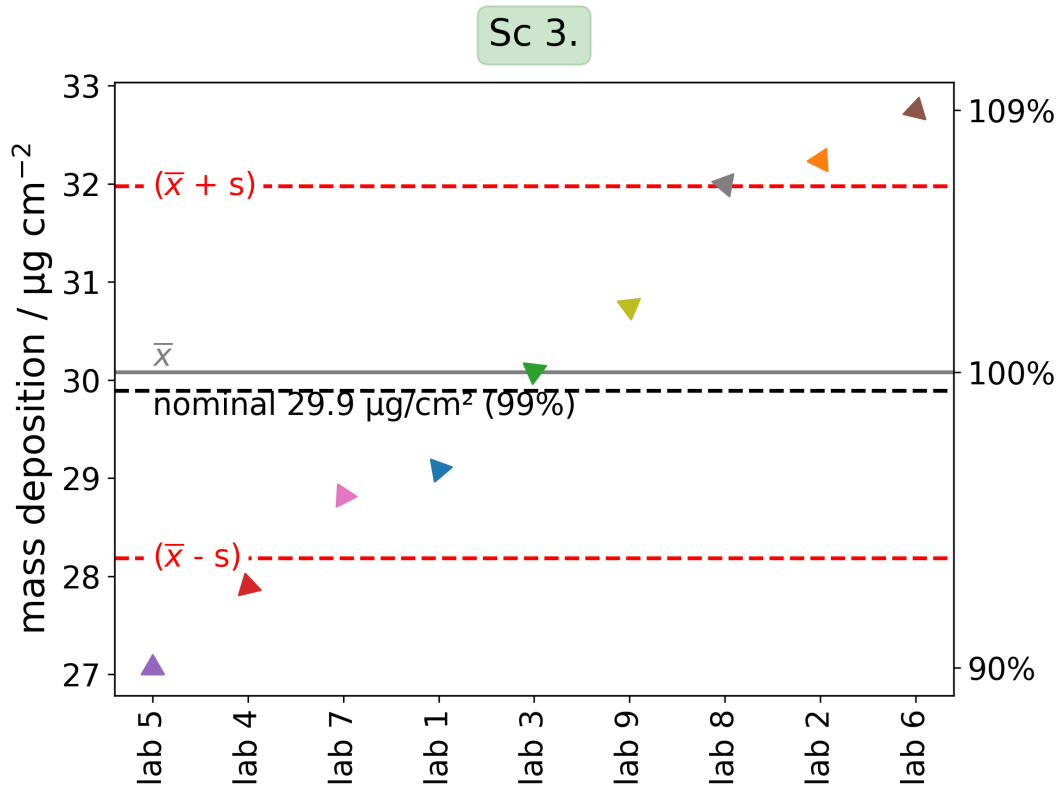
participant	result / $\mu\text{g cm}^{-2}$
lab 1	3.37
lab 2	3.39
lab 3	3.60
lab 4	3.40
lab 5	3.22
lab 6	3.45
lab 7	3.19
lab 8	3.89
lab 9	3.63
\bar{x}	3.46
s	0.21
$s_r = s / \bar{x}$	5.9 %

SI-2.2 Results for sample #2 “Sc 2.”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



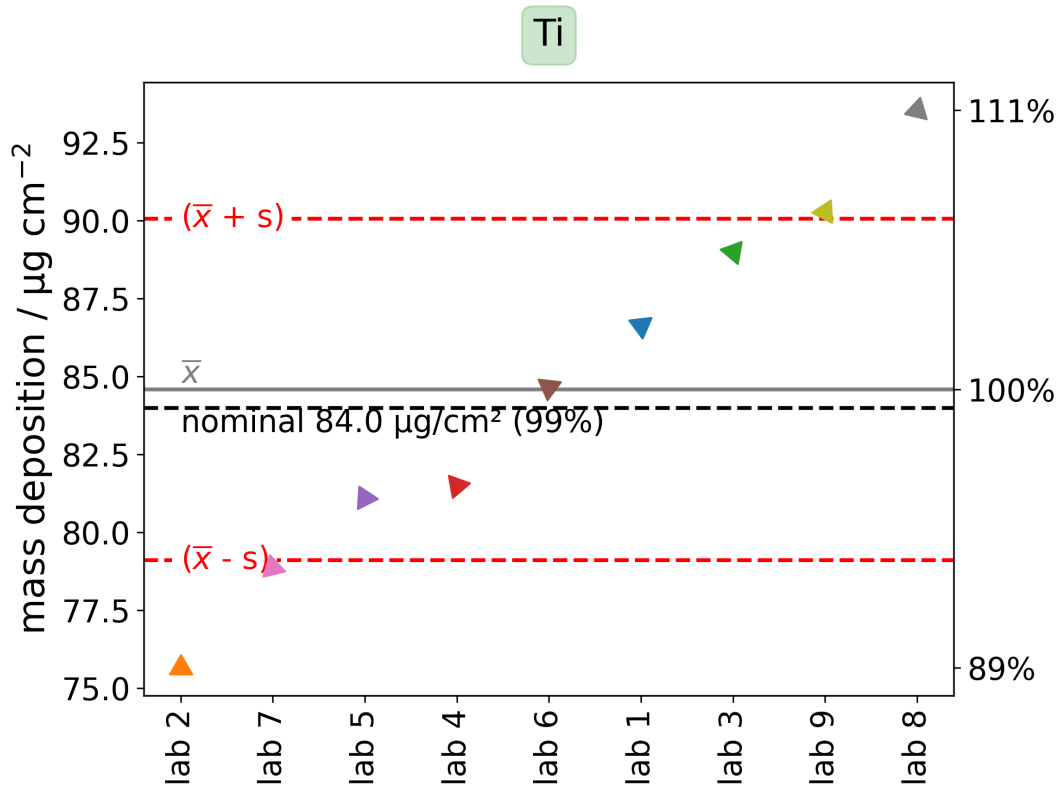
participant	result / $\mu\text{g cm}^{-2}$
lab 1	16.3
lab 2	17.8
lab 3	17.4
lab 4	16.2
lab 5	15.5
lab 6	18.1
lab 7	16.6
lab 8	18.6
lab 9	17.5
\bar{x}	17.1
s	0.95
$s_r = s / \bar{x}$	5.6 %

SI-2.3 Results for sample #3 “Sc 3.,” including mean \bar{x} , standard deviation s , and relative standard deviation s_r



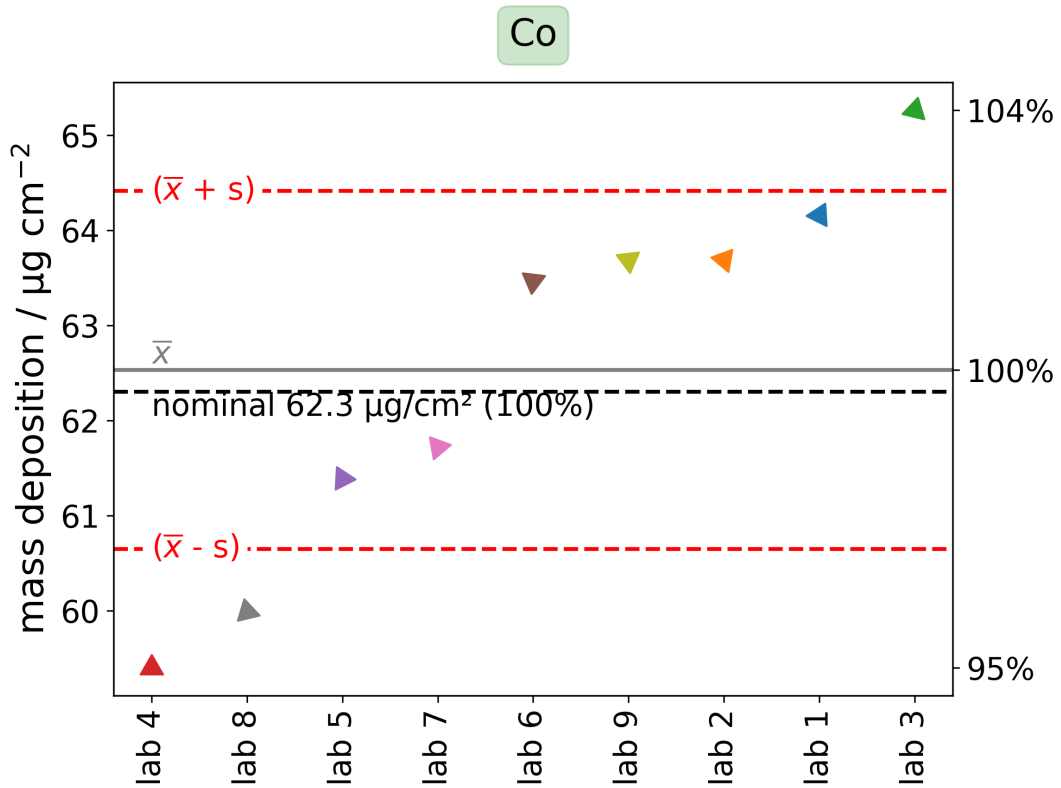
participant	result / $\mu\text{g cm}^{-2}$
lab 1	29.1
lab 2	32.2
lab 3	30.1
lab 4	27.9
lab 5	27.1
lab 6	32.8
lab 7	28.8
lab 8	32.0
lab 9	30.8
\bar{x}	30.1
s	1.9
$s_r = s / \bar{x}$	6.3 %

SI-2.4 Results for sample #4 “Ti”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



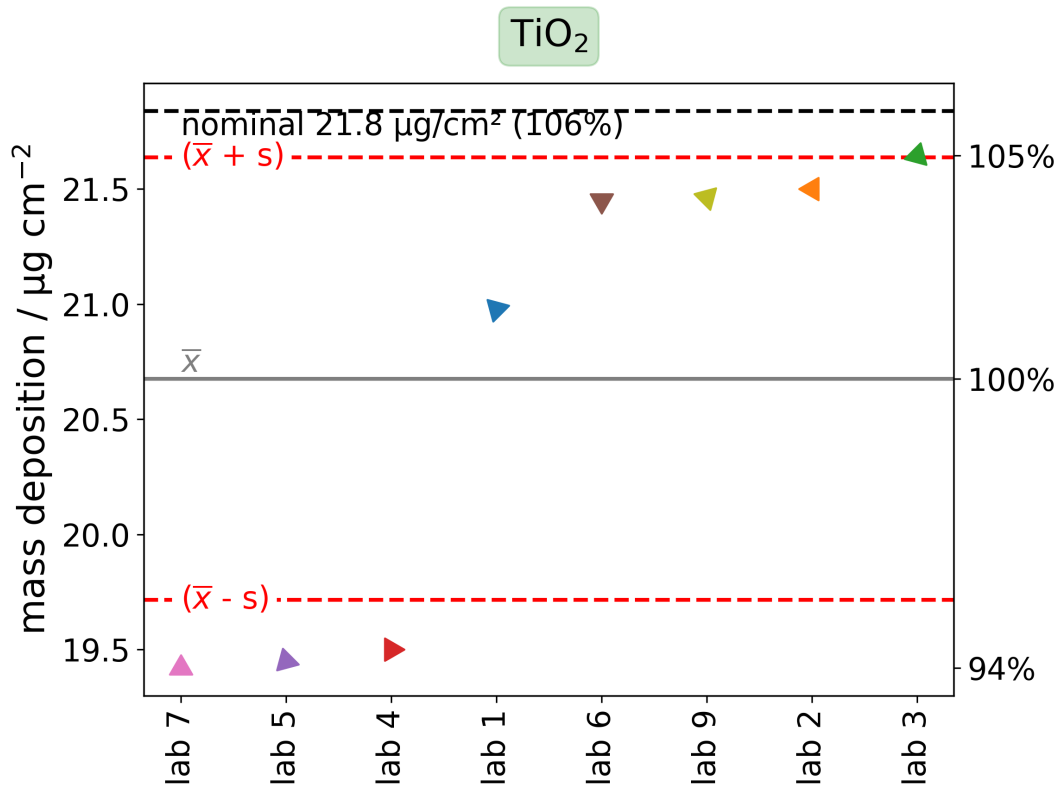
participant	result / $\mu\text{g cm}^{-2}$
lab 1	86.6
lab 2	75.7
lab 3	89.0
lab 4	81.5
lab 5	81.1
lab 6	84.7
lab 7	78.9
lab 8	93.5
lab 9	90.3
\bar{x}	84.6
s	5.5
$s_r = s / \bar{x}$	6.5 %

SI-2.5 Results for sample #5 “Co”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



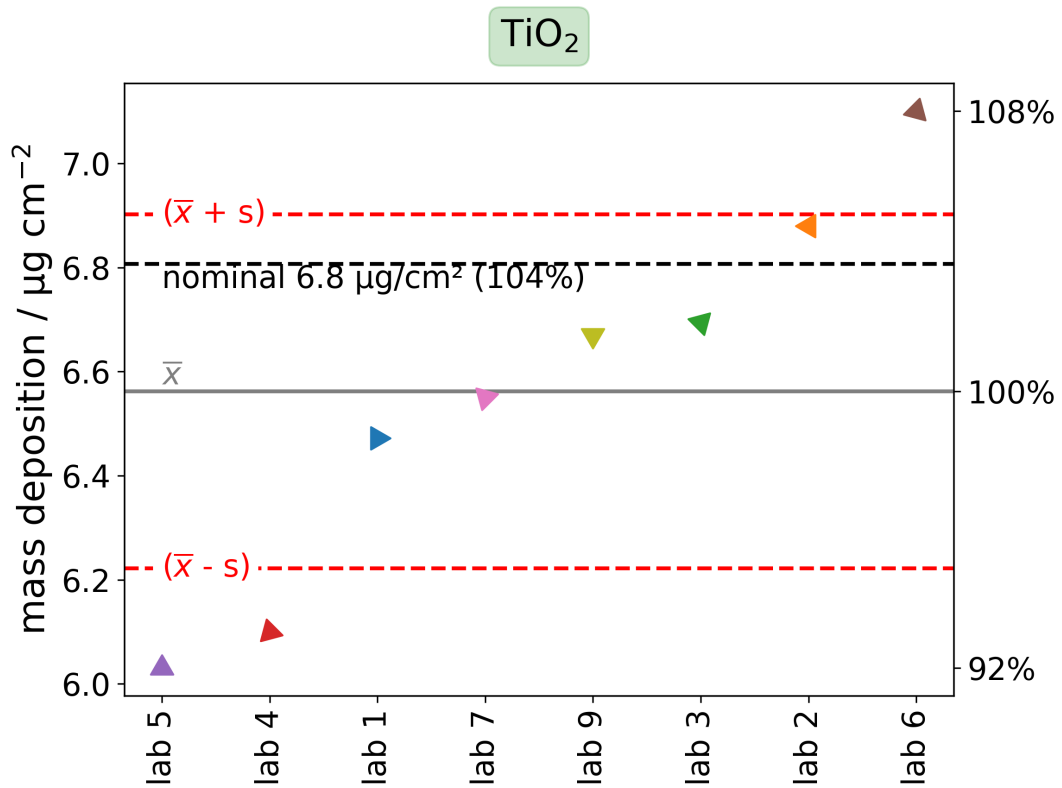
participant	result / $\mu\text{g cm}^{-2}$
lab 1	64.2
lab 2	63.7
lab 3	65.3
lab 4	59.4
lab 5	61.4
lab 6	63.5
lab 7	61.7
lab 8	60.0
lab 9	63.7
\bar{x}	62.5
s	1.9
$s_r = s / \bar{x}$	3.0 %

SI-2.6 Results for sample #6 “TiO2 1.,” including mean \bar{x} , standard deviation s , and relative standard deviation s_r



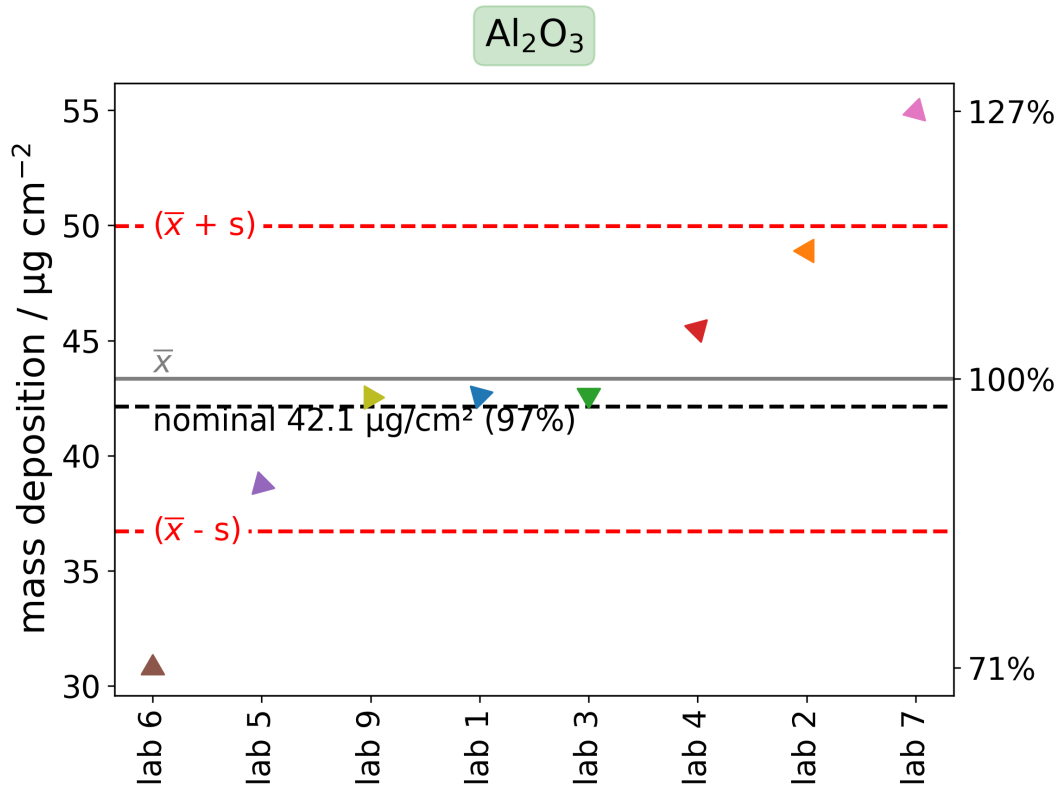
participant	result / $\mu\text{g cm}^{-2}$
lab 1	21.0
lab 2	21.5
lab 3	21.6
lab 4	19.5
lab 5	19.5
lab 6	21.5
lab 7	19.4
lab 9	21.5
\bar{x}	20.7
s	0.96
$s_r = s / \bar{x}$	4.7 %

SI-2.7 Results for sample #7 “TiO2 2.,” including mean \bar{x} , standard deviation s , and relative standard deviation s_r



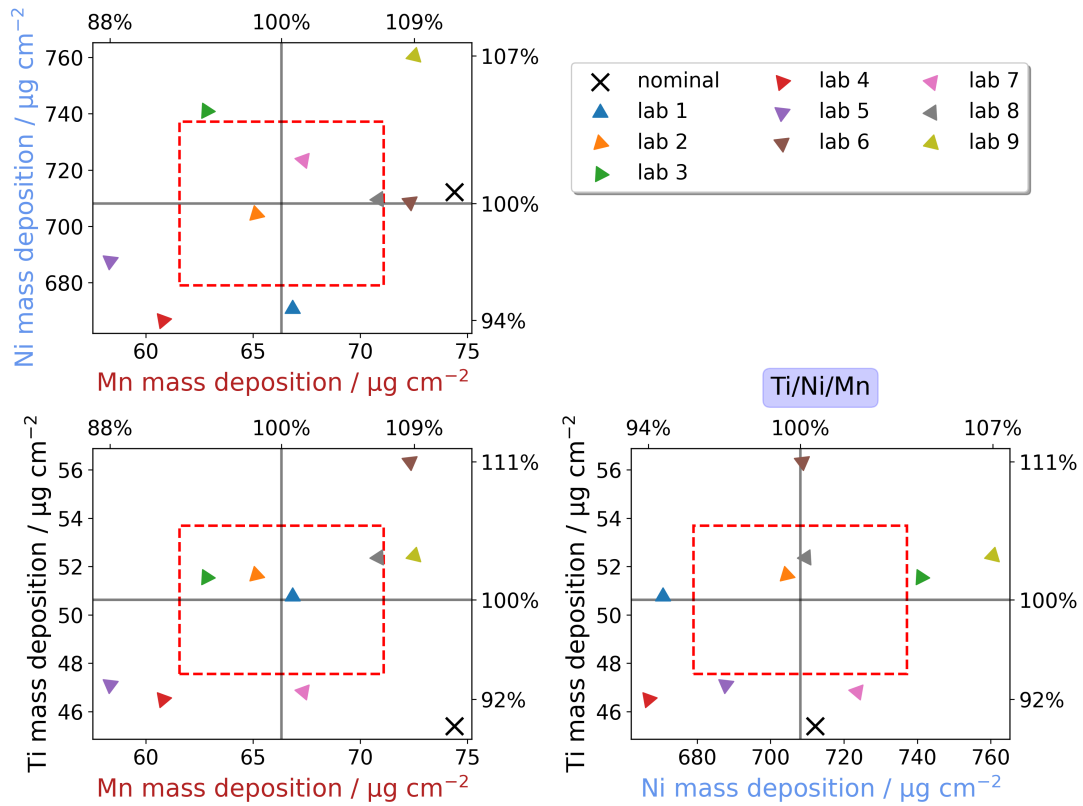
participant	result / $\mu\text{g cm}^{-2}$
lab 1	6.47
lab 2	6.88
lab 3	6.69
lab 4	6.10
lab 5	6.03
lab 6	7.10
lab 7	6.55
lab 9	6.67
\bar{x}	6.56
s	0.34
$s_r = s / \bar{x}$	5.2 %

SI-2.8 Results for sample #8 “Al₂O₃”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



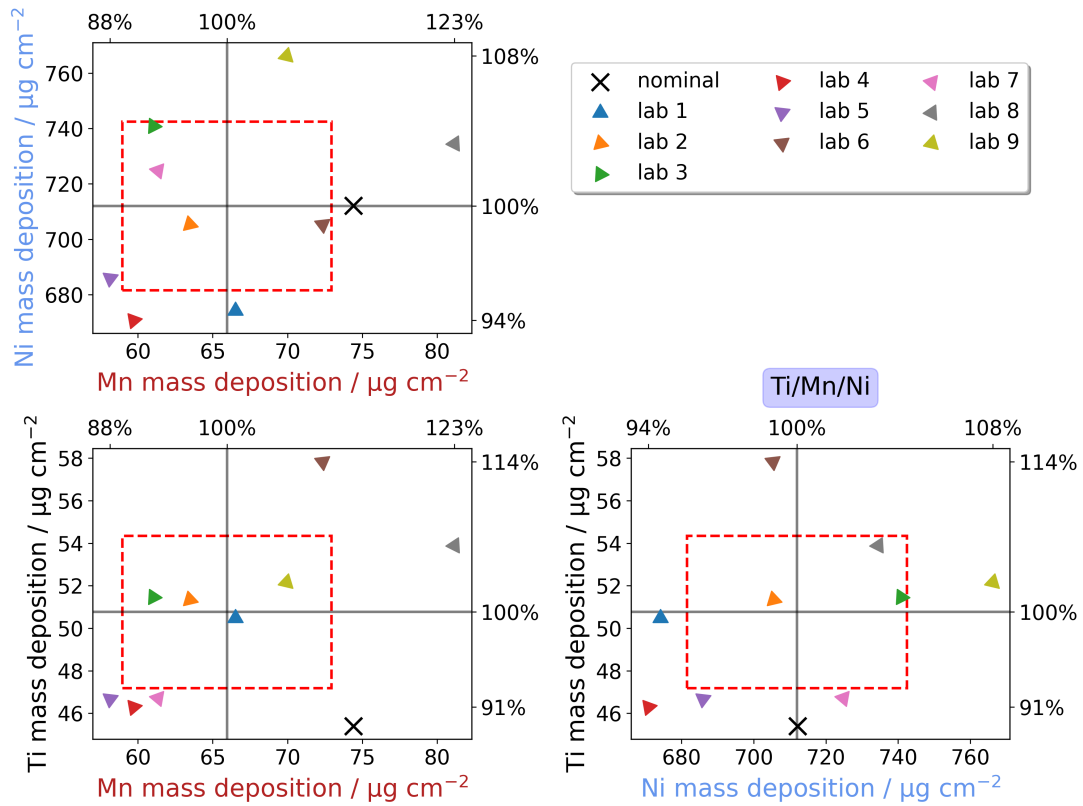
participant	result / $\mu\text{g cm}^{-2}$
lab 1	42.6
lab 2	48.9
lab 3	42.6
lab 4	45.5
lab 5	38.8
lab 6	30.8
lab 7	55.0
lab 9	42.5
\bar{x}	43.3
s	6.6
$s_r = s / \bar{x}$	15 %

SI-2.9 Results for sample #9 “Ti/Ni/Mn”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



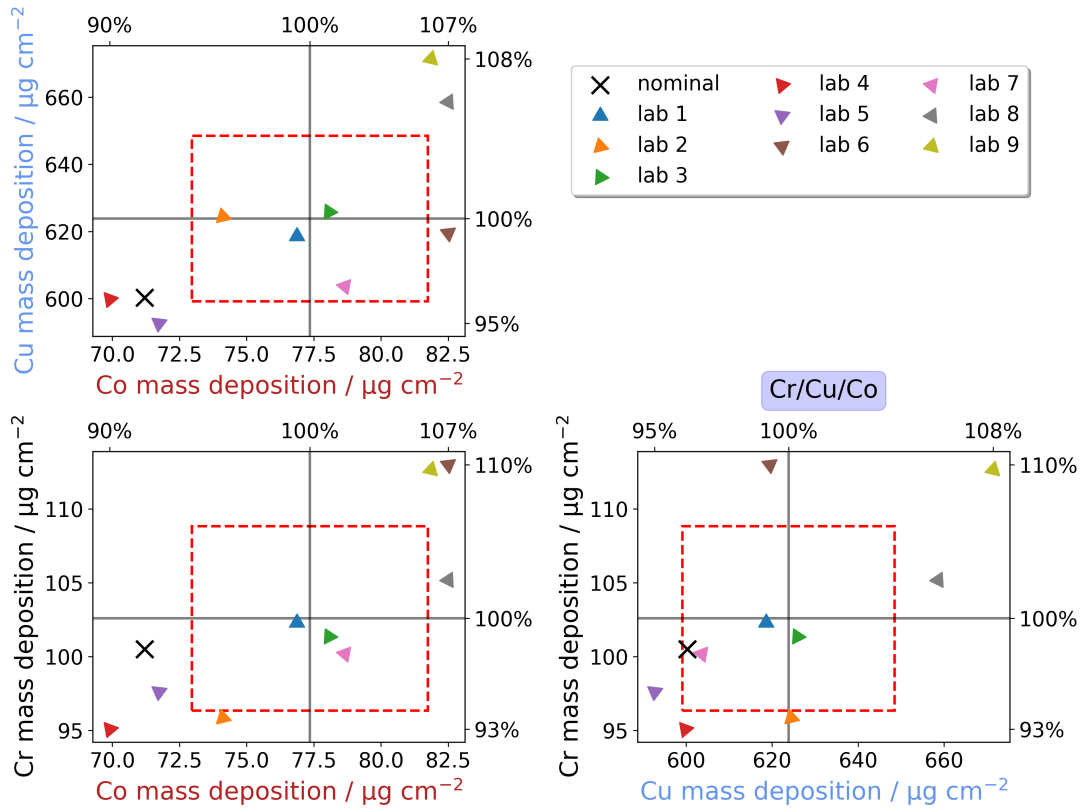
participant	Mn / $\mu\text{g cm}^{-2}$	Ni / $\mu\text{g cm}^{-2}$	Ti / $\mu\text{g cm}^{-2}$
lab 1	66.9	671	50.8
lab 2	65.1	704	51.7
lab 3	62.8	741	51.6
lab 4	60.8	667	46.5
lab 5	58.3	688	47.1
lab 6	72.3	709	56.3
lab 7	67.4	724	46.8
lab 8	70.9	710	52.4
lab 9	72.5	761	52.5
\bar{x}	66.3	708	50.6
s	4.8	29	3.1
$s_r = s / \bar{x}$	7.2 %	4.1 %	6.1 %

SI-2.10 Results for sample #10 “Ti/Mn/Ni”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



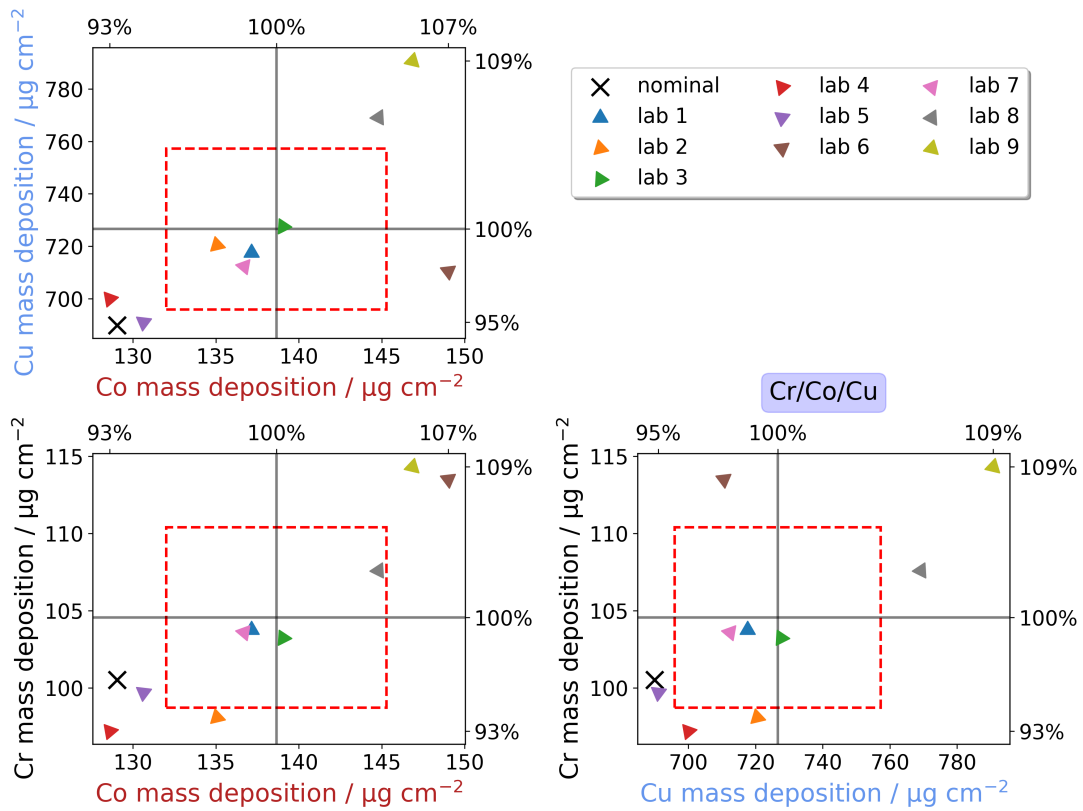
participant	Mn / $\mu\text{g cm}^{-2}$	Ni / $\mu\text{g cm}^{-2}$	Ti / $\mu\text{g cm}^{-2}$
lab 1	66.5	674	50.5
lab 2	63.5	705	51.4
lab 3	61.0	741	51.5
lab 4	59.7	671	46.3
lab 5	58.1	686	46.7
lab 6	72.3	705	57.8
lab 7	61.3	725	46.7
lab 8	81.2	735	53.9
lab 9	69.9	766	52.2
\bar{x}	66.0	712	50.8
s	7.0	30	3.6
$s_r = s / \bar{x}$	11 %	4.3 %	7.1 %

SI-2.11 Results for sample #11 “Cr/Cu/Co”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



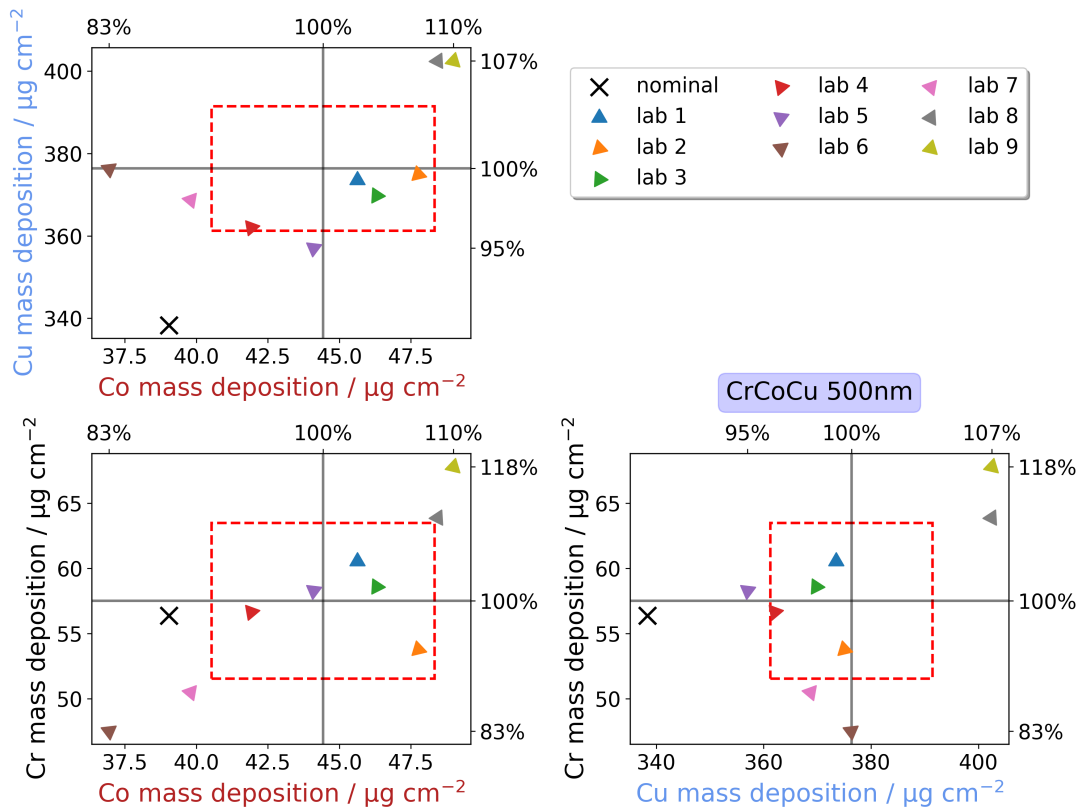
participant	Co / $\mu\text{g cm}^{-2}$	Cu / $\mu\text{g cm}^{-2}$	Cr / $\mu\text{g cm}^{-2}$
lab 1	76.9	619	102
lab 2	74.1	624	95.9
lab 3	78.1	626	101
lab 4	69.9	600	95.1
lab 5	71.7	593	97.6
lab 6	82.5	619	113
lab 7	78.7	604	100
lab 8	82.5	659	105
lab 9	81.9	671	113
\bar{x}	77.4	624	103
s	4.4	25	6.2
$s_r = s / \bar{x}$	5.7 %	4.0 %	6.1 %

SI-2.12 Results for sample #12 “Cr/Co/Cu”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



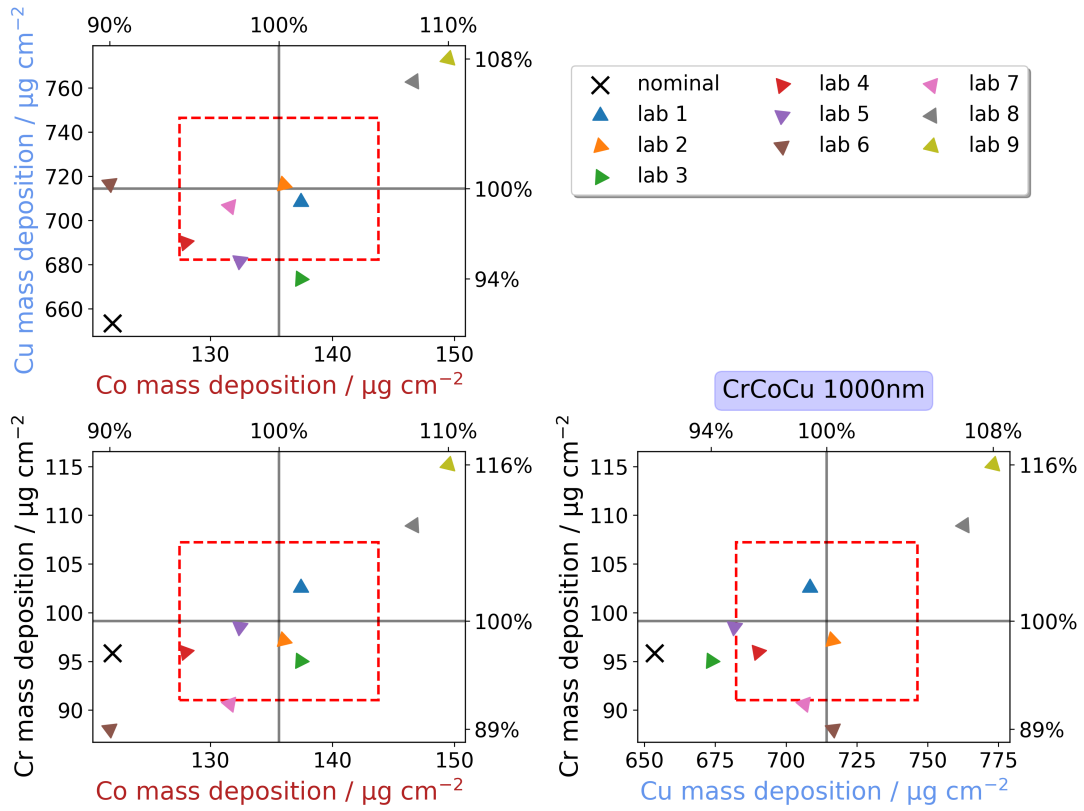
participant	Co / $\mu\text{g cm}^{-2}$	Cu / $\mu\text{g cm}^{-2}$	Cr / $\mu\text{g cm}^{-2}$
lab 1	137	718	104
lab 2	135	720	98.1
lab 3	139	728	103
lab 4	129	700	97.2
lab 5	131	691	99.7
lab 6	149	711	114
lab 7	137	712	104
lab 8	145	769	108
lab 9	147	791	114
\bar{x}	139	727	105
s	6.6	31	5.8
$s_r = s / \bar{x}$	4.8 %	4.2 %	5.6 %

SI-2.13 Results for sample #13 “CrCoCu 500nm”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



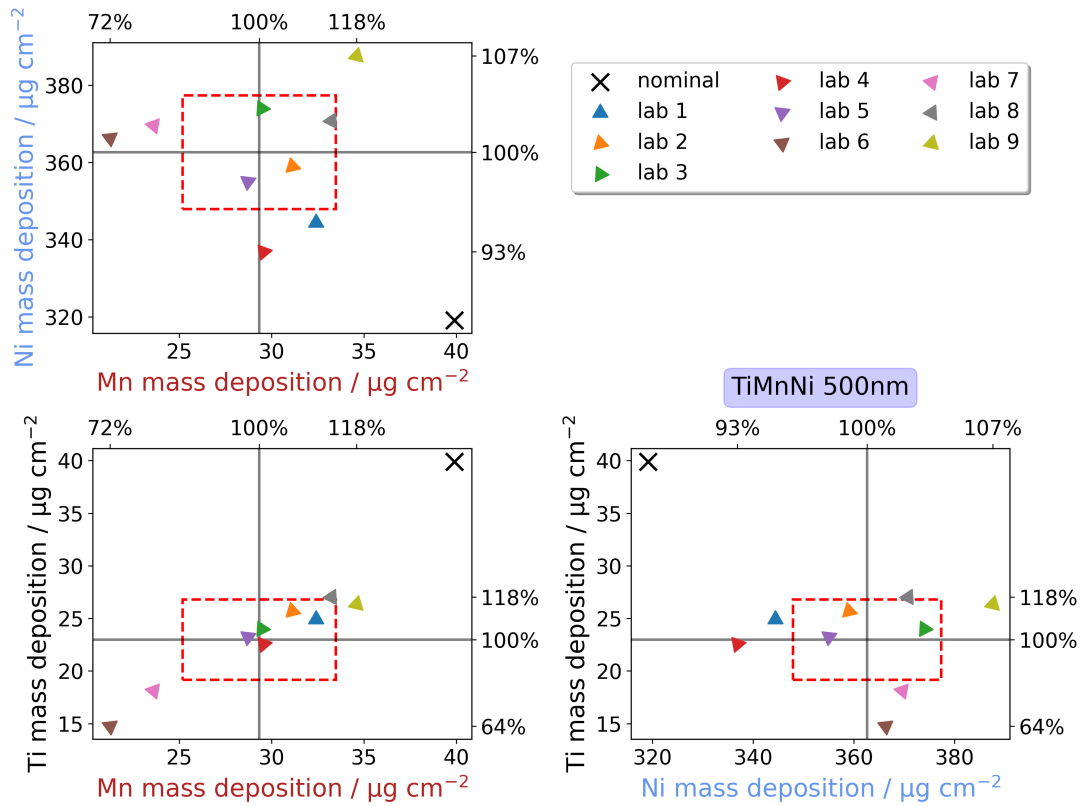
participant	Co / $\mu\text{g cm}^{-2}$	Cu / $\mu\text{g cm}^{-2}$	Cr / $\mu\text{g cm}^{-2}$
lab 1	45.6	373	60.5
lab 2	47.8	375	53.8
lab 3	46.3	370	58.6
lab 4	41.9	362	56.7
lab 5	44.1	357	58.3
lab 6	36.9	376	47.5
lab 7	39.8	369	50.5
lab 8	48.4	402	63.9
lab 9	49.0	402	67.8
\bar{x}	44.4	376	57.5
s	3.9	15	6.0
$s_r = s / \bar{x}$	8.8 %	4.0 %	10 %

SI-2.14 Results for sample #14 “CrCoCu 1000nm”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



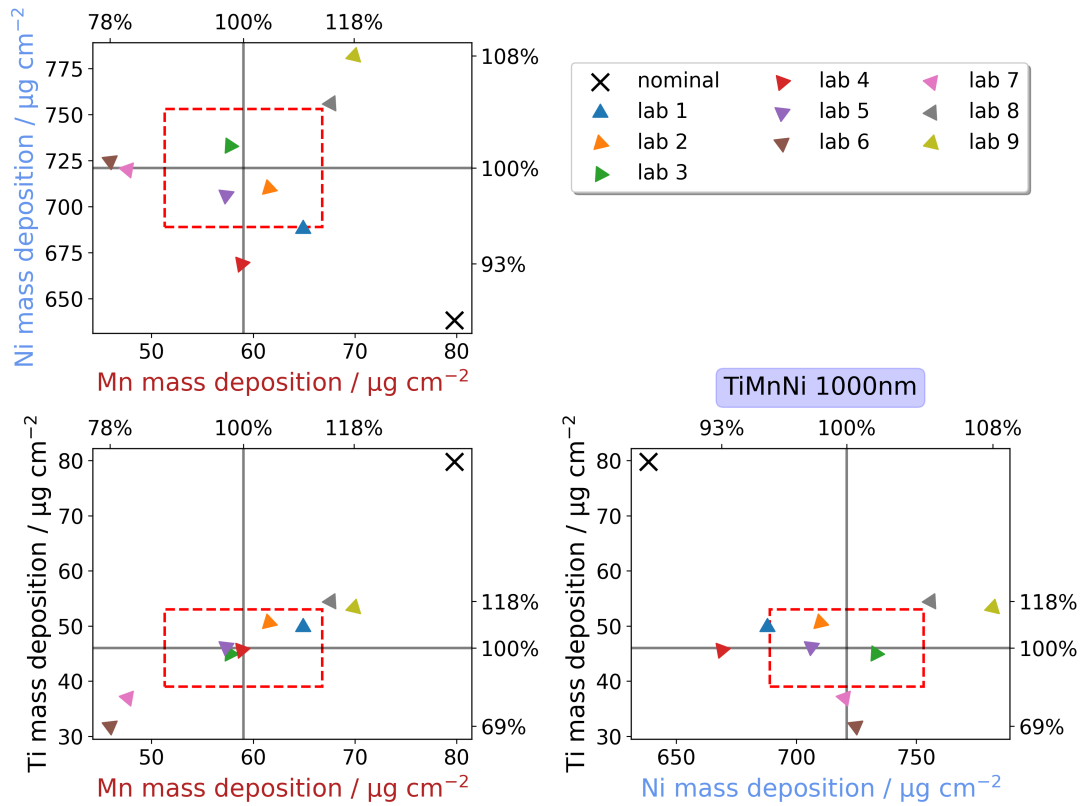
participant	Co / $\mu\text{g cm}^{-2}$	Cu / $\mu\text{g cm}^{-2}$	Cr / $\mu\text{g cm}^{-2}$
lab 1	137	708	103
lab 2	136	716	97.2
lab 3	137	674	95.0
lab 4	128	690	96.0
lab 5	132	682	98.6
lab 6	122	717	88.1
lab 7	132	706	90.6
lab 8	147	763	109
lab 9	149	773	115
\bar{x}	136	714	99.1
s	8.1	32	8.1
$s_r = s / \bar{x}$	6.0 %	4.5 %	8.2 %

SI-2.15 Results for sample #15 “TiMnNi 500nm”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



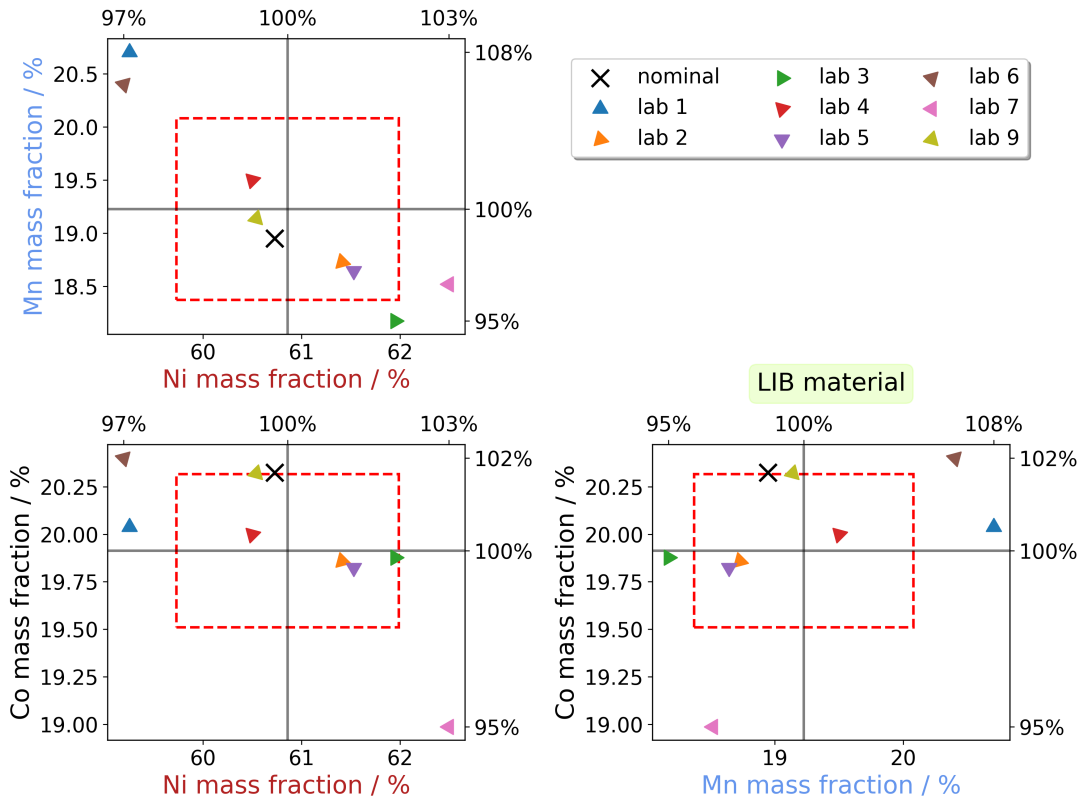
participant	Mn / $\mu\text{g cm}^{-2}$	Ni / $\mu\text{g cm}^{-2}$	Ti / $\mu\text{g cm}^{-2}$
lab 1	32.4	344	24.9
lab 2	31.1	359	25.7
lab 3	29.5	374	24.0
lab 4	29.6	337	22.6
lab 5	28.7	355	23.2
lab 6	21.3	366	14.8
lab 7	23.6	370	18.1
lab 8	33.2	371	27.0
lab 9	34.6	388	26.4
\bar{x}	29.3	363	23.0
s	4.1	15	3.8
$s_r = s / \bar{x}$	14 %	4.1 %	17 %

SI-2.16 Results for sample #16 “TiMnNi 1000nm”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



participant	Mn / $\mu\text{g cm}^{-2}$	Ni / $\mu\text{g cm}^{-2}$	Ti / $\mu\text{g cm}^{-2}$
lab 1	64.9	688	49.8
lab 2	61.5	710	50.7
lab 3	57.7	733	45.0
lab 4	58.8	669	45.7
lab 5	57.3	706	46.2
lab 6	45.9	725	31.9
lab 7	47.6	720	37.0
lab 8	67.6	756	54.5
lab 9	69.9	782	53.4
\bar{x}	59.0	721	46.0
s	7.7	32	7.0
$s_r = s / \bar{x}$	13 %	4.4 %	15 %

SI-2.17 Results for sample #17 “LIB material”, including mean \bar{x} , standard deviation s , and relative standard deviation s_r



participant	Ni / wt. %	Mn / wt. %	Co / wt. %
lab 1	59.3	20.7	20.0
lab 2	61.4	18.7	19.9
lab 3	61.9	18.2	19.9
lab 4	60.5	19.5	20.0
lab 5	61.5	18.6	19.8
lab 6	59.2	20.4	20.4
lab 7	62.5	18.5	19.0
lab 9	60.5	19.1	20.3
\bar{x}	60.9	19.2	19.9
s	1.1	0.85	0.40
$s_r = s / \bar{x}$	1.9 %	4.4 %	2.0 %

SI-3 Principal component analysis of samples #9-10 and #15-16

Figure SI-3.1 below shows the principal component analysis (PCA) of the samples containing Mn, Ni, and Ti, complementing Figure 12 of the main document. Please refer to the main text for further details.

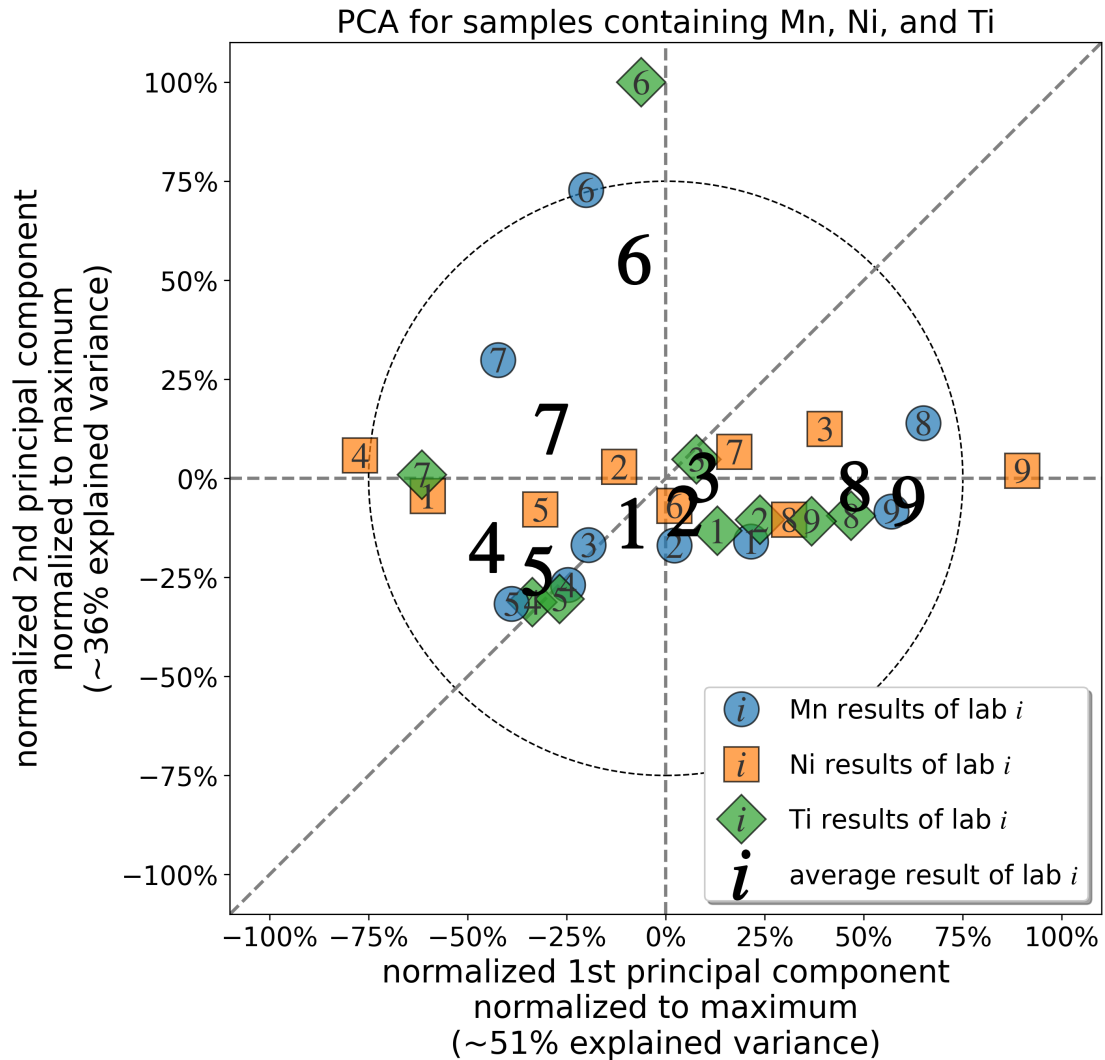


Figure SI-3.1: Principal component analysis of samples #9-10 and #15-16, which contain Mn, Ni, and Ti. Only the first two principal components are shown. The averages for individual laboratories are indicated as large numbers.

SI-4 Lateral XRF scans of thin film samples

Five of the 17 samples were scanned laterally by PTB by moving them through the monochromatized synchrotron beam ($E_0 = 9 \text{ keV}$) in steps of 2 mm, much larger than the spot size of the excitation radiation (about $300 \mu\text{m}$ FWHM). This ensured that individual measurements probed entirely different locations on the samples. Figure SI-4.1 shows the spectra obtained from such a scan with five lateral positions on the same sample, all normalized to their respective livetimes (about 5 min each) and to the incident photon flux monitored with an upstream thin photodiode in transmission. Similarly, Table SI-4.1 shows the (normalized) deviations of the individual spectra from the mean value of all five locations and its expected uncertainty (based on a Poisson distribution). Evidently, the sample is extremely homogenous over a large lateral range, as no deviations beyond the expected photon noise can be observed. Equivalent results were obtained for the other samples.

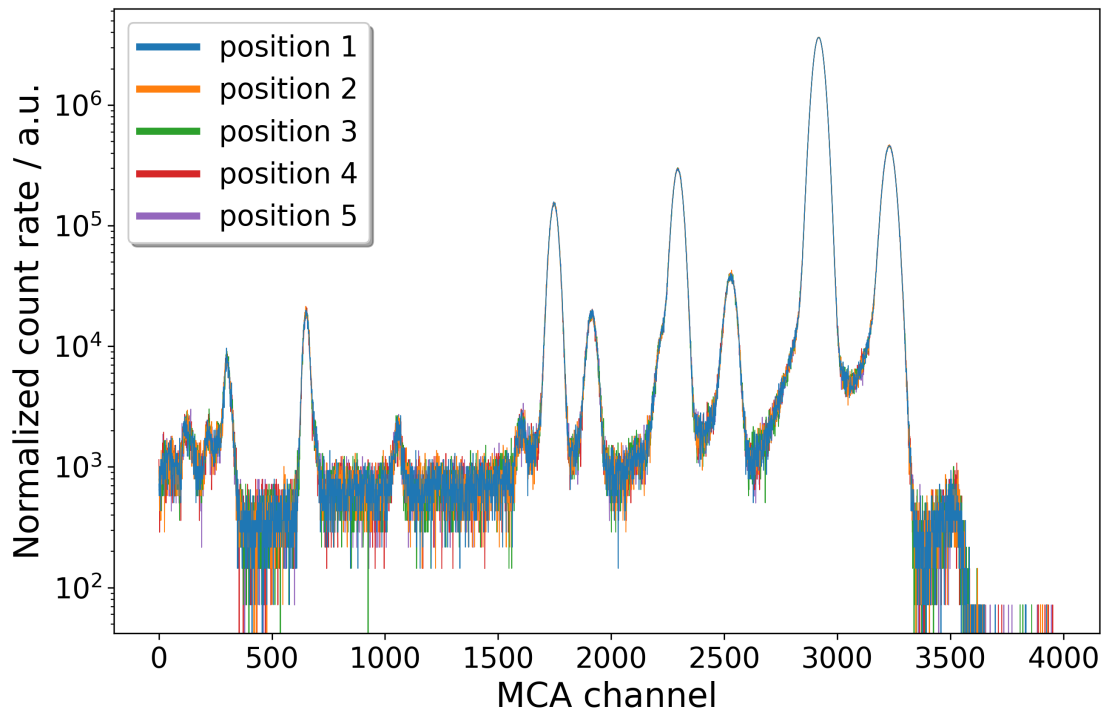


Figure SI-4.1: XRF spectra of a lateral scan with five different lateral positions over sample #9, a multilayer sample containing Ti, Ni, Mn (in that order).

	Relative deviation from the mean at...					expected
	location 1	location 2	location 3	location 4	location 5	1σ -deviation
sum	-0.159 %	0.078 %	0.004 %	0.034 %	0.042 %	0.051 %
Ni	-0.155 %	0.094 %	-0.005 %	0.027 %	0.038 %	0.054 %
Ti	-0.314 %	-0.106 %	0.058 %	0.032 %	0.331 %	0.295 %

Table SI-4.1: Quantitative results from the spectra in Figure SI-4.1. The individual relative deviations of different parts of the spectra are calculated as $\frac{x_i - M}{M}$, where x_i is either the sum of the total spectrum (first row), the Ni- $K\alpha$ and Ni- $K\beta$ intensity (second row), or the Ti- $K\alpha$ and Ti- $K\beta$ intensity (third row). M is the respective mean of all 5 measurements locations. The last column gives the expected (1σ) deviation for the measured count rates based on a Poisson distribution. All observed relative deviations from the mean are within a few permille, explainable by the photon noise of the experiment.

SI-5 Measurement protocol

For the sake of transparency, we have included on the following pages the full measurement protocol received by the participants in the interlaboratory comparison.

Measurement protocol for a round robin test on thin film XRF analysis

(In the context of the German WIPANO KALIB-RFA project, August 2021 – July 2023)

Objective: The German WIPANO KALIB-RFA project is aiming on both the definition and validation of thin film calibration samples for the standardization of reliable X-ray fluorescence analysis (XRF), in particular with respect to the quantification. Project partners involve the German National Metrology Institute PTB in Berlin, the German research center Helmholtz Centre for Materials and Energy (HZB) in Berlin, the battery research institute MEET and the laboratory for surface analysis TASCAN in Münster, the two X-ray instrument manufacturers Bruker Nano in Berlin (collaborator) and Helmut Fischer in Sindelfingen, the X-ray optics company AXO DRESDEN and the German Fraunhofer Institute for Material and Beam Technology IWS in Dresden.

In order to assess thin film XRF quantification, four different types of sample systems shall be investigated within a round robin activity by selected partners to compare the characterization results obtained by PTB, Bruker Nano and Helmut Fischer GmbH with external international round robin participants, such as major XRF instrument manufacturers (e.g., Rigaku, Malvern Panalytical, Bruker AXS, ...), and other XRF specialists. The results of the round robin test shall underpin German DIN and international ISO TC201 SC10 standardization activities aiming at a pre-normative technical specification for a reliable XRF quantification of thin films.

Round Robin Test: The test shall be performed on an appropriate selection of thin film samples at suitable XRF instrumentation. The main goal of this interlaboratory comparison is to get an accurate set of characterization results in order to qualify the investigated specimens as mono- or multielement thin film calibration samples for XRF and other applications. Furthermore, the results shall validate the approach of manufacturing of this kind of samples. For this purpose, several sets of ready to measure samples will be provided by MEET, Fraunhofer IWS and AXO DRESDEN.

An influence of the specific calibration and quantification schemes at the individual participant's site may be expected regarding determined thicknesses and elemental compositions. Thus, different types of samples were arranged for. The round robin partners are kindly requested to provide detailed information about their measurement process and the respective thin film XRF quantification. These details will be treated confidentially by PTB. Only anonymized results will be made public.

Sample description: A total of 17 different samples are intended for the round robin activity. The samples are Si wafer pieces of 18×18 mm² size and 0.4 mm to 0.7 mm thickness, coated with different layers from a few nm up to a few μm thickness. They do not require any special treatment or handling, but, of course, any contamination must be avoided. The different types of samples can be categorized as follows:

Type 1: Thin film deposition of a single **pure** element/oxide on a silicon wafer substrate. There are 3 scandium (Sc) samples of different thicknesses, two titanium oxide (TiO₂) samples, one aluminum oxide (Al₂O₃), one titanium (Ti) sample and one cobalt (Co) sample, for a total of 8 samples.

The mass deposition of the Co layer is 63.7 µg/cm². This value may serve to validate the pre-calibration of the XRF device.

Type 2: Thin film deposition of a **multilayer** system on a silicon wafer substrate, where each individual sub-layer consists of a single pure element. One sample of Ti/Ni/Mn/Substrate, one sample of Ti/Mn/Ni/Substrate, one sample of Cr/Cu/Co/Substrate, one sample of Cr/Co/Cu/Substrate, for a total of 4 different samples.

Type 3: Thin film deposition of an **alloy** system on a silicon wafer substrate. Two samples of (CrCoCu)/Substrate and two samples of (TiMnNi)/Substrate, for a total of 4 different samples.

Type 4: Battery electrode material (NMC, LiNi_xMn_yCo_zO₂) on a 15 µm thick aluminum (Al) substrate (also 18×18 mm² in size), produced at a pilot production line at MEET. In the production process 3 wt.% binder material (Polyvinylidene difluoride PVdF) and 2 wt.% conductive agent material (Super C65 carbon black) are used. The battery electrode is more than 50 µm thick.

In view of the lateral homogeneity of these samples (type 4) please use a beam size of at least 150 µm, or, if only smaller beam sizes are to be used, please perform an averaging lateral scan of the sample with at least 10 points.

All samples on Si substrates (type 1 to type 3) are labeled on the back side with a number or a simple dot. The front side of the battery electrode is black. Only the respective **front sides** shall be measured.

Measurement: The XRF analysis of all provided samples is kindly requested. For type 1 to 3 samples this means determining the elemental mass depositions (µg/cm²) of each layer of the thin films. For type 4 samples (battery material) elemental concentration (wt.%) shall be determined. If some samples cannot be measured, please note the reasons in the documentation. For the measurements, please proceed as described below:

- The XRF device should be an energy-dispersive or wavelength-dispersive spectrometer suitable for the analysis of thin film samples.
- The XRF analysis shall be performed in a conventional beam geometry, avoiding grazing incidence or observation schemes. If possible, please note the actually used geometry in the documentation.
- If possible, please try to ensure that the incident beam spot is located roughly in the center of the sample.
- Please make sure that the XRF device is operated such that the relevant K fluorescence radiation of the chemical elements from Al up to Cu are excited by the incident X-ray radiation.
- The XRF analysis of each individual sample shall be based on at least 10 repeated measurements. Each individual measurement shall detect at least 20'000 events in each relevant K α fluorescence line.

Documentation:

- Please provide information about the laboratory site, instrument, operator and responsible person.
- Please save each spectrum separately and provide it together with the results in a plain text format, e.g., ASCII.
- For the quantification process, each spectrum of the 10 repetitions shall be considered.
- Quantification results should be provided as a table in $\mu\text{g}/\text{cm}^2$ (type 1 to 3) or wt.% (type 4), please also give a reasonable number of digits reflecting the respective uncertainty of each measurement. These values may be based on a qualified estimate or a detailed uncertainty analysis. Complementary to this accuracy information you may provide information on your repeatability in the form of a standard deviation.
- Please note any anomalies you might encounter, which might help to assert problems.

Please provide the measurement results no later than October 12th, 2022, to André Wählich (e-mail: andre.waehlich@PTB.de) and to Burkhard Beckhoff (e-mail: burkhard.beckhoff@PTB.de)

In case of any questions, please do not hesitate to contact us.

Thank you for your kind assistance,
we look forward to receiving your round robin results,

Rainer Unterumsberger, André Wählich and Burkhard Beckhoff

SI-6 Additional data for Figure 3 and Figure 6

The XRR data used to create Figure 3 of the main manuscript has been published at the following location:

A. Wählisch, 'Interlaboratory comparison of XRF analysis on thin films, including alloys, oxides, multilayers, and a lithium-ion battery material'. Zenodo, Mar. 09, 2026. doi: 10.5281/zenodo.18928508.

<https://doi.org/10.5281/zenodo.18928508>

The ToF-SIMS data used to create Figure 6 of the main manuscript has been published at the following location:

A. Wählisch, 'Interlaboratory comparison of XRF analysis on thin films, including alloys, oxides, multilayers, and a lithium-ion battery material'. Zenodo, Mar. 09, 2026. doi: 10.5281/zenodo.18928293

<https://doi.org/10.5281/zenodo.18928293>