

DATA REPOSITORY ITEM 2009107

Raiswell et al.: Schwertmannite in wet, acid and oxic microenvironments beneath polar and polythermal glaciers

1. Chemical Methodology and Data.

All ice samples were melted through filter paper to separate the sediments and meltwaters (see Raiswell et al., 2008). Each sample of air-dried sediment was treated for 24 h by an ascorbate solution buffered at pH 7.5. The extractant was a deoxygenated solution of 50 g L⁻¹ sodium citrate and 50 g L⁻¹ sodium bicarbonate to which ~10 g L⁻¹ of ascorbic acid was added. About 30 mg of sample were mixed with 10 ml of ascorbate solution, shaken for 24 h at room temperature and then filtered through a 0.45µm membrane filter. The Fe removed by ascorbate is termed FeA. The residual sediment was treated for 2 h with a solution of 50 g L⁻¹ sodium dithionite in 0.35M acetic acid and 0.2M sodium citrate, buffered at pH 4.8 (Raiswell et al., 1994). This extraction removes iron present as residual, aged ferrihydrite (following the ascorbate extraction of fresh ferrihydrite), goethite, hematite and lepidocrocite and is termed FeD. Iron was analyzed by Atomic Absorption Spectroscopy with an analytical precision of 3% (FeA) and 10% (FeD) (Raiswell et al., 2008).

Hyacinthe and Van Cappellen (2004) have found that suspensions of fresh 2 line and 6 line ferrihydrite are >97% dissolved by ascorbate but aged and freeze-dried material are only 5-50% extracted. The results in Table DR1 are consistent with this data. Additionally Table DR1 shows that freeze-dried schwertmannite is 20-30% soluble in ascorbate and 85-100% soluble in dithionite (schwertmannite Total Fe data from Davidson, 2007). The ratios (%FeA)/(%FeA + %FeD) in our dried sediments compared to the synthetic, freeze-dried ferrihydrite and schwertmannite, and a range

of iron oxide minerals, confirm that ferrihydrite and schwertmannite are the main phases being extracted.

TABLE DR1. MEAN CHEMICAL COMPOSITIONS OF ICEBERG AND GLACIAL SEDIMENTS (INCLUDING DATA FROM RAISWELL ET AL., 2008), SYNTHETIC NANOPARTICULATE FE-BEARING PHASES AND FE-BEARING MINERALS.

Sample	%FeA	%FeD	FeA/(FeA+FeD)	Fe Minerals
Icebergs S1-4	0.19	0.91	0.16 ± 0.06	FH, GT
KG1-2	0.057	0.47	0.12 ± 0.05	FH, GT
Glaciers T1-3	0.026	0.11	0.19 ± 0.03	SCH, FH, GT
C1	0.023	0.25	0.09	SCH FH, GT
SV1-2	0.05	0.21	0.21 ± 0.03	SCH, FH, GT
Ice Stream 2B, 3B, 3T	0.049	0.14	0.26 ± 0.04	Unidentified*
Aged 2 line FH	12.3	39.0	0.24 (100%)	–
Freeze-dried SCH	12.2	30.0	0.29 (100%)	–
Freeze-dried As-rich SCH	8.4	29.5	0.22 (85%)	–
Freeze-dried 6 line FH	4.0	47.4	0.08(100%)	–
LP	0.42	54.0	<0.01 (87%)	–
GT	0.03	42.5	<0.01 (68%)	–
HM	0.01	23.5	< 0.01 (65.7)	–

Note: SCH—schwertmannite; FH—ferrihydrite; GT—goethite; LP—lepidocrocite; HM—hematite. Data in brackets give % of total Fe extracted as FeA and FeD. Total Fe data for schwertmannite from Davidson (2007). *Fe phases with Ti and Si.

2.High Resolution Microscopy and Data

High-resolution imaging, quantitative nanodiffraction and elemental analysis of the particulates was carried out using a Philips CM200 Field-Emission Gun - Transmission Electron Microscope (FEG-TEM) equipped with an Oxford Instrument Energy Dispersive X-ray spectrometer (EDS) and selected area electron diffraction (SAED) capabilities. The dried samples were re-suspended in ethanol by ultrasonication and deposited on standard holey carbon support films on copper grids and imaged at 197 keV. These techniques were used to identify schwertmannite in the sediments from Canada and Monaco Glaciers by their morphology, X-ray Diffraction Lines and elemental composition (see Figs. DR1 and DR2).

References

- Davidson, L.E., 2007. The formation and transformation of schwertmannite: kinetics and the effect of toxic trace contaminants [Ph.D. thesis]: University of Leeds, 168p.
- Hyacinthe, C., and Van Cappellen, P., 2004. An authigenic iron phosphate phase in estuarine sediments: composition, formation and chemical reactivity. *Marine Chemistry*, v. 91, p. 227-251.
- Raiswell, R., Canfield., D.E., and Berner, R.A.,1994. A comparison of iron extraction methods for the determination of degree of pyritization and recognition of iron-limited pyrite formation. *Chemical Geology*, v. 111, p. 101-111.
- Raiswell, R., Benning, L.G., Tranter, M., and Tulaczyk, S., 2008. Bioavailable iron in the Southern Ocean: The significance of the iceberg conveyor belt. *Geochemical Transactions*, v. 9:7 doi:10:1186/1467-4866-9-7.

Fig. DR1. Canada Glacier TEM, SAED and EDS data.

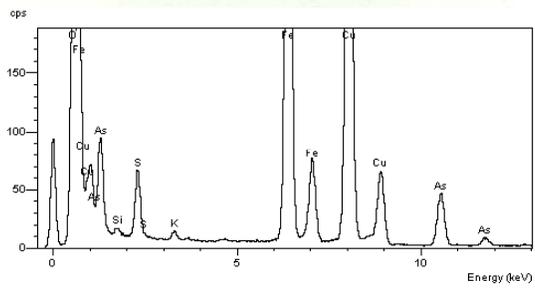
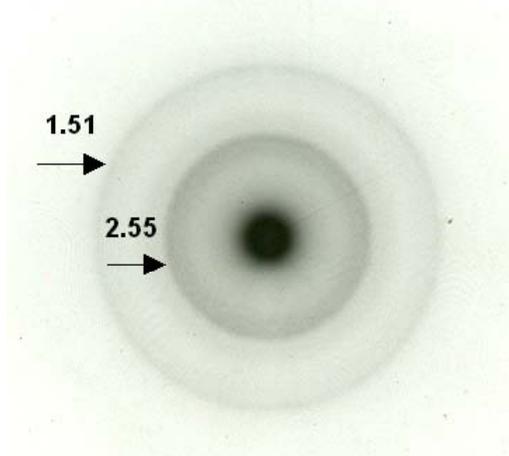
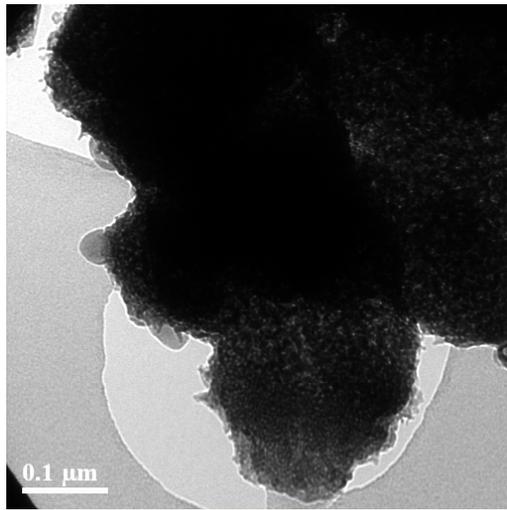


Fig. DR2. Monaco Glacier TEM, SAED and EDS data.

