American Mineralogist Jan 2014. AM-14-105. 8 pages.

SUPPORTING INFORMATION

XAS Evidence for Ni Sequestration by Siderite in a Lateritic Ni-Deposit from New Caledonia.

Gabrielle Dublet[1,2]*, Farid Juillot[1,3], Guillaume Morin[1], Emmanuel Fritsch[1], Vincent Noel[1], Jessica Brest[1], and Gordon E. Brown Jr.[2,4]

[1]Institut de Minéralogie et de Physique des Milieux Condensés (IMPMC), UMR CNRS 7590, UR IRD 206, Université Pierre et Marie Curie (UPMC), Campus Jussieu, 75252, Paris Cedex 05, France

[2]Department of Geological & Environmental Sciences, Stanford University, Stanford CA 94305-2115, USA

[3] UFR STEP, Université Paris Diderot - IPGP, Bâtiment Lamarck, 75013 Paris, France

[4]Stanford Synchrotron Radiation Lightsource, 2575 Sand Hill Road, Menlo Park, California, 94025, USA

*Corresponding author: gdublet@stanford.edu

Principal Component Analysis (PCA) of EXAFS data from the natural samples collected along the regolith.

Table S1. Quantitative results of the PCA analysis performed on the 9 EXAFS spectra from the natural samples collected along the regolith.

Component	Individual Variance	Cumulative variance	Factor Indicator Function (IND)
First	60%	60%	0.496
Second	19%	79%	0.350
Third	5%	84%	0.288
Fourth	4%	88%	0.288
Fifth	1%	89%	0.365

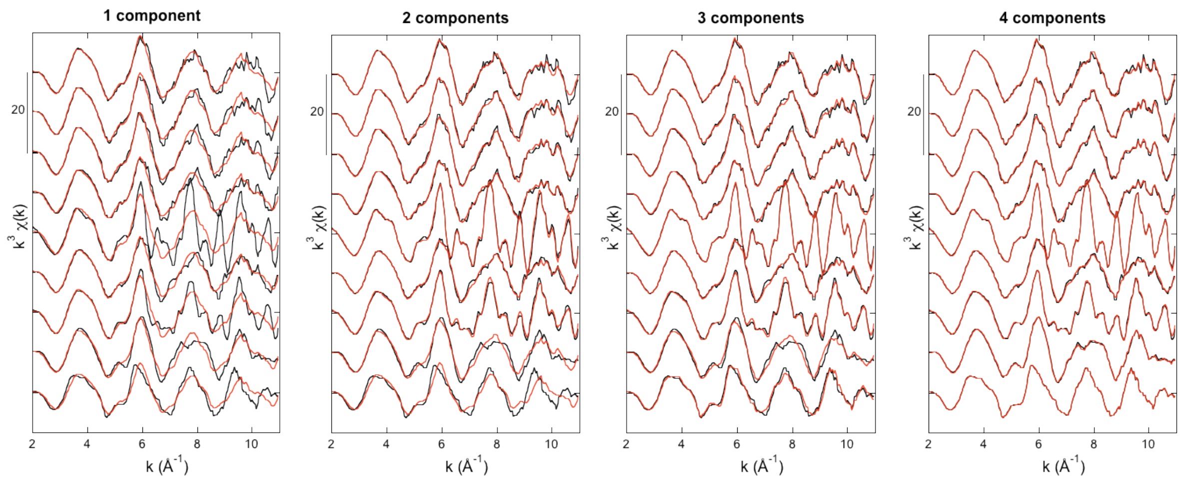

Figure S1. Comparison of the reconstruction for the 9 experimental EXAFS spectra performed with the first, the two first, the three first, and the four first components obtained after PCA analysis.

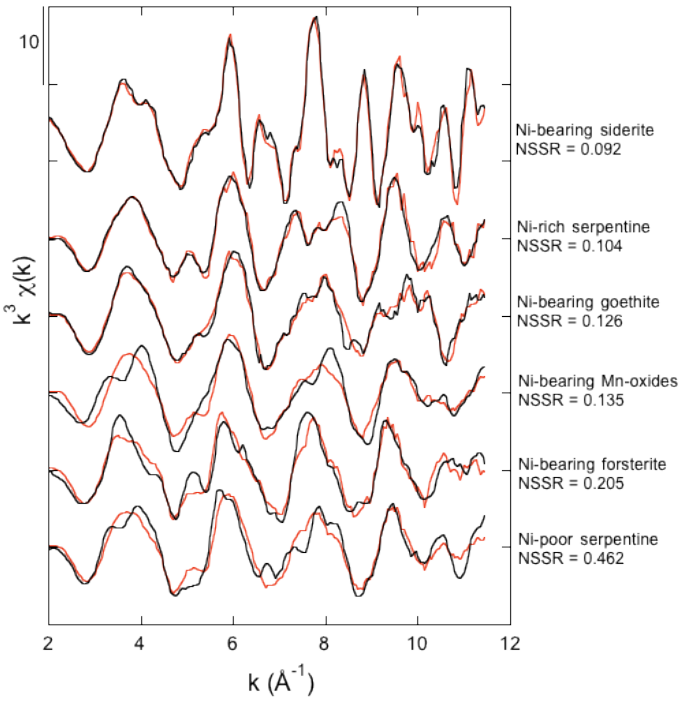

Figure S2. Results of the TT operation performed during the PCA analysis on the Ni K-edge EXAFS spectra of the best candidates model compounds (black lines = target and red lines = transform).

Complements on chemical and mineralogical analyses.

Table S2. EPMA results for the siderite and goethite grains in the sample from 36.1 m (upper part of the sideritic horizon, see Fig. 1 and Fig. 3) in the New Caledonian laterite.

Wt%	FeO	MnO	NiO	CoO	MgO	SiO_2	TOTAL[(1)]	MgO/SiO_2
Siderite								
	54.08	3.99	0.88	0.37	0.92	<0.11	60.27	30
	53.21	3.70	0.96	0.36	0.87	<0.11	59.11	87
	53.70	3.99	0.99	0.47	0.96	<0.11	60.11	---
	53.66	3.93	1.02	0.58	0.87	<0.11	60.12	15
	53.28	3.84	1.07	0.34	0.84	<0.11	59.38	84
	53.48	4.19	0.88	0.42	0.98	<0.11	59.95	---
	52.71	4.43	0.91	0.37	1.05	<0.11	59.53	18
	53.59	4.09	0.77	0.43	1.07	<0.11	59.98	35
	53.30	4.59	0.58	0.37	1.13	<0.11	59.99	56
	55.10	3.00	0.69	0.35	0.94	<0.11	60.12	23
	55.64	3.30	0.67	0.44	0.85	<0.11	60.90	---
	57.95	3.82	0.94	0.33	0.75	0.13	63.92	6
Mean	*54.14*	*3.90*	*0.86*	*0.40*	*0.94*	*<0.11*	*60.27*	*31*
Goethite								
	70.22	3.36	1.89	0.67	0.53	0.19	76.86	2.7
	70.37	3.45	2.09	0.72	0.66	0.16	77.45	4.1
	67.98	3.79	2.17	0.80	0.83	0.52	76.09	1.6
	68.13	5.14	2.21	0.85	0.88	0.81	78.02	1.1
	65.74	5.71	1.99	0.98	0.64	0.59	75.65	1.1
	65.27	5.78	1.99	0.88	0.60	0.61	75.13	1.0
	64.65	6.06	2.03	0.91	0.68	0.60	74.93	1.1
	65.65	6.33	1.85	0.99	0.63	0.65	76.10	1.0
	65.07	6.53	1.83	1.09	0.69	0.62	75.83	1.1
	66.04	7.21	1.66	0.99	0.75	0.62	77.27	1.2
	64.29	7.33	1.79	1.08	0.72	0.69	75.90	1.0
	65.49	5.87	1.74	0.99	0.57	0.74	75.40	0.8
	66.00	5.98	1.82	0.94	0.52	0.53	75.79	1.0
Mean	*66.53*	*5.58*	*1.93*	*0.91*	*0.67*	*0.56*	*76.18*	*1.2*
Detection limit	0.25	0.22	0.18	0.23	0.06	0.11		

[(1)]: Ca, K, Al and Cr also detected by EPMA at trace levels (< 0.10 wt%) are not included.

Table S3. Chemical composition of the core samples, obtained by ICP-AES after digestion (see text)

Depth (m)	NiO (wt%)	CoO (wt%)	Fe_2O_3 (wt%)	SiO_2 (wt%)	MgO (wt%)	Al_2O_3 (wt%)	Cr_2O_3 (wt%)	MnO (wt%)
0.5	0.32	0.01	75.00	0.48	0.23	6.33	3.51	0.16
1.5	0.32	0.02	77.30	0.46	0.17	5.75	3.40	0.19
2.5	0.28	0.02	76.90	0.61	0.32	5.46	3.40	0.18
3.5	0.62	0.03	74.30	0.84	0.21	6.43	3.53	0.34
4.5	0.69	0.04	73.20	0.96	0.27	5.90	3.50	0.34
5.5	0.48	0.03	75.90	0.62	0.19	5.43	4.25	0.30
6.2	0.42	0.02	76.90	0.67	0.22	5.63	4.11	0.27
6.7	0.40	0.03	75.80	0.63	0.15	5.08	4.06	0.32
7.3	0.52	0.03	74.10	0.74	0.18	5.57	3.67	0.33
7.8	0.73	0.03	73.80	0.98	0.27	6.02	3.72	0.37
8.4	0.61	0.03	75.10	0.86	0.21	5.89	3.91	0.32
9.7	0.66	0.02	76.70	1.13	0.18	5.13	3.64	0.26
11.3	0.90	0.02	76.00	1.36	0.21	5.23	3.01	0.29
12.8	0.97	0.01	72.80	1.85	0.45	4.88	3.94	0.19
13.8	0.66	0.01	73.30	1.96	0.40	6.19	3.11	0.18
14.4	0.78	0.01	74.50	1.85	0.47	6.06	3.92	0.22
15.4	0.60	0.03	73.50	0.96	0.24	6.18	3.69	0.30
16.5	0.64	0.02	72.50	1.61	0.43	7.06	3.60	0.24
17.5	0.60	0.02	70.30	1.86	0.74	6.61	4.93	0.22
18.5	0.69	0.02	71.00	1.74	0.49	6.03	3.89	0.25
19.5	0.53	0.01	71.10	2.08	0.65	6.12	4.09	0.18
20.5	0.72	0.01	73.20	2.10	0.49	5.46	3.61	0.22
21.5	0.69	0.02	70.90	2.06	0.53	5.85	3.63	0.23
22.5	0.71	0.02	71.40	2.69	0.44	6.00	3.05	0.22
23.5	0.69	0.03	73.10	1.41	0.33	5.43	3.51	0.29
24.5	0.85	0.02	72.10	2.11	0.51	5.46	3.52	0.22
25.5	1.09	0.02	73.00	2.19	0.50	4.74	3.55	0.18
26.5	0.81	0.04	72.40	1.16	0.42	6.54	4.49	0.39
27.7	0.83	0.03	72.00	1.49	0.45	6.07	4.31	0.34
28.7	0.92	0.04	72.40	1.18	0.32	6.12	4.04	0.41
30.0	1.17	0.03	72.00	2.35	0.74	5.11	4.00	0.21
31.5	1.05	0.10	56.60	14.30	6.46	4.98	3.19	0.13
32.7	1.02	0.12	48.60	19.80	10.10	5.62	4.77	0.10
33.7	1.27	0.04	61.50	11.30	4.02	5.89	3.63	0.14
34.5	1.30	0.04	64.90	8.71	2.49	4.92	4.00	0.11
35.4	1.30	0.17	55.20	11.10	4.48	6.96	3.88	0.75
36.1	1.22	0.44	51.32	9.37	6.67	0.77	0.95	2.53
36.9	1.64	0.07	61.40	14.70	3.56	4.02	2.57	0.13
37.6	1.06	0.12	27.19	30.27	22.11	0.95	0.41	0.72
38.6	0.52	0.04	10.73	41.39	36.85	0.68	0.44	0.34
39.4	1.36	0.20	29.70	29.60	19.80	0.54	0.39	1.04
39.7	1.70	0.24	32.13	27.85	17.78	1.14	0.59	1.24
40.3	2.37	0.13	46.80	22.70	11.90	3.00	2.11	0.39
41.0	0.43	0.03	8.80	42.00	39.30	0.52	0.37	0.27
42.0	0.31	0.02	8.37	41.10	41.90	0.51	0.40	0.18
43.0	0.29	0.01	8.04	39.80	42.20	0.45	0.38	0.12

Depth (m)	Cu (ppm)	Zn (ppm)	LOI	%Moist	Thickness (m)
0.5	65	180	12.4	0.10	1.00
1.5	65	195	12.3	0.09	1.00
2.5	50	175	13.0	0.09	1.05
3.5	60	300	12.8	0.22	0.95
4.5	60	350	12.3	0.21	1.00
5.5	65	310	12.2	0.14	1.00
6.2	70	290	12.1	0.14	0.40
6.7	65	260	12.6	0.12	0.60
7.3	80	310	13.1	0.14	0.50
7.8	70	360	12.3	0.18	0.50
8.4	60	320	12.6	0.17	0.80
9.7	60	330	12.5	0.22	1.70
11.3	60	380	12.6	0.26	1.50
12.8	60	550	12.4	0.37	1.50
13.8	80	550	13.0	0.41	0.50
14.4	55	550	13.0	0.37	0.72
15.4	85	360	13.5	0.19	1.28
16.5	75	450	13.4	0.34	1.00
17.5	65	480	12.9	0.37	1.00
18.5	85	450	13.3	0.33	1.00
19.5	70	420	14.0	0.46	1.00
20.5	75	480	13.0	0.41	1.00
21.5	85	460	13.2	0.40	1.00
22.5	45	480	13.4	0.43	1.00
23.5	85	390	12.6	0.29	1.00
24.5	55	480	12.4	0.42	1.00
25.5	55	500	12.2	0.28	1.00
26.5	65	420	12.0	0.20	1.00
27.7	60	440	11.8	0.35	1.30
28.7	75	440	11.9	0.20	0.70
30.0	80	430	11.7	0.45	2.00
31.5	80	360	10.6	0.50	1.00
32.7	140	380	8.3	0.46	1.37
33.7	85	460	10.5	0.47	0.63
34.5	95	500	11.0	0.51	1.00
35.4	105	490	13.6	0.38	0.70
36.1	10	306	25.1	0.34	0.80
36.9	40	380	10.9	0.55	0.88
37.6	13	118	16.6	0.17	0.45
38.6	5	63	9.5	0.04	1.47
39.4	5	120	17.8	0.12	0.13
39.7	10	185	17.5	0.26	0.57
40.3	45	350	11.4	0.49	0.50
41.0	5	65	8.4	0.03	0.95
42.0	10	55	7.8	0.01	1.05
43.0	10	55	8.0	0.01	1.00

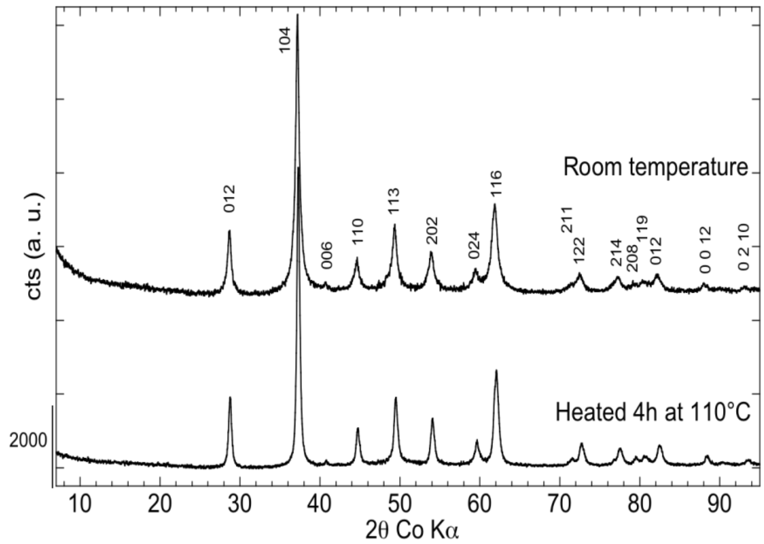

Figure S3. Comparison between the diffraction patterns of the synthetic Ni-free siderite before and after the heating procedure, showing the purity of the mineral phase at room temperature and an increase of the crystallinity after the heat treatment. The siderite peaks are indexed according to the JCDD # 00-029-0696.

Evidence of the occurrence of hematite in the sideritic horizon

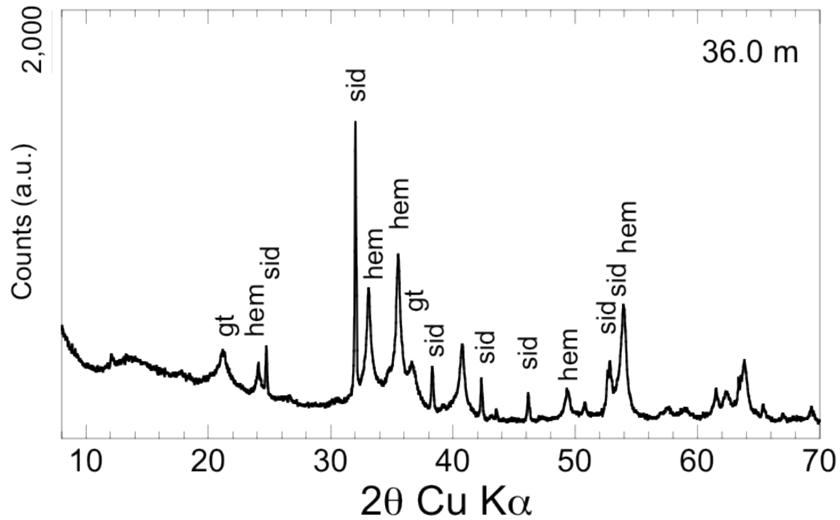

Figure S4. XRD analysis of a 5 cm length core complementary sample taken at the top of the sideritic horizon, and grounded to powder.

REFRENCES

Ressler, T., Wong, J., Roos, J. and Smith, I.L. (2000) Quantitative speciation of Mn-bearing particulates emitted from autos burning (methylcyclopentadienyl)manganese tricarbonyl-added gasolines using XANES spectroscopy. *Environmental Science & Technology*, 34, 950-958.

Webb, S.M. (2005) SIXpack: a graphical user interface for XAS analysis using IFEFFIT. *Physica Scripta*, T115, 1011-1014.