

supplementary information

XANES at Cl K-edge as relevant technique to reveal the iron archaeological artefact dechlorination treatments

Received 00th January 20xx,
Accepted 00th January 20xx

Solenn Reguer^{a*}, Florian Kergourlay^{a,b}, Eddy Foy^b, Delphine Neff^b, Delphine Vantelon^a, Marine Cotte^{c,d}, Francois Mirambet^e and Philippe Dillmann^b

DOI: 10.1039/x0xx00000x

Supplementary Information

Table 2: Results of the LCFs analysis of XANES spectra from POIs located in the XRF maps of A_Wa archaeological sample (SM9-8523, see figure 7). POIs are ordered according to their distance to the metal / oxides interface. Results of phases content are in %

POIs	salty goethite	ferrous hydroxylchloride	akaganeite Cl 12%wt	akaganeite Cl 4%wt	R factor	reduced Chi-square
3	0	88	12	0	0.0157	0.0028
2	19	81	0	0	0.0066	0.0009
4	0	85	10	5	0.0159	0.0028
6	0	85	15	0	0.0161	0.0028
7	0	85	0	15	0.0153	0.0026
5	0	77	23	0	0.0132	0.0023
8	43	39	18	0	0.0083	0.0011
9	52	39	9	0	0.0087	0.0012
10	67	33	0	0	0.0040	0.0005
11	66	34	0	0	0.0102	0.0013
12	76	24	0	0	0.0053	0.0007
13	63	27	0	10	0.0053	0.0007
15	75	19	0	6	0.0073	0.0010
14	80	14	0	6	0.0027	0.0004
16	47	29	0	24	0.0032	0.0004
17	60	0	0	40	0.0218	0.0031

Table 3: Results of the LCFs analysis of XANES spectra from POIs located in the XRF maps of A_NoWa archaeological sample (SM9-8541, see figure 11). POIs are ordered according to their distance to the metal / oxides interface.

POIs	salty goethite	salty lepidocrocite	ferrous hydroxylchloride	akaganeite Cl 12%wt	akaganeite Cl 4%wt	NaCl	R factor	reduced Chi-square
1	0	0	100	0	0	0	0.0139	0.0026
2	0	0	80	20	0	0	0.0071	0.0012
8	0	0	82	0	18	0	0.0131	0.0024
7	0	0	60	0	27	13	0.0058	0.0009
3	0	0	87	4	9	0	0.0098	0.0017
15	0	0	89	0	11	0	0.0168	0.0031
16	0	0	90	0	10	0	0.0173	0.0032
10	0	0	83	17	0	0	0.0105	0.0018
17	0	0	88	12	0	0	0.0163	0.0029
18	0	0	67	33	0	0	0.0135	0.0022
19	0	0	58	42	0	0	0.0094	0.0015
4	31	0	0	45	0	24	0.0057	0.0008
20	0	0	79	18	3	0	0.0125	0.0021
21	35	0	17	48	0	0	0.0038	0.0006
5	29	0	0	52	0	19	0.0047	0.0007
22	38	0	0	62	0	0	0.0125	0.0017
23	13	24	0	63	0	0	0.0129	0.0017
6	25	0	0	61	0	14	0.0039	0.0006

^a DiffAbs beamline, Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, 91192 Gif-sur-Yvette cedex, France.

^b LAPA NIMBE UMR3685 LMC – IRAMAT UMR 5060, CEA/CNRS, Université Paris Saclay, Bât. 637 CEA Saclay, 91191 Gif sur Yvette cedex, France.

^c ESRF, 6 rue Jules Horowitz BP 220, 38043 Grenoble cedex 9, France

^d Sorbonne Université, CNRS, Laboratoire d'archéologie moléculaire et structurale, LAMS, 4 place Jussieu, 75005, Paris, France.

^e C2RMF, Palais du Louvre - Porte des Lions 14 Quai François Mitterrand 75001, Institut de Recherche de Chimie Paris (IRCP) Chimie Paris Tech PSL Université 75006, Paris, France.

Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x