

Traceability of Spectrometer Chemical Analysis

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Spectrosource Pty Ltd



Atomic physics – How photons are emitted

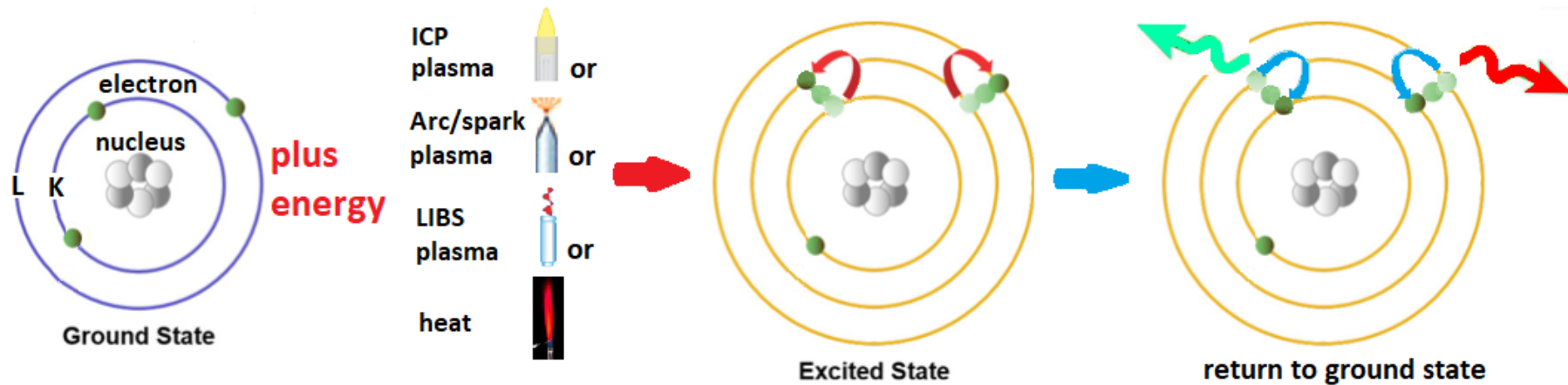
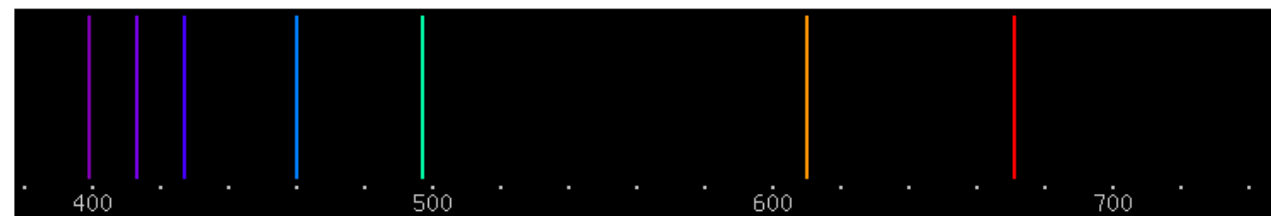


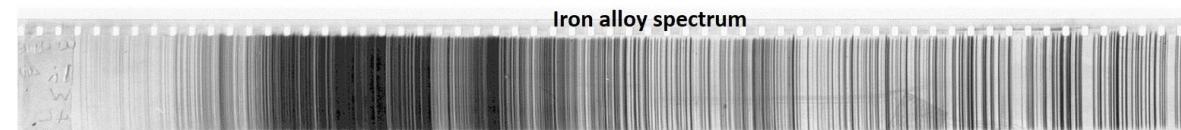
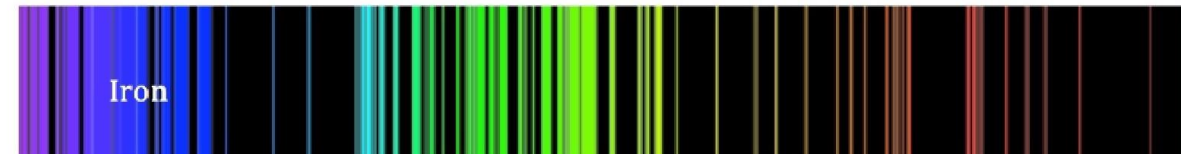
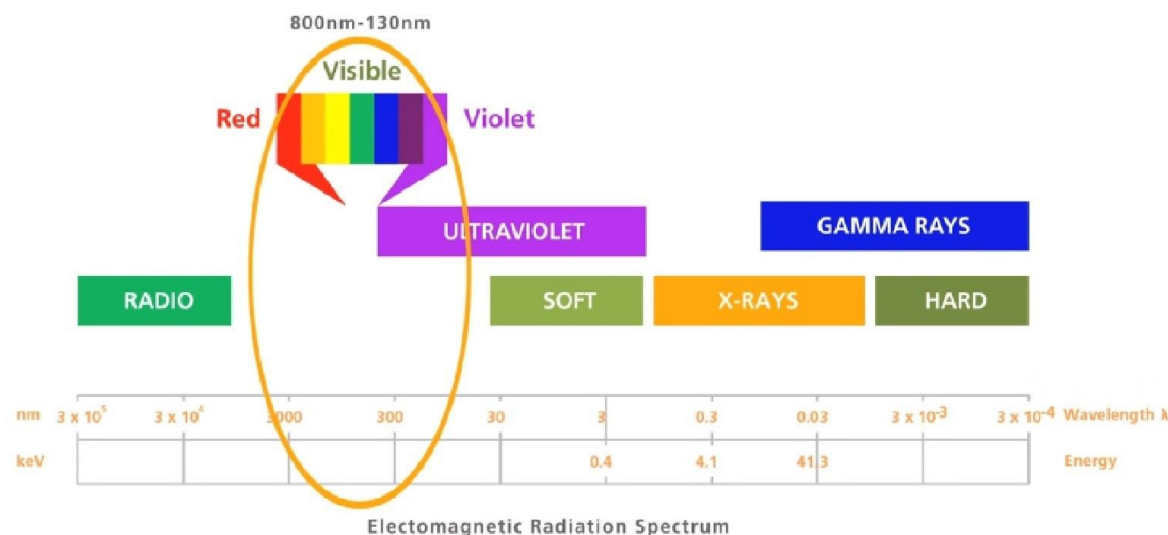
Figure 1: Bohr model (1913) Lithium --> excitation --> relaxation --> photon emission



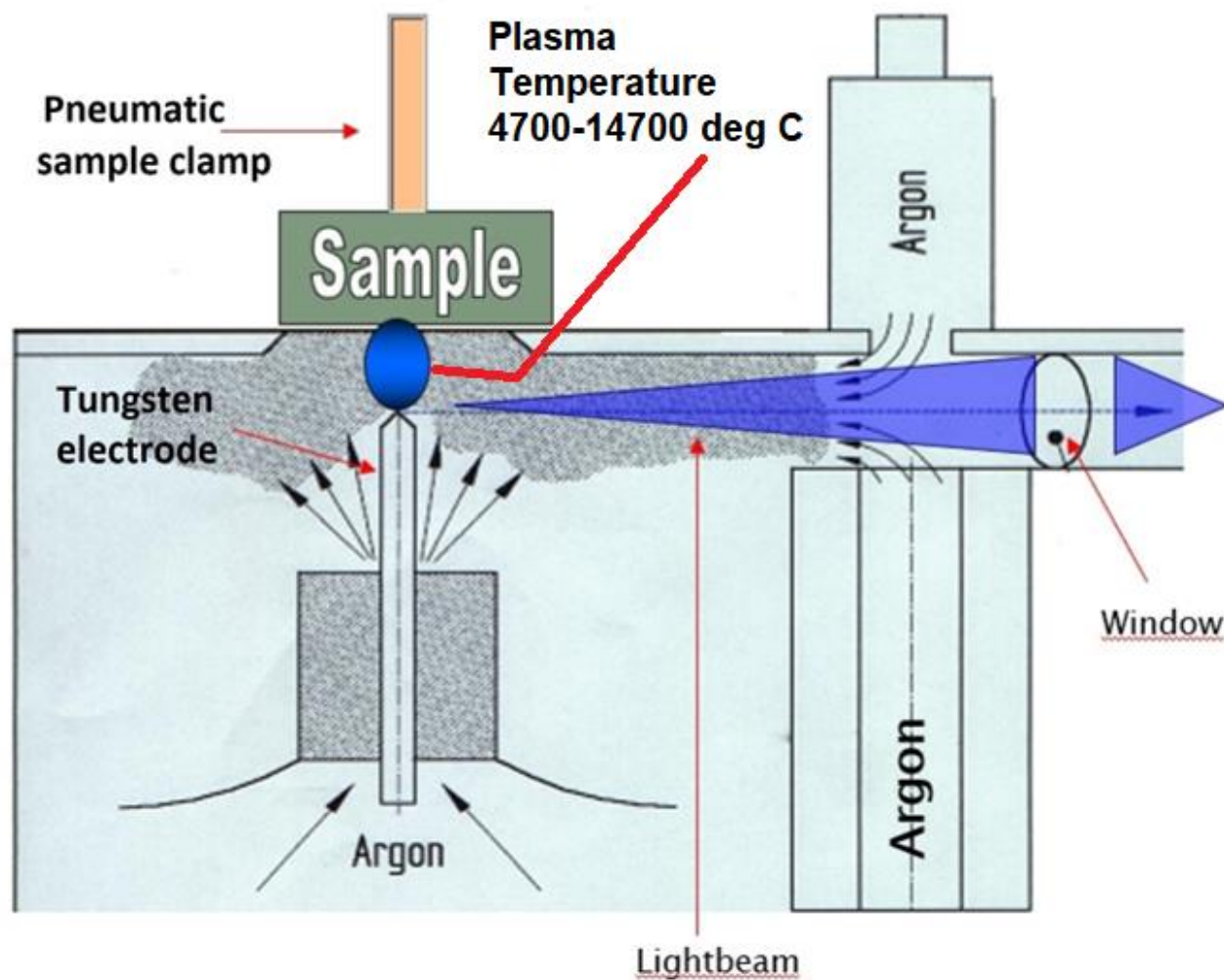
3	2	K
Li	1	L
Lithium		
6.941		

Figure 2: Lithium emission spectrum

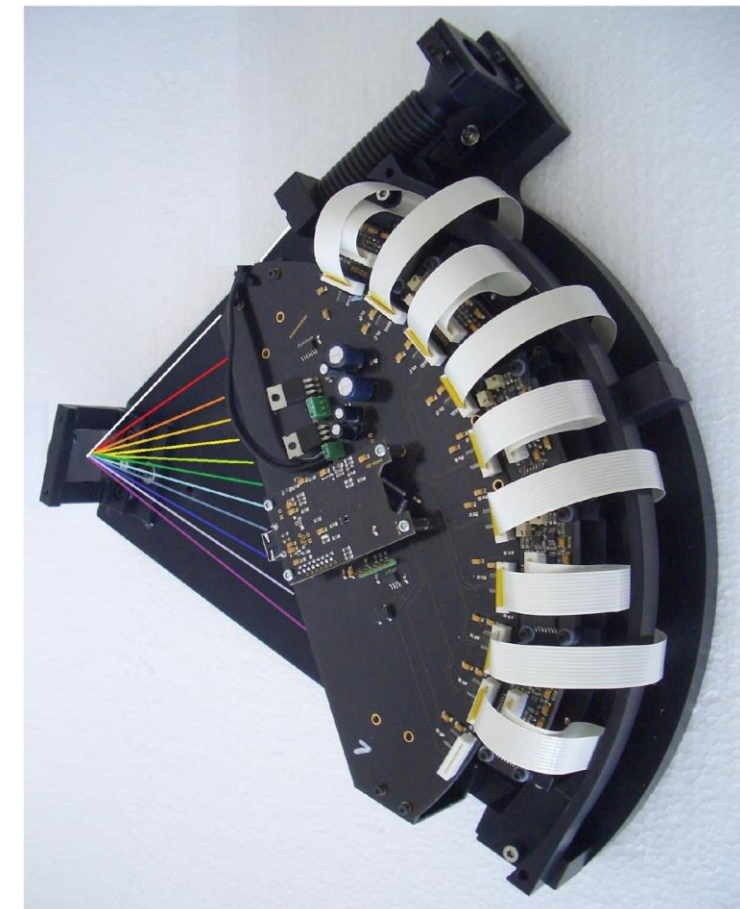
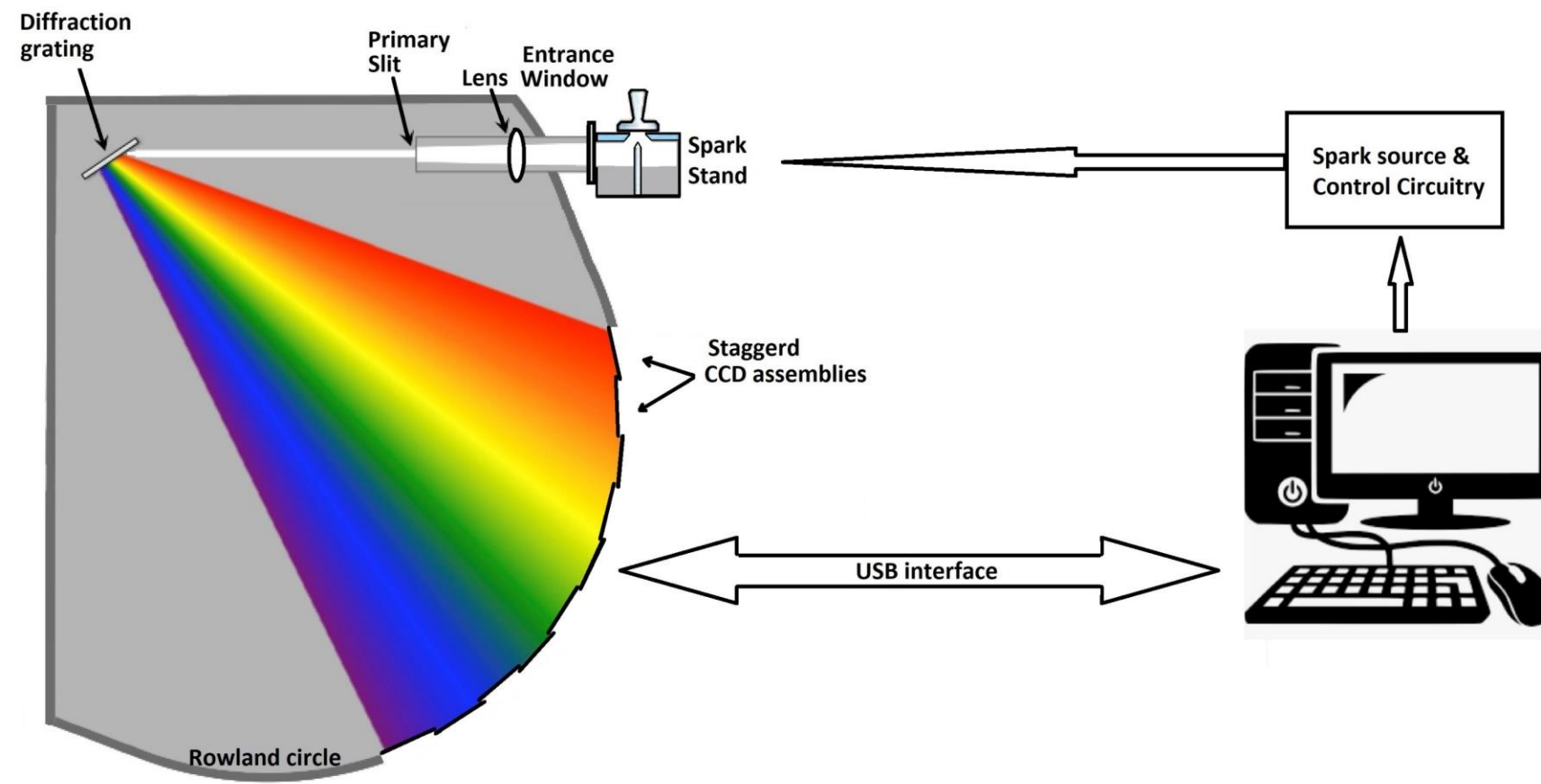
Spark OES Spectrum 130nm – 800nm



Spark Stand architecture



CCD based Spark OES architecture



Reference material hierarchy

Primary Certified Reference Material (CRM) standards : Certified Reference Materials standards are considered to provide the best level of accuracy, uncertainty and traceability for Spark OES. Results from >5 participating ISO 17034 accredited (NATA) laboratories provide results for the certificate of analysis of a CRM standard.

Secondary Reference Materials (RMs): Reference Materials are produced or analysed by an ISO 17034 accredited (NATA) accredited facility. The certificate of analysis (COA) must reference the facility's NATA accreditation.

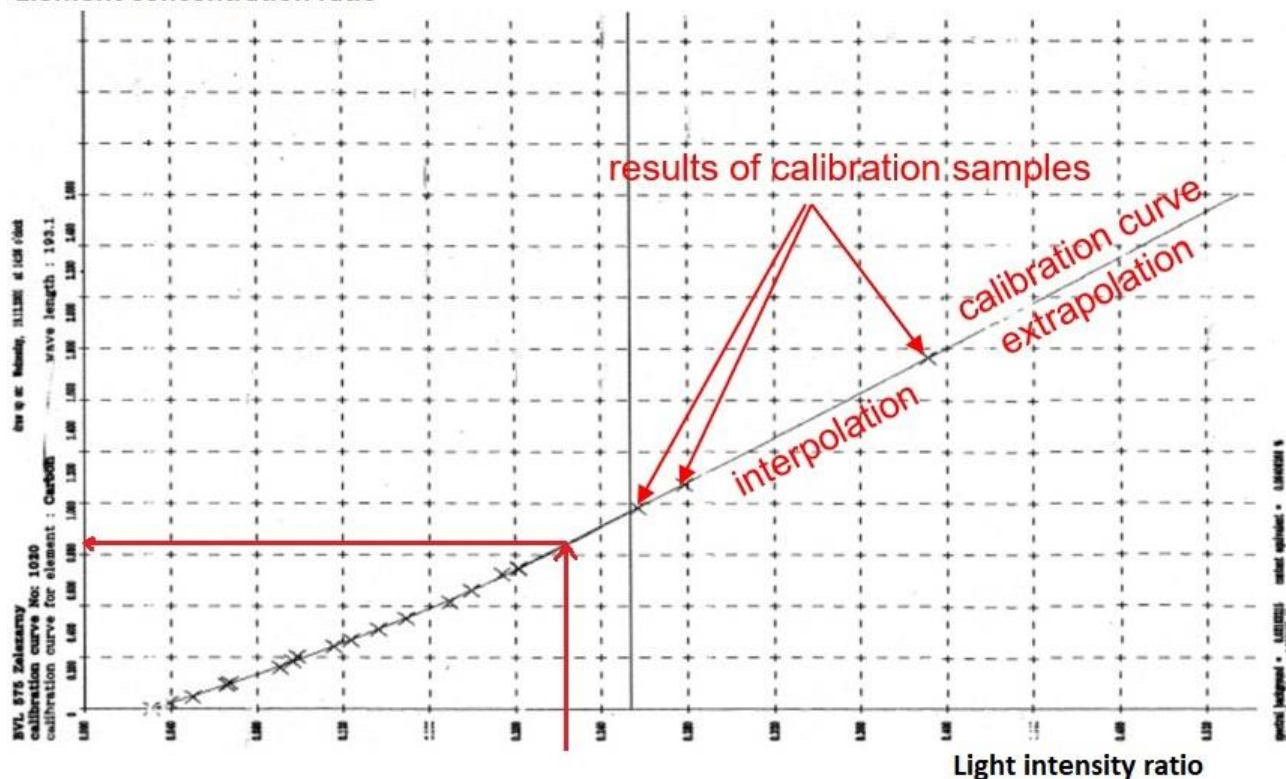
Set Up sample (SUS) standard: standards produced and certified by ISO 17034 accredited manufacturers for the purpose of calibrating Spark Optical Emission Spectrometers.

In House Material standard: These are prepared by an internal non accredited laboratory (Foundry) for use in daily operations. Ideally the COA should be linked to CRM or RM standards. Their preparation, homogeneity, and stability must be carefully documented to prove their link to CRM or RM standards. They are used to preserve CRM or RM standards.

Calculation of results from Calibration Curve

Calibration curve for Carbon in low alloy steel

Element concentration ratio



result comparison to previously
measured set of calibration samples

Spectrosource Pty Ltd copyright 2026

standard analyse measuring program

measuring program	program no	sample identification	measurement no.	grade no.	description
low alloyed steel	11	demo software	average	1.7131	16 MnCr 5

no.	C %	Si %	Mn %	P %	S %	Cu %	Al %	Cr %	Mo %
1	0.18	0.30	1.26	0.015	0.022	0.09	0.106	1.06	0.06
2	0.18	0.30	1.26	0.015	0.022	0.09	0.106	1.06	0.06
3	0.18	0.30	1.26	0.015	0.022	0.09	0.106	1.09	0.06
4	0.18	0.30	1.26	0.015	0.022	0.09	0.106	1.16	0.06
5	0.18	0.30	1.26	0.015	0.022	0.09	0.106	1.09	0.06
6	0.18	0.30	1.26	0.015	0.022	0.09	0.106	1.09	0.06
mitte	0.18	0.30	1.26	0.015	0.022	0.09	0.106	1.08	0.06

no.	Ni %	V %	Ti %	Nb %	Co %	W %	Pb %
1	0.04	0.02	0.029	0.039	0.05	0.06	0.003
2	0.04	0.02	0.029	0.039	0.05	0.06	0.003
3	0.04	0.02	0.029	0.039	0.05	0.06	0.003
4	0.04	0.02	0.029	0.039	0.05	0.06	0.003
5	0.04	0.02	0.029	0.039	0.05	0.06	0.003
6	0.04	0.02	0.029	0.039	0.05	0.06	0.003
mitte	0.04	0.02	0.029	0.039	0.05	0.06	0.003

start end P-Prot H-Prot A-Prot prog desc aver standard Correct calc direct print print save

Emission spectrometry is a
relative measurement method

Traceability in Spark optical emission spectrometers

Spark OES is a relative technique; it measures light intensity rather than absolute quantities

Lookup Light intensity of an element in its calibration curve to determine % weight result

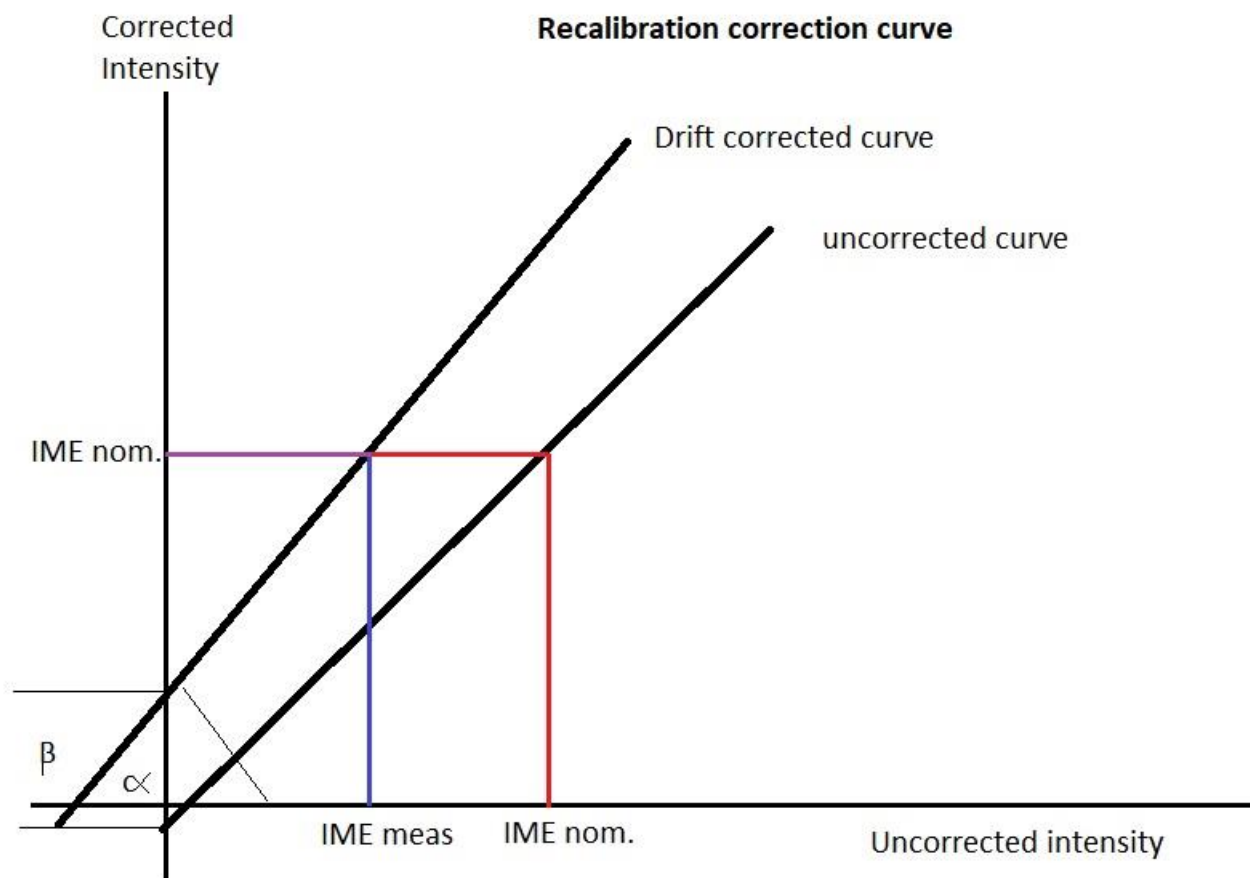
Need to establish a link between primary CRM standards and the chemical analysis results

Calibrations using CRM's, RM's, SUS and Internal reference materials.

Instrument Drift Correction/Standardisation/Recalibration – link to calibration curves.

Type calibration/Type measurement/Type grade check – control link to CRM's.

Recalibration, Standardization or Drift correction



Type Calibration

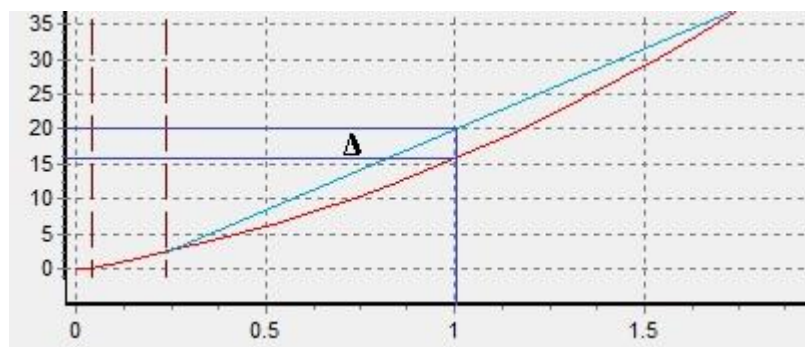


Illustration of exaggerated concentration error Δ in a calibration curve where Type calibration correction can be used to improve accuracy.

Type - Calibration

type no. 12 type description SS 2205 measuring-no average- measuring program High alloyed Cr>5% Ni>4% Program No. 13

No	C %	Si %	Mn %	P %
nom	0.017	0.360	1.420	0.009
1	0.011	0.356	1.416	0.008
2	0.008	0.350	1.417	0.008
3	0.011	0.364	1.417	0.008
4	0.008	0.347	1.409	0.008
mittel	0.009	0.354	1.415	0.008

Type Correction Value—
Type No: 122
additive multiplicative

Element	additive	multiplicative
C	0.0076	
Si	0.0057	
Mn		1.003581
P	0.0034	
S	0.0010	
Cr		1.007635
Mo		1.009992
Ni		0.992337
N	-0.0011	
Fe	0.1324	

do you want to save this values ?

No	Ni %	V %	Ti %	Nb %
nom	5.930			
1	5.98	0.076	0.010	0.004
2	5.98	0.076	0.011	0.004
3	5.95	0.077	0.011	0.004
4	5.99	0.076	0.010	0.004
mittel	5.98	0.076	0.010	0.005

% Mo	% Fe
450	3.180
17	3.163
34	3.162
28	3.164
33	3.106
28	3.149
66.417	
66.37	
66.18	
66.29	
66.30	
66.28	

Start End printprotocol file protocol Type aver. Standart calc. rect pr direct print save

Type Calibration and measure program

type no.550

type description11X15295

measuring no. average

measuring programCast iron Co5%

Program No.52

No	C %	Si %	Mn %	P %
nom	2.520	0.589	0.491	0.1
1	2.276	0.84	0.49	0.1
2	2.297	0.82	0.48	0.1
mittel	2.286	0.83	0.48	0.1

Type Correction Value

Element

Type No: 550

additive

multiplicativ

Fe.

2.4969

C

1.182235

Si

0.708146

Mn

0.0079

P

0.0086

S

0.0014

Cu

-0.0090

Al

-0.0019

Cr.

0.964182

Ni

0.0197

Nb

0.0245

Co

0.0113

W

-0.0086

Mg

-0.0748

Fe

0.0070

do you want to save this values ?

Yes

No

No	Ni %	V %	Ti %	Nb %	Co %	W %	Mg %	Fe %
nom	0.304	0.201		0.036	1.510	0.195		67.203
1	0.28	0.193	0.00	0.05	1.60	0.20	0.000	64.64
2	0.28	0.187	0.00	0.04	1.57	0.18	0.000	64.77
mittel	0.28	0.190	0.00	0.04	1.58	0.19	0.000	64.71

type Measuring

measuring programCast iron Co5%

Program No.52

type description11X15295

type no.550

measuring no. average

Grade-No.no grade found

Grade-Description

No	C %	Si %	Mn %	P %	S %	Cu %	Al %	Cr. %	Mo %
1	2.493	0.61	0.49	0.050	0.039	0.20	0.196	27.45	0.39
2	2.425	0.61	0.49	0.050	0.037	0.20	0.196	27.47	0.39
mittel	2.459	0.61	0.49	0.050	0.038	0.20	0.196	27.46	0.39

type listing

550

11X15295

52

15

element	nominal%	meas. value%	kind of correction
Fe.	67.2030	64.7061	additiv
C	2.5200	2.2863	multiplikativ
Si	0.5890	0.8317	multiplikativ
Mn	0.4910	0.4831	additiv
P	0.0504	0.0418	additiv
S	0.0413	0.0399	additiv
Cu	0.1970	0.2060	additiv
Al	0.1900	0.1919	additiv
Cr.	27.5300	28.5527	multiplikativ
Mo	0.3910	0.3713	additiv
Ni	0.3040	0.2795	additiv
V	0.2010	0.1897	additiv
Nb	0.0360	0.0446	additiv
Co	1.5100	1.5848	additiv
W	0.1950	0.1880	additiv
Sn	0.0470	0.0000	additiv
Pb	0.0150	0.0000	additiv

15

back

choose

close

Start

End

printprotocol

File protocol

Type

aver.

Standard

direct print

save

10:30 AM

13/10/2025

Start

End

printprotocol

File protocol

Type

desc.

aver.

Standard

Correct

calc.

Sample identification

20251013 TM

direct print

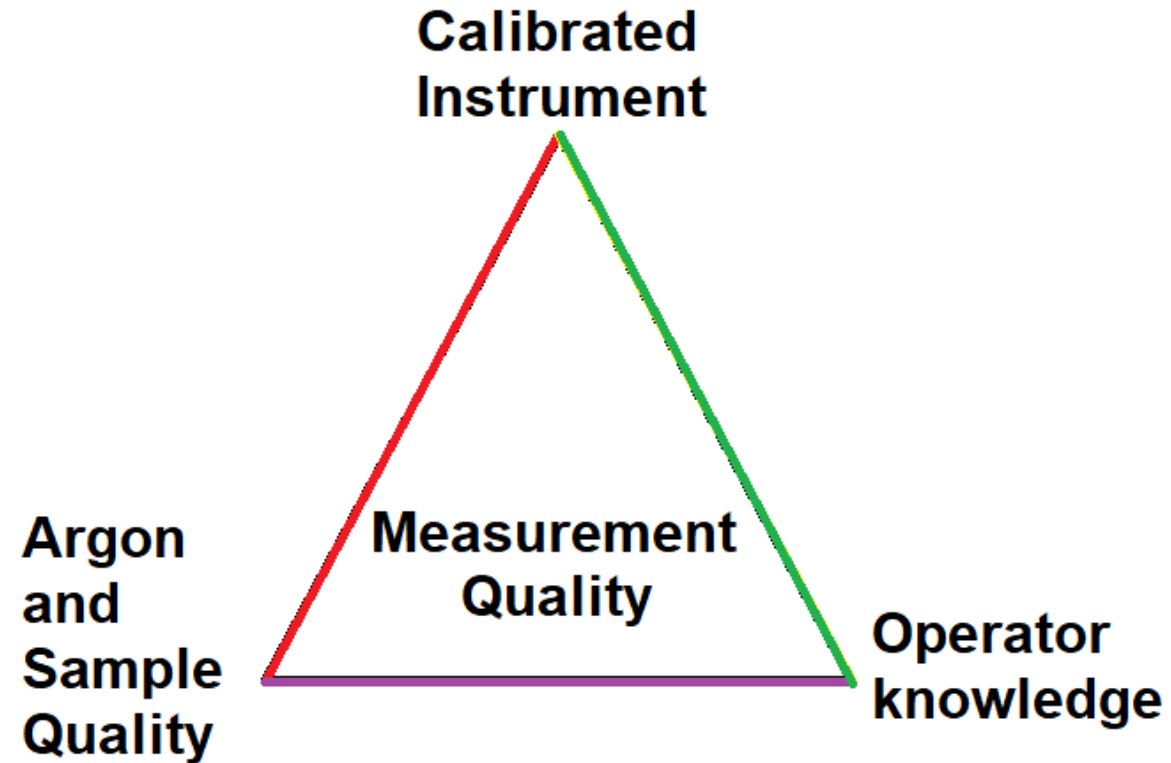
print

save

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Measurement Quality Triangle



Argon Purity

Ultra High Argon purity 99.999% improves to > 99.9999% after oxiclear purifier.
Hard to couple materials need ideal plasma conditions.
Highest purity argon and a flat 60 grit ground sample surface results in good coupling to the hard sample - good material vaporisation.
Less energy wastage on contaminants (O, H₂O, N) improves coupling and assists a good condensate ring.
Free C inhibits coupling to iron – higher pre spark time is required.



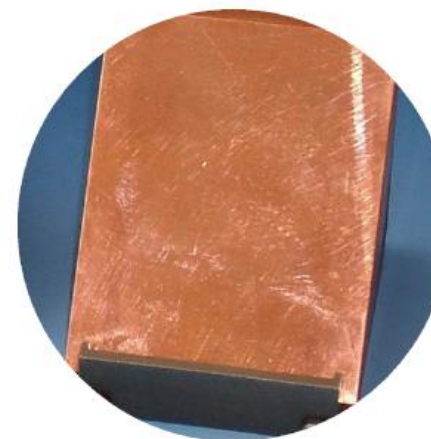
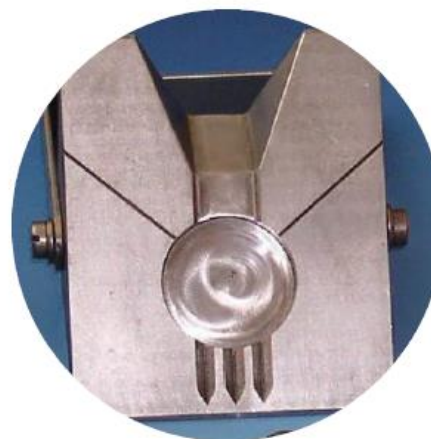
**Sg iron burns
99.99% argon vs
Oxiclear purified
>99.9999% argon**

Sample Quality

Special mould for grey and nodular Cast Iron CAST-150

Mould with 45° casting angle in combined Steel/Copper construction

- Mould form from steel, casting on copper block ensures unidirectional chill cast solidification on the analytical side of the sample only
- Spectro sample and pins for analysis of C + S simultaneously from same sample cast
- Pin samples of about 0.4 g each to be broken off easily and ready for analysis
- Most simple mounting for tight joining by putting mould form on copper block, no mechanism, no moving parts, self locking
- Copper block designed as flat surface block, enabling easy resurfacing and thus giving extended life time of mould
- Standard size of sample: Ø 34-36 x 5 mm.



Sample Quality



Samplers

Cast iron can solidify white or grey. White samples are quickly chilled and obtained by built-in cooling plates. Grey samples are exposed to a slow, normal cooling rate. The white chilled samples are further analysed by spectro analysis. The grey samples are for acoustic (block) and porosity analysis (cross).

WHITE SAMPLERS

SAF



SAF-Disc Only



Manufacturing Internal material standards

CRM and RM standards often do not match the alloy chemical composition requirements for the many metal grades manufactured by Foundries.

When the chemical composition of a melt matches the chemical composition of a specific grade then 5 chilled cast samples should be taken.

The 5 chilled cast samples must be analysed on the spark OES (minimum 3 x sparks per sample). The chemical analysis results of each sample should closely match each other. Results must be retained,

One of the chilled cast samples must be set to a NATA accredited laboratory for chemical analysis. The returned sample together with its certificate of analysis must be held as the Reference material standard. The remaining samples can be used as IN house reference standards. Periodic control checks RM standard vs IN house reference standard

Chemical analysis results CRM standard vs Furnace sample

standard analyse measuring program

measuring program	program no	sample identification	measurement no.	grade no.	description					
Cast iron Cr>5%	52	20251013	average		no grade found					
no.	C %	Si %	Mn %	P %	S %	Cu %	Al %	Cr. %	Mo %	
1	2.295	0.83	0.48	0.041	0.041	0.21	0.198	28.62	0.37	
2	2.281	0.85	0.49	0.041	0.043	0.21	0.204	28.57	0.38	
3	2.470	0.71	0.48	0.004	0.035	0.10	0.000	28.58	0.50	
4	2.419	0.70	0.48	0.004	0.032	0.10	0.000	28.64	0.49	
AVE 1-2	2.288	0.84	0.49	0.041	0.042	0.21	0.201	28.60	0.37	
AVE 3-4	2.419	0.70	0.48	0.004	0.032	0.10	0.000	28.64	0.49	

no.	Ni %	V %	Ti %	Nb %	Co %	W %	Mg %	Fe. %	
1	0.28	0.189	0.00	0.04	1.58	0.18	0.000	64.63	
2	0.28	0.191	0.00	0.05	1.60	0.20	0.000	64.61	
3	0.22	0.060	0.00	0.04	0.06	0.00	0.000	66.75	
4	0.22	0.060	0.00	0.04	0.05	0.00	0.000	66.75	
AVE 1-2	0.28	0.190	0.00	0.05	1.59	0.19	0.000	64.62	
AVE 3-4	0.22	0.060	0.00	0.04	0.05	0.00	0.000	66.75	

Alloy type: 27% Cr iron

Element	CRM 11X15295 Nominal	CRM 11X15295 Measured	CRM 11X15295 Nominal correction factor	27% Cr measured	27% Cr iron Corrected	27% Cr Grade min	27% Cr Grade Max	Pass/ Fail
C	2.520	2.288	0.232	2.419	2.651	2.600	2.900	✓
Si	0.589	0.840	-0.251	0.700	0.449	0.600	0.700	✗
Mn	0.491	0.490	0.001	0.480	0.481	0.600	0.900	✗
P	0.050	0.041	0.009	0.004	0.013	0.000	0.080	✓
S	0.041	0.042	-0.001	0.032	0.031	0.000	0.080	✓
Mo	0.391	0.370	0.021	0.490	0.511	0.250	0.500	✗
Cr	27.530	28.600	-1.070	28.640	27.570	26.000	28.000	✓
Ni	0.304	0.280	0.024	0.220	0.244	0.000	2.000	✓
Fe	68.083	67.049		67.015	68.049	69.950	64.840	✓

Measurements made on spectrometer nearing its annual service cycle which is evident in the results being less than desired .

Type Calibration

Type - Calibration

type no. 550 type description 11X15295 R4 measuring-no average- measuring program Cast iron Cr>5% Program No. 52

No	C %	Si %	Mn %	P %
nom	2.520	0.589	0.491	0.010
1	2.357	0.83	0.49	0.010
2	2.359	0.84	0.49	0.010
mittel	2.358	0.83	0.49	0.010

Type Correction Value

Element Type No: 550 additive multiplicativ

Fe	3.1086	
C	1.068714	
Si	0.706800	
Mn	-0.0035	
P	0.0126	
S	0.0018	
Cu	0.0024	
Al	-0.0141	
Cr	0.948435	
Mo	0.0226	
Ni	0.0330	
U	0.0091	
Nb	-0.0114	
Co	-0.1266	
W	-0.0032	

do you want to save this values ?

Yes No

No	Ni %	V %	Ti %	Nb %	Co %	W %	Mg %	Fe %
nom	0.304	0.201		0.036	1.510	0.195		67.203
1	0.27	0.192	0.00	0.05	1.66	0.20	0.000	64.12
2	0.27	0.192	0.00	0.05	1.6	type correction measuring value		64.07
mittel	0.27	0.192	0.00	0.05	1.64	0.20	0.000	64.09

Start End printprotocol Type aver. Standard direct print save

4:17 PM 30/09/2026

Type Grade Check Control sample

	C	Si	Mn	P	S	Cu	Al	Cr	Mo
min	2.42	0.489	0.391	0.02	0.02	0.097	0.1	27	0.291
max	2.62	0.589	0.591	0.07	0.06	0.297	0.3	28	0.491

	Ni	V	Ti	Nb	Co	W	Mg	Fe
min	0.2	0.1	0	0.01	1.4	0.1	0	0
max	0.4	0.3	0.1	0.06	1.6	0.3	0.1	1000000

no.	C	%	Si	%	Mn	%	P	%	S	%	Cu	%	Al	%	Cr	%	Mo	%
1	2.533		0.57		0.48		0.051		0.039		0.20		0.183		27.29		0.39	

no.	Ni	%	V	%	Ti	%	Nb	%	Co	%	W	%	Mg	%	Fe	%
1	0.30		0.200		0.00		0.03		1.50		0.19		0.000		66.03	

grade no.
11X15295

description
CRM 27%

good

bad


measurement
good

52 550
sample
20260930
measurement no.
1

start end print report file report grade desc aver stand autoGC direct print print save

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30/09/2026

Type Grade Check Ladle sample

	C	Si	Mn	P	S	Cu	Al	Cr	Mo
min	2.6	0.6	0.6	0	0	0	0	26	0.25
max	2.9	0.7	0.9	0.08	0.08	0.4	0.4	28	0.5

	Ni	V	Ti	Nb	Co	W	Mg	Fe
min	0	0	0	0	0	0	0	0
max	2	0.3	0.1	0.1	0.4	0.4	0.1	1000000

no.	C %	Si %	Mn %	P %	S %	Cu %	Al %	Cr %	Mo %
1	2.533	0.57	0.48	0.051	0.039	0.20	0.183	27.29	0.39
2	2.609	0.38	0.73	0.020	0.031	0.10	0.000	25.08	0.64
3	2.609	0.38	0.72	0.020	0.029	0.10	0.000	25.32	0.63
4	2.599	0.38	0.72	0.020	0.029	0.10	0.000	25.43	0.63
mittel	2.606	0.38	0.72	0.020	0.030	0.10	0.000	25.28	0.63
asd	0.006	0.00	0.00	0.000	0.001	0.00	0.000	0.18	0.01
rsd	0.23	1.09	0.54	1.44	3.82	2.17	0.00	0.70	0.93

no.	Ni %	V %	Ti %	Nb %	Co %	W %	Mg %	Fe %
1	0.30	0.200	0.00	0.03	1.50	0.19	0.000	66.03
2	0.23	0.055	0.00	0.06	0.00	0.00	0.000	70.07
3	0.23	0.054	0.00	0.06	0.00	0.00	0.000	69.85
4	0.23	0.054	0.00	0.06	0.00	0.00	0.000	69.76
mittel	0.23	0.054	0.00	0.06	0.00	0.00	0.000	69.89
asd	0.00	0.001	0.00	0.00	0.00	0.00	0.000	0.16
rsd	0.62	1.65	1.56	1.51	0.00	0.00	0.00	0.23

grade no.
27% Cr

description
27% Cr iron

good

1

bad

1

no grade



measurement
bad

52 550

sample
20260930

measurement no.
4

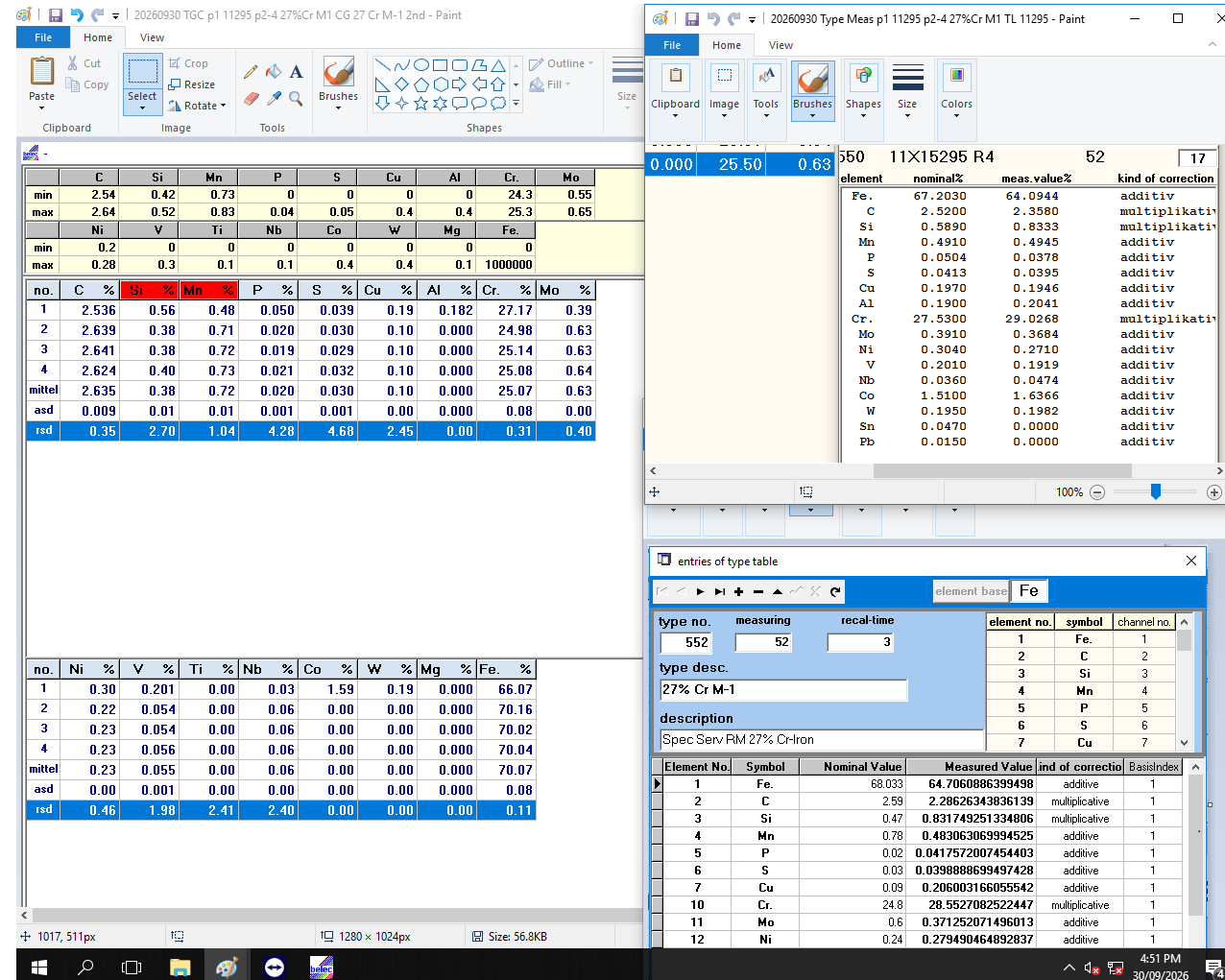
start end print report file report grade desc

aver standard autoGC

direct print print save

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Complete Type Grade process



The screenshot displays two windows from the Spectrosource software. The left window, titled '20260930 TGC p1 11295 p2-4 27%Cr M1 CG 27 Cr M-1 2nd - Paint', shows a table of chemical analysis results for various elements (C, Si, Mn, P, S, Cu, Al, Cr, Mo) with minimum, maximum, and average values. The right window, titled '20260930 Type Meas p1 11295 p2-4 27%Cr M1 TL 11295 - Paint', shows a table of chemical analysis results for various elements (Fe, C, Si, Mn, P, S, Cu, Al, Cr, Mo) with nominal and measured values, and a kind of correction. Below these tables, there is a section for 'entries of type table' which includes a table of element data and a table of element data with nominal and measured values.

	C	Si	Mn	P	S	Cu	Al	Cr	Mo
min	2.54	0.42	0.73	0	0	0	0	24.3	0.55
max	2.64	0.52	0.83	0.04	0.05	0.4	0.4	25.3	0.65
min	0.2	0	0	0	0	0	0	0	0
max	0.28	0.3	0.1	0.1	0.4	0.4	0.1	100000	

no.	C %	Si %	Mn %	P %	S %	Cu %	Al %	Cr %	Mo %
1	2.536	0.56	0.48	0.050	0.039	0.19	0.182	27.17	0.39
2	2.639	0.38	0.71	0.020	0.030	0.10	0.000	24.98	0.63
3	2.641	0.38	0.72	0.019	0.029	0.10	0.000	25.14	0.63
4	2.624	0.40	0.73	0.021	0.032	0.10	0.000	25.08	0.64
mittel	2.635	0.38	0.72	0.020	0.030	0.10	0.000	25.07	0.63
asd	0.009	0.01	0.01	0.001	0.001	0.00	0.000	0.08	0.00
rsd	0.35	2.70	1.04	4.28	4.68	2.45	0.00	0.31	0.40

no.	Ni %	V %	Ti %	Nb %	Co %	W %	Mg %	Fe %
1	0.30	0.201	0.00	0.03	1.59	0.19	0.000	66.07
2	0.22	0.054	0.00	0.06	0.00	0.00	0.000	70.16
3	0.23	0.054	0.00	0.06	0.00	0.00	0.000	70.02
4	0.23	0.056	0.00	0.06	0.00	0.00	0.000	70.04
mittel	0.23	0.055	0.00	0.06	0.00	0.00	0.000	70.07
asd	0.00	0.001	0.00	0.00	0.00	0.00	0.000	0.08
rsd	0.46	1.98	2.41	2.40	0.00	0.00	0.00	0.11

element	nominal%	meas.value%	kind of correction
Fe.	67.2030	64.0944	additiv
C	2.5200	2.3580	multiplikativ
Si	0.5890	0.8333	multiplikativ
Mn	0.4910	0.4945	additiv
P	0.0504	0.0378	additiv
S	0.0413	0.0395	additiv
Cu	0.1970	0.1946	additiv
Al	0.1900	0.2041	additiv
Cr.	27.5300	29.0268	multiplikativ
Mo	0.3910	0.3684	additiv
Ni	0.3040	0.2710	additiv
V	0.2010	0.1919	additiv
Nb	0.0360	0.0474	additiv
Co	1.5100	1.6366	additiv
W	0.1950	0.1982	additiv
Sn	0.0470	0.0000	additiv
Pb	0.0150	0.0000	additiv

type no.	measuring	recal-time	element no.	symbol	channel no.
552	52	3	1	Fe.	1
			2	C	2
			3	Si	3
			4	Mn	4
			5	P	5
			6	S	6
			7	Cu	7

Element No.	Symbol	Nominal Value	Measured Value	ind of correctio	BasisIndex
1	Fe.	68.033	64.7060886399498	additive	1
2	C	2.59	2.28626343836139	multiplicative	1
3	Si	0.47	0.831749251334806	multiplicative	1
4	Mn	0.78	0.483063069994525	additive	1
5	P	0.02	0.0417572007454403	additive	1
6	S	0.03	0.0398888693497428	additive	1
7	Cu	0.09	0.206003166055542	additive	1
10	Cr.	24.8	28.5527082522447	multiplicative	1
11	Mo	0.6	0.371252071496013	additive	1
12	Ni	0.24	0.279490464892837	additive	1

Material Data Base / Grade Table

grade table

delete save Load print close

226 Copy convert

index	grade no.	grade identification
12880	1.2880	1.2880
13202	1.3202	S 12-1-4-5
13247	1.3247	HS2-9-1-8
13316	1.3316	S 9-1-2
13318	1.3318	S 12-1-2
13333	1.3333	S 3-3-2
13342	1.3342	SC 6-5-2
13343	1.3343	S 6-5-2
13505	1.3505	100 Cr 6 (W3)
13520	1.3520	100 CrMn 6
13533	1.3533	17 NiCrMo 14
14001	1.4001	1.4001

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grade table entries

print close

index	grade no.	element no.	symbol
13505	1.3505	1	Fe.
		2	C
		3	Si
		4	Mn
		5	P
		6	S

grade identification

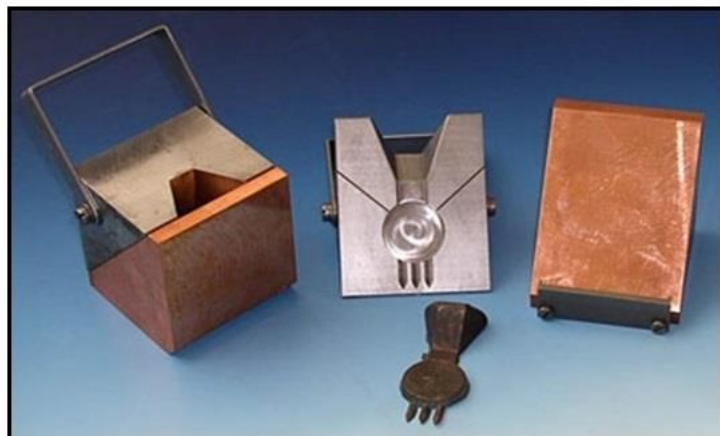
100 Cr 6 (W3)

element no	minimal	maximal	extended minir	extended maximal	do not check
2	0,9	1,05	0,81	1,155	Air probe
3	0,15	0,35	0,135	0,385	never
4	0,25	0,45	0,225	0,495	never
7	0	0,3	0	0,33	never
9	1,35	1,65	1,3	1,805	never
12	0	0,3	0	0,33	never

- software compares analysis results with element concentration ranges and reports grade matches
- virtually unlimited material data entries

- international material standards as well as customised data base can be loaded
- Specific material data base can be linked to a measuring program

Summary of The analytical Process



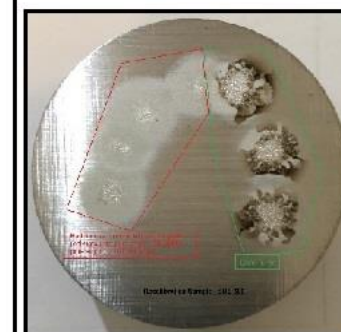
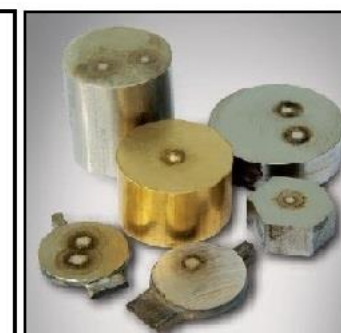
Sample taking



Sample preparation



Chemical analysis



Thank you.

For more information or feedback contact Glen Thiele

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email: info@spectrosource.com.au

- References
- (1) V. Thomsen, Modern Spectrochemical Analysis of Metals: An Introduction for Users of Arc/Spark Instrumentation (ASM International, Materials Park, Ohio, 1996).
- (2) Power Point Presentations – definitions and images: Belec Spectrometrie Opto-Electronik (2012 – 2023).
- (3) Various definitions and images: Wikipedia and Manufacturers website data.
- (4) Melting Spectro Analysis Version 6: G Henderieckx – Gietech BV