Supplementary information: Quantifying uncertainty from mass-peak overlaps in atom probe microscopy

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S.1 Introduction

This document supports the paper titled "Quantifying uncertainty from mass-peak overlaps in atom probe microscopy". Raw data is available on request from PublicationsManager@ccfe.ac.uk, this includes the knitr file (https://yihui.name/knitr/) and data used to produce the figures in R.

Data processing was performed using MATLAB with the functions and scripts available from atomprobelab.sourceforge.net.

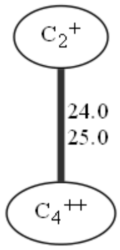

Figure S.1: Overlap diagram of the overlap of C_2^+/C_4^{2+} overlap at 24 Da.

S.2 C_2/C_4 Overlap

Table 2 (in the main manuscript) lists the details of the peak overlap at 24 Da including the peak positions, ions and natural abundance of C_2 and C_4, using data from Sha et al., 1992. The overlap graph for this overlap is shown in figure S.1. The numbers on the connecting link between C_2 and C_4 show that these ions overlap at m/z positions 24 and 25 Da. A full mass spectrum for this data can be found in the original reference (Sha et al. 1992).

S.3 FeTiYO ODS overlap

The mass spectrum with the peaks labelled with the ions which contribute to them, is shown in Figure S.2. For each position bin in Figure 6b (in the main paper), a details table is given in Table S.1.

The table contains the counts of each ion (and residual) for each m/z range for every histogram bin in the composition line profile. Labelled sections give the position range, e.g. “19.2–22.4 nm”, that the composition profile details refer to. The m/z range gives the mass-peak window used. Counts are the background subtracted counts for each peak. For each range the ions and their peak-overlap solved counts are given as well as the residual for the fit (last column).

The error bars shown Figure 6b (in the main paper) are calculated from the ionic composition and therefore cannot easily be shown along side the counts of each ion in each mass-peak. However, Table S.1 does show all of the data used in the profile.

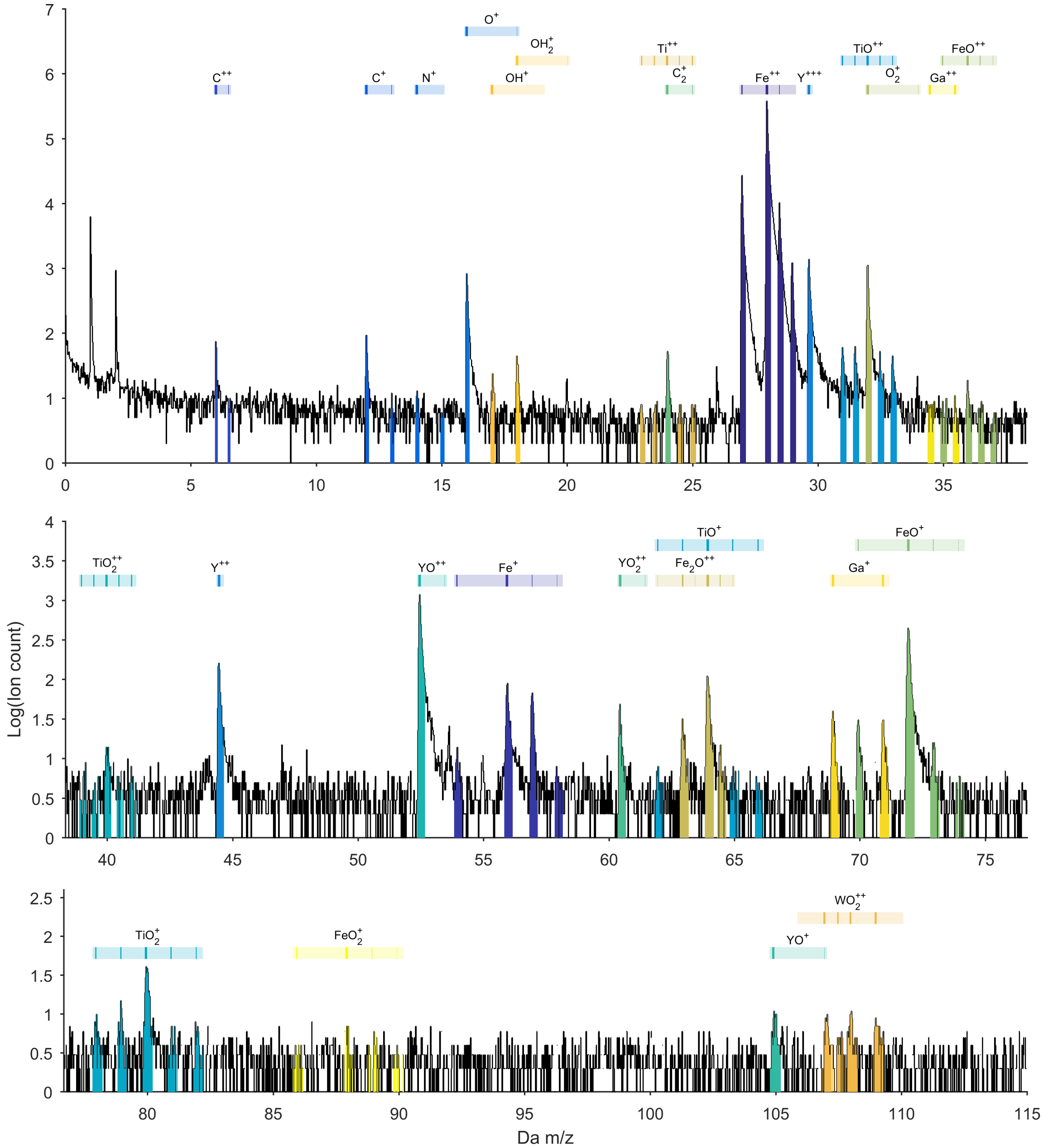

Figure S.2: Mass spectrum of a Fe-Ti-Y2O3 ODS with ion labels. The line thickness in the label indicates the intensity of the natural abundance in that peak, thicker line = higher natural abundance.

m/z Range	Counts	Ion1	Ion1 Count	Ion2	Ion2 Count	Residual
0.0–3.2 nm						
6.0 – 6.1 Da	8.8	C++	8.8			0
6.5 – 6.6 Da	0.8	C++	0.8			0
11.9 – 12.1 Da	7.7	C+	7.7			0
12.9 – 13.1 Da	1.5	C+	1.5			0
13.9 – 14.1 Da	1.2	N+	1.2			0
14.9 – 15.1 Da	4.2	N+	4.2			0
15.9 – 16.1 Da	61.6	O+	61.6			0
16.9 – 17.1 Da	2.3	OH+	2.3			0
17.9 – 18.1 Da	11	OH2+	11			0
22.9 – 23.1 Da	0					0
23.4 – 23.6 Da	0					0
23.9 – 24.1 Da	11.2	C2+	4.9	Ti++	6.3	0
24.4 – 24.6 Da	1.6	Ti++	0.5			1.1
24.9 – 25.2 Da	1.1	C2+	0.1	Ti++	0.4	0.5
26.9 – 27.1 Da	4183.7	Fe++	4183.7			0
27.9 – 28.1 Da	66273.8	Fe++	66273.8			0
28.4 – 28.6 Da	1552.6	Fe++	1552.6			0
28.9 – 29.1 Da	196.1	Fe++	196.1			0
29.6 – 29.8 Da	82.3	Y+++	82.3			0
30.9 – 31.1 Da	4.5	TiO++	1.7			2.8
31.4 – 31.6 Da	0					0
31.9 – 32.2 Da	14.1	TiO++	14.9	O2+	0	-0.8
32.4 – 32.6 Da	5.9	TiO++	1.1			4.8
32.9 – 33.1 Da	4.8	TiO++	1			3.8
34.4 – 34.6 Da	1.7	Ga++	1.7			0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	0					0
35.9 – 36.1 Da	2.7	FeO++	2.7			0
36.4 – 36.6 Da	2.6	FeO++	2.6			0
36.9 – 37.1 Da	0					0
38.9 – 39.2 Da	0					0
39.4 – 39.7 Da	0					0
39.9 – 40.2 Da	8.4	TiO2++	8.4			0
40.4 – 40.7 Da	0					0
40.9 – 41.2 Da	1.6	TiO2++	1.6			0
44.4 – 44.7 Da	9.3	Y++	9.3			0
52.3 – 52.7 Da	59.7	YO++	59.7			0
53.8 – 54.2 Da	4.7	Fe+	4.7			0
55.8 – 56.2 Da	31.3	Fe+	31.3			0
56.8 – 57.2 Da	23.2	Fe+	23.2			0
57.8 – 58.2 Da	0	Fe+	0			0
60.3 – 60.7 Da	2.9	YO2++	2.9			0
61.8 – 62.2 Da	1.1	TiO+	0.6	Fe2O++	0	0.6
62.8 – 63.2 Da	0.8	TiO+	0.5	Fe2O++	0	0.3
63.8 – 64.2 Da	4.8	TiO+	5	Fe2O++	0	-0.2
64.3 – 64.7 Da	0					0
64.8 – 65.2 Da	2	TiO+	0.4	Fe2O++	0	1.6
65.8 – 66.2 Da	0					0
68.8 – 69.2 Da	24.8	Ga+	24.8			0
69.8 – 70.2 Da	4.1	FeO+	4.1			0
70.8 – 71.2 Da	11	Ga+	11			0
71.8 – 72.2 Da	25.7	FeO+	25.7			0
72.8 – 73.2 Da	4.6	FeO+	4.6			0
73.8 – 74.2 Da	0.1	FeO+	0.1			0
77.8 – 78.2 Da	0.2	TiO2+	0.2			0
78.8 – 79.2 Da	3.7	TiO2+	3.7			0
79.8 – 80.2 Da	4.2	TiO2+	4.2			0
80.8 – 81.2 Da	0					0
81.8 – 82.2 Da	5	TiO2+	5			0
85.8 – 86.2 Da	0					0
87.8 – 88.2 Da	0					0
88.8 – 89.2 Da	0					0
89.8 – 90.2 Da	0					0
104.7 – 105.2 Da	0					0
106.8 – 107.3 Da	0					0
107.3 – 107.8 Da	2	WO2++	2			0
107.8 – 108.3 Da	2	WO2++	2			0
108.8 – 109.3 Da	3.1	WO2++	3.1			0
3.2–6.4 nm						
6.0 – 6.1 Da	16.5	C++	16.5			0
6.5 – 6.6 Da	0.9	C++	0.9			0
11.9 – 12.1 Da	11.6	C+	11.6			0
12.9 – 13.1 Da	0.1	C+	0.1			0
13.9 – 14.1 Da	4.4	N+	4.4			0
14.9 – 15.1 Da	7.1	N+	7.1			0
15.9 – 16.1 Da	105.3	O+	105.3			0
16.9 – 17.1 Da	9	OH+	9			0
17.9 – 18.1 Da	2	OH2+	2			0
22.9 – 23.1 Da	3.2	Ti++	1.1			2.1
23.4 – 23.6 Da	1	Ti++	1			0
23.9 – 24.1 Da	9.3	C2+	0	Ti++	9.8	-0.4
24.4 – 24.6 Da	0.5	Ti++	0.7			-0.2
24.9 – 25.2 Da	2.1	C2+	0	Ti++	0.7	1.4
26.9 – 27.1 Da	6126.8	Fe++	6126.8			0
27.9 – 28.1 Da	93157.8	Fe++	93157.8			0
28.4 – 28.6 Da	2209.9	Fe++	2209.9			0
28.9 – 29.1 Da	294.2	Fe++	294.2			0
29.6 – 29.8 Da	93.7	Y+++	93.7			0
30.9 – 31.1 Da	3.4	TiO++	1.4			2
31.4 – 31.6 Da	8.5	TiO++	1.3			7.3
31.9 – 32.2 Da	10.9	TiO++	12.6	O2+	0	-1.7
32.4 – 32.6 Da	3.1	TiO++	0.9			2.1
32.9 – 33.1 Da	9.9	TiO++	0.9			9.1
34.4 – 34.6 Da	0					0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	6.7	Ga++	6.7			0
35.9 – 36.1 Da	0.2	FeO++	0.2			0
36.4 – 36.6 Da	0.5	FeO++	0.5			0
36.9 – 37.1 Da	0					0
38.9 – 39.2 Da	0					0
39.4 – 39.7 Da	0					0
39.9 – 40.2 Da	11.9	TiO2++	11.9			0
40.4 – 40.7 Da	3.3	TiO2++	3.3			0
40.9 – 41.2 Da	0					0
44.4 – 44.7 Da	9.2	Y++	9.2			0
52.3 – 52.7 Da	81.4	YO++	81.4			0
53.8 – 54.2 Da	1.4	Fe+	1.4			0
55.8 – 56.2 Da	42.9	Fe+	42.9			0
56.8 – 57.2 Da	30.9	Fe+	30.9			0
57.8 – 58.2 Da	0					0
60.3 – 60.7 Da	0.5	YO2++	0.5			0
61.8 – 62.2 Da	0.7	TiO+	1.1	Fe2O++	0	-0.5
62.8 – 63.2 Da	4.3	TiO+	1	Fe2O++	0	3.3
63.8 – 64.2 Da	9.4	TiO+	10	Fe2O++	0	-0.6
64.3 – 64.7 Da	0					0
64.8 – 65.2 Da	5.6	TiO+	0.7	Fe2O++	0	4.9
65.8 – 66.2 Da	0					0
68.8 – 69.2 Da	24.7	Ga+	24.7			0
69.8 – 70.2 Da	4	FeO+	4			0
70.8 – 71.2 Da	19	Ga+	19			0
71.8 – 72.2 Da	57.5	FeO+	57.5			0
72.8 – 73.2 Da	2.3	FeO+	2.3			0
73.8 – 74.2 Da	1.6	FeO+	1.6			0
77.8 – 78.2 Da	0.5	TiO2+	0.5			0
78.8 – 79.2 Da	0.3	TiO2+	0.3			0
79.8 – 80.2 Da	0.7	TiO2+	0.7			0
80.8 – 81.2 Da	0					0
81.8 – 82.2 Da	0.7	TiO2+	0.7			0
85.8 – 86.2 Da	0					0
87.8 – 88.2 Da	0					0
88.8 – 89.2 Da	0.1	FeO2+	0.1			0
89.8 – 90.2 Da	3.5	FeO2+	3.5			0
104.7 – 105.2 Da	0					0
106.8 – 107.3 Da	4.7	WO2++	4.7			0
107.3 – 107.8 Da	0					0
107.8 – 108.3 Da	0					0
108.8 – 109.3 Da	1.1	WO2++	1.1			0
6.4–9.6 nm						
6.0 – 6.1 Da	19.8	C++	19.8			0
6.5 – 6.6 Da	0					0
11.9 – 12.1 Da	10	C+	10			0
12.9 – 13.1 Da	1	C+	1			0
13.9 – 14.1 Da	2.3	N+	2.3			0
14.9 – 15.1 Da	0					0
15.9 – 16.1 Da	136.3	O+	136.3			0
16.9 – 17.1 Da	9.7	OH+	9.7			0
17.9 – 18.1 Da	13.1	OH2+	13.1			0
22.9 – 23.1 Da	0.2	Ti++	1.1			-0.9
23.4 – 23.6 Da	1.9	Ti++	1			0.9
23.9 – 24.1 Da	9.8	C2+	0	Ti++	9.8	0
24.4 – 24.6 Da	0					0
24.9 – 25.2 Da	2.3	C2+	0	Ti++	0.7	1.6
26.9 – 27.1 Da	5977.5	Fe++	5977.5			0
27.9 – 28.1 Da	92077.8	Fe++	92077.8			0
28.4 – 28.6 Da	2376.3	Fe++	2376.3			0
28.9 – 29.1 Da	291.5	Fe++	291.5			0
29.6 – 29.8 Da	154.3	Y+++	154.3			0
30.9 – 31.1 Da	2	TiO++	4.7			-2.7
31.4 – 31.6 Da	2.7	TiO++	4.2			-1.5
31.9 – 32.2 Da	81.6	TiO++	41.8	O2+	39.6	0.1
32.4 – 32.6 Da	2.6	TiO++	3.1			-0.5
32.9 – 33.1 Da	7.7	TiO++	2.9			4.7
34.4 – 34.6 Da	1.8	Ga++	1.8			0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	1.5	Ga++	1.5			0
35.9 – 36.1 Da	4	FeO++	4			0
36.4 – 36.6 Da	1.5	FeO++	1.5			0
36.9 – 37.1 Da	3.8	FeO++	3.8			0
38.9 – 39.2 Da	0.9	TiO2++	0.9			0
39.4 – 39.7 Da	1.9	TiO2++	1.9			0
39.9 – 40.2 Da	8.3	TiO2++	8.3			0
40.4 – 40.7 Da	0					0
40.9 – 41.2 Da	1.3	TiO2++	1.3			0
44.4 – 44.7 Da	21.8	Y++	21.8			0
52.3 – 52.7 Da	150.2	YO++	150.2			0
53.8 – 54.2 Da	5.4	Fe+	5.4			0
55.8 – 56.2 Da	24	Fe+	24			0
56.8 – 57.2 Da	37.9	Fe+	37.9			0
57.8 – 58.2 Da	1.9	Fe+	1.9			0
60.3 – 60.7 Da	2.2	YO2++	2.2			0
61.8 – 62.2 Da	0					0
62.8 – 63.2 Da	13.1	TiO+	0	Fe2O++	1.8	11.3
63.8 – 64.2 Da	12.9	TiO+	0	Fe2O++	14.3	-1.5
64.3 – 64.7 Da	1.5	Fe2O++	0.7			0.8
64.8 – 65.2 Da	0					0
65.8 – 66.2 Da	0					0
68.8 – 69.2 Da	21.8	Ga+	21.8			0
69.8 – 70.2 Da	6.6	FeO+	6.6			0
70.8 – 71.2 Da	18.4	Ga+	18.4			0
71.8 – 72.2 Da	89.2	FeO+	89.2			0
72.8 – 73.2 Da	1	FeO+	1			0
73.8 – 74.2 Da	0					0
77.8 – 78.2 Da	1.7	TiO2+	1.7			0
78.8 – 79.2 Da	4	TiO2+	4			0
79.8 – 80.2 Da	1.3	TiO2+	1.3			0
80.8 – 81.2 Da	2.3	TiO2+	2.3			0
81.8 – 82.2 Da	0					0
85.8 – 86.2 Da	1	FeO2+	1			0
87.8 – 88.2 Da	3.5	FeO2+	3.5			0
88.8 – 89.2 Da	3.6	FeO2+	3.6			0
89.8 – 90.2 Da	3.9	FeO2+	3.9			0
104.7 – 105.2 Da	4.4	YO+	4.4			0
106.8 – 107.3 Da	5.5	WO2++	5.5			0
107.3 – 107.8 Da	0					0
107.8 – 108.3 Da	0.7	WO2++	0.7			0
108.8 – 109.3 Da	0					0
9.6–12.8 nm						
6.0 – 6.1 Da	16.5	C++	16.5			0
6.5 – 6.6 Da	5	C++	5			0
11.9 – 12.1 Da	24.2	C+	24.2			0
12.9 – 13.1 Da	0.9	C+	0.9			0
13.9 – 14.1 Da	0					0
14.9 – 15.1 Da	2.6	N+	2.6			0
15.9 – 16.1 Da	400.5	O+	400.5			0
16.9 – 17.1 Da	4	OH+	4			0
17.9 – 18.1 Da	14	OH2+	14			0
22.9 – 23.1 Da	0					0
23.4 – 23.6 Da	0.5	Ti++	1.5			-1
23.9 – 24.1 Da	14.7	C2+	0	Ti++	14.7	0
24.4 – 24.6 Da	6.5	Ti++	1.1			5.5
24.9 – 25.2 Da	0					0
26.9 – 27.1 Da	5650.1	Fe++	5650.1			0
27.9 – 28.1 Da	86286.2	Fe++	86286.2			0
28.4 – 28.6 Da	2133.6	Fe++	2133.6			0
28.9 – 29.1 Da	286.4	Fe++	286.4			0
29.6 – 29.8 Da	1078.7	Y+++	1078.7			0
30.9 – 31.1 Da	11.1	TiO++	4.1			7
31.4 – 31.6 Da	0					0
31.9 – 32.2 Da	746.5	TiO++	36.5	O2+	710	0
32.4 – 32.6 Da	1.9	TiO++	2.7			-0.8
32.9 – 33.1 Da	0					0
34.4 – 34.6 Da	0					0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	0					0
35.9 – 36.1 Da	3.4	FeO++	3.4			0
36.4 – 36.6 Da	5.3	FeO++	5.3			0
36.9 – 37.1 Da	0					0
38.9 – 39.2 Da	0					0
39.4 – 39.7 Da	2	TiO2++	2			0
39.9 – 40.2 Da	10.7	TiO2++	10.7			0
40.4 – 40.7 Da	7	TiO2++	7			0
40.9 – 41.2 Da	5.8	TiO2++	5.8			0
44.4 – 44.7 Da	194.3	Y++	194.3			0
52.3 – 52.7 Da	1356	YO++	1356			0
53.8 – 54.2 Da	10.2	Fe+	10.2			0
55.8 – 56.2 Da	46.9	Fe+	46.9			0
56.8 – 57.2 Da	27	Fe+	27			0
57.8 – 58.2 Da	3.3	Fe+	3.3			0
60.3 – 60.7 Da	55.5	YO2++	55.5			0
61.8 – 62.2 Da	5.3	TiO+	2.9	Fe2O++	0	2.3
62.8 – 63.2 Da	14.1	TiO+	2.7	Fe2O++	0.3	11.1
63.8 – 64.2 Da	27.1	TiO+	26.3	Fe2O++	2.2	-1.4
64.3 – 64.7 Da	0					0
64.8 – 65.2 Da	4.3	TiO+	1.9	Fe2O++	0	2.3
65.8 – 66.2 Da	0.3	TiO+	1.9			-1.6
68.8 – 69.2 Da	24	Ga+	24			0
69.8 – 70.2 Da	15.7	FeO+	15.7			0
70.8 – 71.2 Da	18	Ga+	18			0
71.8 – 72.2 Da	278.4	FeO+	278.4			0
72.8 – 73.2 Da	19.3	FeO+	19.3			0
73.8 – 74.2 Da	0					0
77.8 – 78.2 Da	0					0
78.8 – 79.2 Da	8	TiO2+	8			0
79.8 – 80.2 Da	4	TiO2+	4			0
80.8 – 81.2 Da	4.9	TiO2+	4.9			0
81.8 – 82.2 Da	4.9	TiO2+	4.9			0
85.8 – 86.2 Da	2.7	FeO2+	2.7			0
87.8 – 88.2 Da	0	FeO2+	0			0
88.8 – 89.2 Da	4.5	FeO2+	4.5			0
89.8 – 90.2 Da	2.1	FeO2+	2.1			0
104.7 – 105.2 Da	10.3	YO+	10.3			0
106.8 – 107.3 Da	18.9	WO2++	18.9			0
107.3 – 107.8 Da	8.4	WO2++	8.4			0
107.8 – 108.3 Da	0					0
108.8 – 109.3 Da	11.9	WO2++	11.9			0
12.8–16.0 nm						
6.0 – 6.1 Da	10.3	C++	10.3			0
6.5 – 6.6 Da	2.9	C++	2.9			0
11.9 – 12.1 Da	25.6	C+	25.6			0
12.9 – 13.1 Da	3.1	C+	3.1			0
13.9 – 14.1 Da	0	N+	0			0
14.9 – 15.1 Da	1	N+	1			0
15.9 – 16.1 Da	421.6	O+	421.6			0
16.9 – 17.1 Da	7.9	OH+	7.9			0
17.9 – 18.1 Da	15.7	OH2+	15.7			0
22.9 – 23.1 Da	1.8	Ti++	1.6			0.2
23.4 – 23.6 Da	1.1	Ti++	1.4			-0.3
23.9 – 24.1 Da	14	C2+	0	Ti++	14.3	-0.4
24.4 – 24.6 Da	3.9	Ti++	1.1			2.9
24.9 – 25.2 Da	3.6	C2+	0	Ti++	1	2.6
26.9 – 27.1 Da	5485.9	Fe++	5485.9			0
27.9 – 28.1 Da	84096.5	Fe++	84096.5			0
28.4 – 28.6 Da	2136.4	Fe++	2136.4			0
28.9 – 29.1 Da	271.4	Fe++	271.4			0
29.6 – 29.8 Da	1333.3	Y+++	1333.3			0
30.9 – 31.1 Da	10.3	TiO++	12			-1.7
31.4 – 31.6 Da	1.9	TiO++	10.8			-8.9
31.9 – 32.2 Da	882.3	TiO++	107	O2+	775.3	0
32.4 – 32.6 Da	12	TiO++	7.9			4.1
32.9 – 33.1 Da	14	TiO++	7.5			6.5
34.4 – 34.6 Da	0.6	Ga++	0.6			0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	7.2	Ga++	7.2			0
35.9 – 36.1 Da	10.4	FeO++	10.4			0
36.4 – 36.6 Da	1.1	FeO++	1.1			0
36.9 – 37.1 Da	2	FeO++	2			0
38.9 – 39.2 Da	2.8	TiO2++	2.8			0
39.4 – 39.7 Da	0					0
39.9 – 40.2 Da	6	TiO2++	6			0
40.4 – 40.7 Da	0					0
40.9 – 41.2 Da	2.9	TiO2++	2.9			0
44.4 – 44.7 Da	213.6	Y++	213.6			0
52.3 – 52.7 Da	1616.3	YO++	1616.3			0
53.8 – 54.2 Da	8.3	Fe+	8.3			0
55.8 – 56.2 Da	43.7	Fe+	43.7			0
56.8 – 57.2 Da	28.4	Fe+	28.4			0
57.8 – 58.2 Da	4.6	Fe+	4.6			0
60.3 – 60.7 Da	78.2	YO2++	78.2			0
61.8 – 62.2 Da	1.4	TiO+	0.8	Fe2O++	0.3	0.3
62.8 – 63.2 Da	19.9	TiO+	0.8	Fe2O++	8.1	11
63.8 – 64.2 Da	70	TiO+	7.5	Fe2O++	64.3	-1.9
64.3 – 64.7 Da	13.3	Fe2O++	3.1			10.3
64.8 – 65.2 Da	4.9	TiO+	0.6	Fe2O++	0.4	3.9
65.8 – 66.2 Da	0					0
68.8 – 69.2 Da	8.8	Ga+	8.8			0
69.8 – 70.2 Da	28.2	FeO+	28.2			0
70.8 – 71.2 Da	13.7	Ga+	13.7			0
71.8 – 72.2 Da	350.4	FeO+	350.4			0
72.8 – 73.2 Da	4.5	FeO+	4.5			0
73.8 – 74.2 Da	0.8	FeO+	0.8			0
77.8 – 78.2 Da	3.2	TiO2+	3.2			0
78.8 – 79.2 Da	9.6	TiO2+	9.6			0
79.8 – 80.2 Da	0					0
80.8 – 81.2 Da	2.6	TiO2+	2.6			0
81.8 – 82.2 Da	0					0
85.8 – 86.2 Da	1.1	FeO2+	1.1			0
87.8 – 88.2 Da	5.9	FeO2+	5.9			0
88.8 – 89.2 Da	4.1	FeO2+	4.1			0
89.8 – 90.2 Da	1.4	FeO2+	1.4			0
104.7 – 105.2 Da	17.9	YO+	17.9			0
106.8 – 107.3 Da	21.7	WO2++	21.7			0
107.3 – 107.8 Da	5.8	WO2++	5.8			0
107.8 – 108.3 Da	27.3	WO2++	27.3			0
108.8 – 109.3 Da	13.5	WO2++	13.5			0
16.0–19.2 nm						
6.0 – 6.1 Da	15.8	C++	15.8			0
6.5 – 6.6 Da	0					0
11.9 – 12.1 Da	32.4	C+	32.4			0
12.9 – 13.1 Da	0					0
13.9 – 14.1 Da	2.6	N+	2.6			0
14.9 – 15.1 Da	2.2	N+	2.2			0
15.9 – 16.1 Da	342.8	O+	342.8			0
16.9 – 17.1 Da	11.2	OH+	11.2			0
17.9 – 18.1 Da	17.3	OH2+	17.3			0
22.9 – 23.1 Da	0					0
23.4 – 23.6 Da	4.9	Ti++	0.8			4.1
23.9 – 24.1 Da	7.2	C2+	0	Ti++	7.6	-0.3
24.4 – 24.6 Da	0					0
24.9 – 25.2 Da	1.2	C2+	0	Ti++	0.5	0.7
26.9 – 27.1 Da	5710.3	Fe++	5710.3			0
27.9 – 28.1 Da	85979.3	Fe++	85979.3			0
28.4 – 28.6 Da	2136.4	Fe++	2136.4			0
28.9 – 29.1 Da	293.7	Fe++	293.7			0
29.6 – 29.8 Da	916.3	Y+++	916.3			0
30.9 – 31.1 Da	12.5	TiO++	10.8			1.7
31.4 – 31.6 Da	12.9	TiO++	9.8			3.1
31.9 – 32.2 Da	410	TiO++	96.7	O2+	313.2	0
32.4 – 32.6 Da	9.1	TiO++	7.1			1.9
32.9 – 33.1 Da	0					0
34.4 – 34.6 Da	0.5	Ga++	0.5			0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	5.5	Ga++	5.5			0
35.9 – 36.1 Da	12.8	FeO++	12.8			0
36.4 – 36.6 Da	0.3	FeO++	0.3			0
36.9 – 37.1 Da	2.6	FeO++	2.6			0
38.9 – 39.2 Da	3.4	TiO2++	3.4			0
39.4 – 39.7 Da	0					0
39.9 – 40.2 Da	4.4	TiO2++	4.4			0
40.4 – 40.7 Da	0					0
40.9 – 41.2 Da	1.3	TiO2++	1.3			0
44.4 – 44.7 Da	158	Y++	158			0
52.3 – 52.7 Da	1023.8	YO++	1023.8			0
53.8 – 54.2 Da	12	Fe+	12			0
55.8 – 56.2 Da	44.8	Fe+	44.8			0
56.8 – 57.2 Da	20.8	Fe+	20.8			0
57.8 – 58.2 Da	1.6	Fe+	1.6			0
60.3 – 60.7 Da	27.1	YO2++	27.1			0
61.8 – 62.2 Da	3.3	TiO+	3.5	Fe2O++	0.2	-0.5
62.8 – 63.2 Da	30	TiO+	3.2	Fe2O++	6.6	20.1
63.8 – 64.2 Da	81.9	TiO+	31.7	Fe2O++	52.6	-2.3
64.3 – 64.7 Da	0					0
64.8 – 65.2 Da	5.3	TiO+	2.3	Fe2O++	0.3	2.6
65.8 – 66.2 Da	1.5	TiO+	2.2			-0.7
68.8 – 69.2 Da	7.2	Ga+	7.2			0
69.8 – 70.2 Da	21.7	FeO+	21.7			0
70.8 – 71.2 Da	0					0
71.8 – 72.2 Da	396.9	FeO+	396.9			0
72.8 – 73.2 Da	6.4	FeO+	6.4			0
73.8 – 74.2 Da	3.3	FeO+	3.3			0
77.8 – 78.2 Da	0					0
78.8 – 79.2 Da	7.5	TiO2+	7.5			0
79.8 – 80.2 Da	2.6	TiO2+	2.6			0
80.8 – 81.2 Da	4.7	TiO2+	4.7			0
81.8 – 82.2 Da	5	TiO2+	5			0
85.8 – 86.2 Da	0					0
87.8 – 88.2 Da	4.9	FeO2+	4.9			0
88.8 – 89.2 Da	1.3	FeO2+	1.3			0
89.8 – 90.2 Da	0					0
104.7 – 105.2 Da	16.4	YO+	16.4			0
106.8 – 107.3 Da	14	WO2++	14			0
107.3 – 107.8 Da	0					0
107.8 – 108.3 Da	24.8	WO2++	24.8			0
108.8 – 109.3 Da	15.8	WO2++	15.8			0
19.2–22.4 nm						
6.0 – 6.1 Da	11.6	C++	11.6			0
6.5 – 6.6 Da	0					0
11.9 – 12.1 Da	18.7	C+	18.7			0
12.9 – 13.1 Da	0					0
13.9 – 14.1 Da	2	N+	2			0
14.9 – 15.1 Da	0.2	N+	0.2			0
15.9 – 16.1 Da	158.6	O+	158.6			0
16.9 – 17.1 Da	16	OH+	16			0
17.9 – 18.1 Da	9.1	OH2+	9.1			0
22.9 – 23.1 Da	5.2	Ti++	2.1			3.1
23.4 – 23.6 Da	2.6	Ti++	1.9			0.7
23.9 – 24.1 Da	18	C2+	0	Ti++	18.9	-0.9
24.4 – 24.6 Da	2.9	Ti++	1.4			1.6
24.9 – 25.2 Da	6.2	C2+	0	Ti++	1.3	4.8
26.9 – 27.1 Da	5649.7	Fe++	5649.7			0
27.9 – 28.1 Da	86904.6	Fe++	86904.6			0
28.4 – 28.6 Da	2036	Fe++	2036			0
28.9 – 29.1 Da	316.6	Fe++	316.6			0
29.6 – 29.8 Da	170.3	Y+++	170.3			0
30.9 – 31.1 Da	4.5	TiO++	4.4			0.1
31.4 – 31.6 Da	10.9	TiO++	4			6.9
31.9 – 32.2 Da	38.5	TiO++	39.3	O2+	0	-0.8
32.4 – 32.6 Da	5	TiO++	2.9			2.2
32.9 – 33.1 Da	1.6	TiO++	2.8			-1.2
34.4 – 34.6 Da	4.8	Ga++	4.8			0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	0.4	Ga++	0.4			0
35.9 – 36.1 Da	5.3	FeO++	5.3			0
36.4 – 36.6 Da	2.3	FeO++	2.3			0
36.9 – 37.1 Da	1.8	FeO++	1.8			0
38.9 – 39.2 Da	0					0
39.4 – 39.7 Da	0					0
39.9 – 40.2 Da	1.7	TiO2++	1.7			0
40.4 – 40.7 Da	7.4	TiO2++	7.4			0
40.9 – 41.2 Da	0					0
44.4 – 44.7 Da	26.8	Y++	26.8			0
52.3 – 52.7 Da	173.7	YO++	173.7			0
53.8 – 54.2 Da	0					0
55.8 – 56.2 Da	43.3	Fe+	43.3			0
56.8 – 57.2 Da	23.4	Fe+	23.4			0
57.8 – 58.2 Da	9	Fe+	9			0
60.3 – 60.7 Da	6.4	YO2++	6.4			0
61.8 – 62.2 Da	0					0
62.8 – 63.2 Da	11.7	TiO+	3.1	Fe2O++	8.6	0
63.8 – 64.2 Da	98.7	TiO+	30.8	Fe2O++	67.7	0.2
64.3 – 64.7 Da	0					0
64.8 – 65.2 Da	4.6	TiO+	2.3	Fe2O++	0.4	1.9
65.8 – 66.2 Da	2.3	TiO+	2.2			0.2
68.8 – 69.2 Da	13	Ga+	13			0
69.8 – 70.2 Da	24.6	FeO+	24.6			0
70.8 – 71.2 Da	10.5	Ga+	10.5			0
71.8 – 72.2 Da	302.7	FeO+	302.7			0
72.8 – 73.2 Da	7.2	FeO+	7.2			0
73.8 – 74.2 Da	0.9	FeO+	0.9			0
77.8 – 78.2 Da	2.3	TiO2+	2.3			0
78.8 – 79.2 Da	4.1	TiO2+	4.1			0
79.8 – 80.2 Da	1.5	TiO2+	1.5			0
80.8 – 81.2 Da	2.7	TiO2+	2.7			0
81.8 – 82.2 Da	3.2	TiO2+	3.2			0
85.8 – 86.2 Da	2.7	FeO2+	2.7			0
87.8 – 88.2 Da	3.8	FeO2+	3.8			0
88.8 – 89.2 Da	1.1	FeO2+	1.1			0
89.8 – 90.2 Da	5.7	FeO2+	5.7			0
104.7 – 105.2 Da	9	YO+	9			0
106.8 – 107.3 Da	2.1	WO2++	2.1			0
107.3 – 107.8 Da	3.4	WO2++	3.4			0
107.8 – 108.3 Da	6.3	WO2++	6.3			0
108.8 – 109.3 Da	7.4	WO2++	7.4			0
22.4–25.6 nm						
6.0 – 6.1 Da	9	C++	9			0
6.5 – 6.6 Da	4.5	C++	4.5			0
11.9 – 12.1 Da	12.7	C+	12.7			0
12.9 – 13.1 Da	2	C+	2			0
13.9 – 14.1 Da	0					0
14.9 – 15.1 Da	0					0
15.9 – 16.1 Da	55.5	O+	55.5			0
16.9 – 17.1 Da	1.7	OH+	1.7			0
17.9 – 18.1 Da	19.2	OH2+	19.2			0
22.9 – 23.1 Da	3.7	Ti++	1.2			2.4
23.4 – 23.6 Da	2.8	Ti++	1.1			1.7
23.9 – 24.1 Da	10.5	C2+	0	Ti++	11.1	-0.6
24.4 – 24.6 Da	2	Ti++	0.8			1.2
24.9 – 25.2 Da	2	C2+	0	Ti++	0.8	1.2
26.9 – 27.1 Da	5662.3	Fe++	5662.3			0
27.9 – 28.1 Da	88818.8	Fe++	88818.8			0
28.4 – 28.6 Da	2250.6	Fe++	2250.6			0
28.9 – 29.1 Da	251.3	Fe++	251.3			0
29.6 – 29.8 Da	20.2	Y+++	20.2			0
30.9 – 31.1 Da	9.2	TiO++	6.4			2.7
31.4 – 31.6 Da	12.2	TiO++	5.8			6.4
31.9 – 32.2 Da	55.3	TiO++	57.4	O2+	0	-2.1
32.4 – 32.6 Da	10.6	TiO++	4.2			6.4
32.9 – 33.1 Da	13.7	TiO++	4			9.7
34.4 – 34.6 Da	1.1	Ga++	1.1			0
34.9 – 35.1 Da	0.6	FeO++	0.6			0
35.4 – 35.6 Da	4.5	Ga++	4.5			0
35.9 – 36.1 Da	4	FeO++	4			0
36.4 – 36.6 Da	0.6	FeO++	0.6			0
36.9 – 37.1 Da	0.8	FeO++	0.8			0
38.9 – 39.2 Da	0					0
39.4 – 39.7 Da	0.4	TiO2++	0.4			0
39.9 – 40.2 Da	1.4	TiO2++	1.4			0
40.4 – 40.7 Da	0.7	TiO2++	0.7			0
40.9 – 41.2 Da	0					0
44.4 – 44.7 Da	4.8	Y++	4.8			0
52.3 – 52.7 Da	8.5	YO++	8.5			0
53.8 – 54.2 Da	5.5	Fe+	5.5			0
55.8 – 56.2 Da	33.3	Fe+	33.3			0
56.8 – 57.2 Da	22.3	Fe+	22.3			0
57.8 – 58.2 Da	1.8	Fe+	1.8			0
60.3 – 60.7 Da	0					0
61.8 – 62.2 Da	2.1	TiO+	0.1	Fe2O++	0	2
62.8 – 63.2 Da	1.4	TiO+	0	Fe2O++	0.2	1.1
63.8 – 64.2 Da	1.4	TiO+	0.5	Fe2O++	1.9	-0.5
64.3 – 64.7 Da	8	Fe2O++	0.1			7.9
64.8 – 65.2 Da	1	TiO+	0	Fe2O++	0	0.9
65.8 – 66.2 Da	0.1	TiO+	0			0.1
68.8 – 69.2 Da	7.7	Ga+	7.7			0
69.8 – 70.2 Da	4.1	FeO+	4.1			0
70.8 – 71.2 Da	5.8	Ga+	5.8			0
71.8 – 72.2 Da	19	FeO+	19			0
72.8 – 73.2 Da	6.2	FeO+	6.2			0
73.8 – 74.2 Da	3.4	FeO+	3.4			0
77.8 – 78.2 Da	2	TiO2+	2			0
78.8 – 79.2 Da	0					0
79.8 – 80.2 Da	10	TiO2+	10			0
80.8 – 81.2 Da	3.2	TiO2+	3.2			0
81.8 – 82.2 Da	0					0
85.8 – 86.2 Da	0					0
87.8 – 88.2 Da	1.4	FeO2+	1.4			0
88.8 – 89.2 Da	0.8	FeO2+	0.8			0
89.8 – 90.2 Da	2.4	FeO2+	2.4			0
104.7 – 105.2 Da	0					0
106.8 – 107.3 Da	0					0
107.3 – 107.8 Da	1	WO2++	1			0
107.8 – 108.3 Da	2	WO2++	2			0
108.8 – 109.3 Da	1.9	WO2++	1.9			0
25.6–28.8 nm						
6.0 – 6.1 Da	9.3	C++	9.3			0
6.5 – 6.6 Da	0.5	C++	0.5			0
11.9 – 12.1 Da	14.4	C+	14.4			0
12.9 – 13.1 Da	2.7	C+	2.7			0
13.9 – 14.1 Da	2.1	N+	2.1			0
14.9 – 15.1 Da	0.3	N+	0.3			0
15.9 – 16.1 Da	194.8	O+	194.8			0
16.9 – 17.1 Da	8	OH+	8			0
17.9 – 18.1 Da	10	OH2+	10			0
22.9 – 23.1 Da	2.7	Ti++	3.4			-0.8
23.4 – 23.6 Da	4.7	Ti++	3.1			1.6
23.9 – 24.1 Da	30.6	C2+	0	Ti++	30.8	-0.2
24.4 – 24.6 Da	1.6	Ti++	2.3			-0.7
24.9 – 25.2 Da	4.8	C2+	0	Ti++	2.2	2.7
26.9 – 27.1 Da	5876	Fe++	5876			0
27.9 – 28.1 Da	91260.7	Fe++	91260.7			0
28.4 – 28.6 Da	2194.5	Fe++	2194.5			0
28.9 – 29.1 Da	287.8	Fe++	287.8			0
29.6 – 29.8 Da	322	Y+++	322			0
30.9 – 31.1 Da	71.6	TiO++	68.1			3.5
31.4 – 31.6 Da	51.7	TiO++	61.4			-9.6
31.9 – 32.2 Da	607.9	TiO++	608	O2+	0	-0.1
32.4 – 32.6 Da	61.2	TiO++	44.6			16.6
32.9 – 33.1 Da	34	TiO++	42.7			-8.8
34.4 – 34.6 Da	5	Ga++	5			0
34.9 – 35.1 Da	2.8	FeO++	2.8			0
35.4 – 35.6 Da	1.2	Ga++	1.2			0
35.9 – 36.1 Da	11.1	FeO++	11.1			0
36.4 – 36.6 Da	2.8	FeO++	2.8			0
36.9 – 37.1 Da	7.8	FeO++	7.8			0
38.9 – 39.2 Da	0					0
39.4 – 39.7 Da	5.7	TiO2++	5.7			0
39.9 – 40.2 Da	5	TiO2++	5			0
40.4 – 40.7 Da	4	TiO2++	4			0
40.9 – 41.2 Da	0					0
44.4 – 44.7 Da	30	Y++	30			0
52.3 – 52.7 Da	208.2	YO++	208.2			0
53.8 – 54.2 Da	5.8	Fe+	5.8			0
55.8 – 56.2 Da	45.7	Fe+	45.7			0
56.8 – 57.2 Da	10.8	Fe+	10.8			0
57.8 – 58.2 Da	0					0
60.3 – 60.7 Da	4.6	YO2++	4.6			0
61.8 – 62.2 Da	11.9	TiO+	5.6	Fe2O++	0.3	6.1
62.8 – 63.2 Da	16.8	TiO+	5.1	Fe2O++	7.9	3.8
63.8 – 64.2 Da	111.8	TiO+	50	Fe2O++	62.5	-0.8
64.3 – 64.7 Da	7.4	Fe2O++	3			4.4
64.8 – 65.2 Da	0					0
65.8 – 66.2 Da	5.9	TiO+	3.5			2.4
68.8 – 69.2 Da	5.1	Ga+	5.1			0
69.8 – 70.2 Da	17.2	FeO+	17.2			0
70.8 – 71.2 Da	14.7	Ga+	14.7			0
71.8 – 72.2 Da	260.8	FeO+	260.8			0
72.8 – 73.2 Da	6.3	FeO+	6.3			0
73.8 – 74.2 Da	3.6	FeO+	3.6			0
77.8 – 78.2 Da	13.7	TiO2+	13.7			0
78.8 – 79.2 Da	12.4	TiO2+	12.4			0
79.8 – 80.2 Da	126.9	TiO2+	126.9			0
80.8 – 81.2 Da	9.6	TiO2+	9.6			0
81.8 – 82.2 Da	8.2	TiO2+	8.2			0
85.8 – 86.2 Da	1.3	FeO2+	1.3			0
87.8 – 88.2 Da	3	FeO2+	3			0
88.8 – 89.2 Da	0.3	FeO2+	0.3			0
89.8 – 90.2 Da	0					0
104.7 – 105.2 Da	4.6	YO+	4.6			0
106.8 – 107.3 Da	3.1	WO2++	3.1			0
107.3 – 107.8 Da	0					0
107.8 – 108.3 Da	0					0
108.8 – 109.3 Da	4	WO2++	4			0
28.8–32.0 nm						
6.0 – 6.1 Da	8.6	C++	8.6			0
6.5 – 6.6 Da	0					0
11.9 – 12.1 Da	15	C+	15			0
12.9 – 13.1 Da	0.9	C+	0.9			0
13.9 – 14.1 Da	1.7	N+	1.7			0
14.9 – 15.1 Da	0					0
15.9 – 16.1 Da	284.6	O+	284.6			0
16.9 – 17.1 Da	9	OH+	9			0
17.9 – 18.1 Da	12.3	OH2+	12.3			0
22.9 – 23.1 Da	5.9	Ti++	4.5			1.4
23.4 – 23.6 Da	6.5	Ti++	4.1			2.4
23.9 – 24.1 Da	39.5	C2+	0	Ti++	40.2	-0.8
24.4 – 24.6 Da	2.9	Ti++	3			0
24.9 – 25.2 Da	8	C2+	0	Ti++	2.8	5.1
26.9 – 27.1 Da	5833.2	Fe++	5833.2			0
27.9 – 28.1 Da	91218.1	Fe++	91218.1			0
28.4 – 28.6 Da	2288.1	Fe++	2288.1			0
28.9 – 29.1 Da	332.6	Fe++	332.6			0
29.6 – 29.8 Da	347.1	Y+++	347.1			0
30.9 – 31.1 Da	95.6	TiO++	70.8			24.8
31.4 – 31.6 Da	69	TiO++	63.8			5.1
31.9 – 32.2 Da	628.6	TiO++	632.5	O2+	0	-3.8
32.4 – 32.6 Da	36.7	TiO++	46.4			-9.8
32.9 – 33.1 Da	62.5	TiO++	44.5			18.1
34.4 – 34.6 Da	0					0
34.9 – 35.1 Da	0.2	FeO++	0.2			0
35.4 – 35.6 Da	4.9	Ga++	4.9			0
35.9 – 36.1 Da	9.8	FeO++	9.8			0
36.4 – 36.6 Da	12	FeO++	12			0
36.9 – 37.1 Da	2.7	FeO++	2.7			0
38.9 – 39.2 Da	0					0
39.4 – 39.7 Da	1.4	TiO2++	1.4			0
39.9 – 40.2 Da	10.7	TiO2++	10.7			0
40.4 – 40.7 Da	0					0
40.9 – 41.2 Da	0					0
44.4 – 44.7 Da	29.8	Y++	29.8			0
52.3 – 52.7 Da	227.3	YO++	227.3			0
53.8 – 54.2 Da	12.4	Fe+	12.4			0
55.8 – 56.2 Da	33.1	Fe+	33.1			0
56.8 – 57.2 Da	26.1	Fe+	26.1			0
57.8 – 58.2 Da	6.6	Fe+	6.6			0
60.3 – 60.7 Da	6.7	YO2++	6.7			0
61.8 – 62.2 Da	9.2	TiO+	5.3	Fe2O++	0.4	3.4
62.8 – 63.2 Da	28.7	TiO+	4.8	Fe2O++	13.9	9.9
63.8 – 64.2 Da	156.6	TiO+	47.7	Fe2O++	110.2	-1.3
64.3 – 64.7 Da	7.3	Fe2O++	5.3			2
64.8 – 65.2 Da	0					0
65.8 – 66.2 Da	5.5	TiO+	3.4			2.2
68.8 – 69.2 Da	7.3	Ga+	7.3			0
69.8 – 70.2 Da	24.9	FeO+	24.9			0
70.8 – 71.2 Da	15.1	Ga+	15.1			0
71.8 – 72.2 Da	417.9	FeO+	417.9			0
72.8 – 73.2 Da	16.9	FeO+	16.9			0
73.8 – 74.2 Da	0					0
77.8 – 78.2 Da	15.8	TiO2+	15.8			0
78.8 – 79.2 Da	14.2	TiO2+	14.2			0
79.8 – 80.2 Da	96.6	TiO2+	96.6			0
80.8 – 81.2 Da	6.5	TiO2+	6.5			0
81.8 – 82.2 Da	4.1	TiO2+	4.1			0
85.8 – 86.2 Da	0.8	FeO2+	0.8			0
87.8 – 88.2 Da	0					0
88.8 – 89.2 Da	0					0
89.8 – 90.2 Da	0					0
104.7 – 105.2 Da	11	YO+	11			0
106.8 – 107.3 Da	1.2	WO2++	1.2			0
107.3 – 107.8 Da	0					0
107.8 – 108.3 Da	0.3	WO2++	0.3			0
108.8 – 109.3 Da	4	WO2++	4			0
32.0–35.2 nm						
6.0 – 6.1 Da	9.6	C++	9.6			0
6.5 – 6.6 Da	0					0
11.9 – 12.1 Da	15.2	C+	15.2			0
12.9 – 13.1 Da	3	C+	3			0
13.9 – 14.1 Da	3.7	N+	3.7			0
14.9 – 15.1 Da	0					0
15.9 – 16.1 Da	129.8	O+	129.8			0
16.9 – 17.1 Da	6.6	OH+	6.6			0
17.9 – 18.1 Da	13.6	OH2+	13.6			0
22.9 – 23.1 Da	0.3	Ti++	1.9			-1.5
23.4 – 23.6 Da	0.4	Ti++	1.7			-1.3
23.9 – 24.1 Da	16.6	C2+	0	Ti++	16.7	-0.1
24.4 – 24.6 Da	2.2	Ti++	1.2			1
24.9 – 25.2 Da	6.2	C2+	0	Ti++	1.2	5
26.9 – 27.1 Da	5707.8	Fe++	5707.8			0
27.9 – 28.1 Da	88296.9	Fe++	88296.9			0
28.4 – 28.6 Da	2288.6	Fe++	2288.6			0
28.9 – 29.1 Da	316.2	Fe++	316.2			0
29.6 – 29.8 Da	48.2	Y+++	48.2			0
30.9 – 31.1 Da	12.4	TiO++	9.5			2.9
31.4 – 31.6 Da	11.5	TiO++	8.5			2.9
31.9 – 32.2 Da	84.3	TiO++	84.5	O2+	0	-0.2
32.4 – 32.6 Da	1	TiO++	6.2			-5.2
32.9 – 33.1 Da	5.5	TiO++	5.9			-0.5
34.4 – 34.6 Da	0					0
34.9 – 35.1 Da	2.4	FeO++	2.4			0
35.4 – 35.6 Da	0					0
35.9 – 36.1 Da	9.1	FeO++	9.1			0
36.4 – 36.6 Da	5	FeO++	5			0
36.9 – 37.1 Da	0					0
38.9 – 39.2 Da	2.5	TiO2++	2.5			0
39.4 – 39.7 Da	1.7	TiO2++	1.7			0
39.9 – 40.2 Da	5	TiO2++	5			0
40.4 – 40.7 Da	3	TiO2++	3			0
40.9 – 41.2 Da	5.3	TiO2++	5.3			0
44.4 – 44.7 Da	5.1	Y++	5.1			0
52.3 – 52.7 Da	30	YO++	30			0
53.8 – 54.2 Da	0.6	Fe+	0.6			0
55.8 – 56.2 Da	52.1	Fe+	52.1			0
56.8 – 57.2 Da	36.8	Fe+	36.8			0
57.8 – 58.2 Da	3.6	Fe+	3.6			0
60.3 – 60.7 Da	2.4	YO2++	2.4			0
61.8 – 62.2 Da	3.5	TiO+	1.3	Fe2O++	0.2	2.1
62.8 – 63.2 Da	15.5	TiO+	1.2	Fe2O++	5	9.4
63.8 – 64.2 Da	49.9	TiO+	11.7	Fe2O++	39.5	-1.3
64.3 – 64.7 Da	4.6	Fe2O++	1.9			2.7
64.8 – 65.2 Da	0.3	TiO+	0.9	Fe2O++	0.2	-0.8
65.8 – 66.2 Da	1.3	TiO+	0.8			0.5
68.8 – 69.2 Da	15.7	Ga+	15.7			0
69.8 – 70.2 Da	11.2	FeO+	11.2			0
70.8 – 71.2 Da	9.9	Ga+	9.9			0
71.8 – 72.2 Da	185.7	FeO+	185.7			0
72.8 – 73.2 Da	2.8	FeO+	2.8			0
73.8 – 74.2 Da	3.2	FeO+	3.2			0
77.8 – 78.2 Da	3.9	TiO2+	3.9			0
78.8 – 79.2 Da	3.1	TiO2+	3.1			0
79.8 – 80.2 Da	15.6	TiO2+	15.6			0
80.8 – 81.2 Da	2.3	TiO2+	2.3			0
81.8 – 82.2 Da	3.7	TiO2+	3.7			0
85.8 – 86.2 Da	0					0
87.8 – 88.2 Da	0					0
88.8 – 89.2 Da	0					0
89.8 – 90.2 Da	0					0
104.7 – 105.2 Da	1.5	YO+	1.5			0
106.8 – 107.3 Da	0					0
107.3 – 107.8 Da	0.7	WO2++	0.7			0
107.8 – 108.3 Da	0.6	WO2++	0.6			0
108.8 – 109.3 Da	2.1	WO2++	2.1			0
35.2–38.4 nm						
6.0 – 6.1 Da	11.9	C++	11.9			0
6.5 – 6.6 Da	1.3	C++	1.3			0
11.9 – 12.1 Da	6	C+	6			0
12.9 – 13.1 Da	1.8	C+	1.8			0
13.9 – 14.1 Da	0					0
14.9 – 15.1 Da	0					0
15.9 – 16.1 Da	33.4	O+	33.4			0
16.9 – 17.1 Da	6.9	OH+	6.9			0
17.9 – 18.1 Da	2.4	OH2+	2.4			0
22.9 – 23.1 Da	0					0
23.4 – 23.6 Da	1.4	Ti++	1.1			0.3
23.9 – 24.1 Da	11.1	C2+	0	Ti++	11.3	-0.1
24.4 – 24.6 Da	1.2	Ti++	0.8			0.4
24.9 – 25.2 Da	4	C2+	0	Ti++	0.8	3.2
26.9 – 27.1 Da	3639.1	Fe++	3639.1			0
27.9 – 28.1 Da	57119.9	Fe++	57119.9			0
28.4 – 28.6 Da	1422.5	Fe++	1422.5			0
28.9 – 29.1 Da	163.3	Fe++	163.3			0
29.6 – 29.8 Da	13.9	Y+++	13.9			0
30.9 – 31.1 Da	0					0
31.4 – 31.6 Da	0					0
31.9 – 32.2 Da	22	TiO++	22	O2+	0	0
32.4 – 32.6 Da	6	TiO++	1.6			4.4
32.9 – 33.1 Da	3.6	TiO++	1.5			2.1
34.4 – 34.6 Da	2.3	Ga++	2.3			0
34.9 – 35.1 Da	0					0
35.4 – 35.6 Da	1.3	Ga++	1.3			0
35.9 – 36.1 Da	0.6	FeO++	0.6			0
36.4 – 36.6 Da	0.4	FeO++	0.4			0
36.9 – 37.1 Da	0.8	FeO++	0.8			0
38.9 – 39.2 Da	3.8	TiO2++	3.8			0
39.4 – 39.7 Da	3	TiO2++	3			0
39.9 – 40.2 Da	3.4	TiO2++	3.4			0
40.4 – 40.7 Da	1.9	TiO2++	1.9			0
40.9 – 41.2 Da	1.8	TiO2++	1.8			0
44.4 – 44.7 Da	1.7	Y++	1.7			0
52.3 – 52.7 Da	8.1	YO++	8.1			0
53.8 – 54.2 Da	0					0
55.8 – 56.2 Da	28.8	Fe+	28.8			0
56.8 – 57.2 Da	32.5	Fe+	32.5			0
57.8 – 58.2 Da	0					0
60.3 – 60.7 Da	0.2	YO2++	0.2			0
61.8 – 62.2 Da	0					0
62.8 – 63.2 Da	3	TiO+	0.1	Fe2O++	0.3	2.6
63.8 – 64.2 Da	3.2	TiO+	1	Fe2O++	2.7	-0.4
64.3 – 64.7 Da	3	Fe2O++	0.1			2.9
64.8 – 65.2 Da	0					0
65.8 – 66.2 Da	1.7	TiO+	0.1			1.6
68.8 – 69.2 Da	10.3	Ga+	10.3			0
69.8 – 70.2 Da	0.4	FeO+	0.4			0
70.8 – 71.2 Da	6.9	Ga+	6.9			0
71.8 – 72.2 Da	12.4	FeO+	12.4			0
72.8 – 73.2 Da	0					0
73.8 – 74.2 Da	0.8	FeO+	0.8			0
77.8 – 78.2 Da	2.7	TiO2+	2.7			0
78.8 – 79.2 Da	3	TiO2+	3			0
79.8 – 80.2 Da	4	TiO2+	4			0
80.8 – 81.2 Da	1.6	TiO2+	1.6			0
81.8 – 82.2 Da	2.6	TiO2+	2.6			0
85.8 – 86.2 Da	0.8	FeO2+	0.8			0
87.8 – 88.2 Da	0					0
88.8 – 89.2 Da	2.3	FeO2+	2.3			0
89.8 – 90.2 Da	0					0
104.7 – 105.2 Da	1.8	YO+	1.8			0
106.8 – 107.3 Da	0					0
107.3 – 107.8 Da	0					0
107.8 – 108.3 Da	2	WO2++	2			0
108.8 – 109.3 Da	0.7	WO2++	0.7			0

Table S.1: Details table for the Fe-Ti-Y2O3 ODS composition line profile (Figure 6a).

m/z (Da)	Probability
26.970	0.02610
27.972	0.41274
28.468	0.00990
28.970	0.03540
29.970	0.01305
30.466	0.00057
30.964	0.00180
31.964	0.00046
Not detected	0.50000

Table S.2: The multinomial probability used to simulate peak counts of 90% Fe^{2+} overlapping with 10% Ni^{2+}. The 0.5 probability of non-detection simulates a detection efficiency of 50%.

S.4 Identifying ions with AIC

In the Identifying Ions section, a simulation was made of the overlap between Fe^{2+} and Ni^{2+} ions. The composition was set to 90% Fe and 10% Ni. The simulated peak counts were drawn from a multinomial distribution with a probability in each mass-peak as shown in Table S.2. The multinomial random numbers were generated using the MATLAB function `mnrnd` with 2000 counts, so that on average 1000 counts would fall in the detected m/z ranges. 10,000 simulated spectra were produced and each solved using a combination of MLE or LS with or without Si as a possible species along with Fe and Ni. An empirical cumulative distribution function is shown for the content of fitted Si using MLE and LS in Figure S.3. As described in the main paper, the AIC value for the Fe/Ni/Si and Fe/Ni fit was computed. The AIC can be used to reject tests, and this curve is shown in yellow in Figure S.3.

S.5 Hudson 2011 Example

Hudson et al. 2011 present the m/z spectrum between 25–29 Da for a measurement acquired from ZIRLO aged at 360 °C for 100 days in 18 MPa primary water (see their paper). They state the peak counts are “determined manually for the ‘whole visible area’ of background corrected data” (Hudson et al. 2011). An overlap diagram of the overlapping ions is shown in Figure S.4.

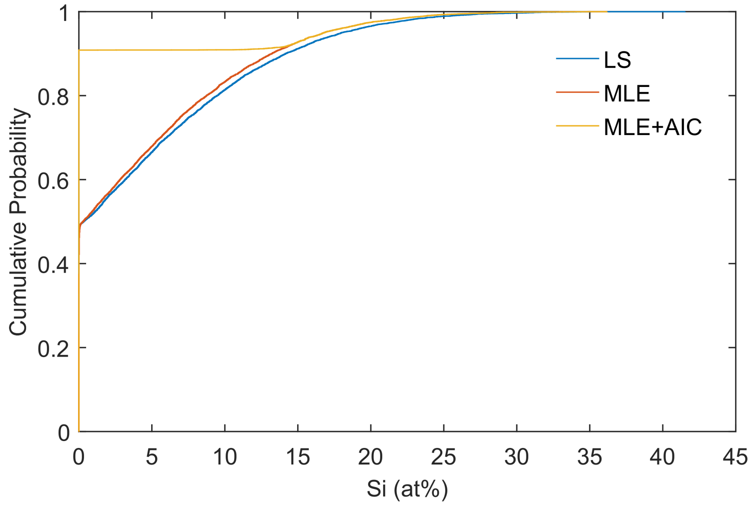

Figure S.3: Empirical cumulative distribution function of the Si content after fitting the Fe/Ni/Si overlap.

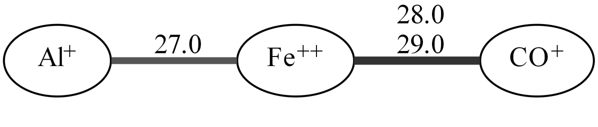

Figure S.4: Overlap diagram of Al^+/Fe^{2+}/CO^+ in a zirconium alloy. The thick line between Fe and CO indicates significantly increased uncertainty arising from this overlap.