Isothermal transition of pyrrhotines into goethite in the atmosphere of the Earth

A.V. MASHUKOV*, V.V. ONUFRIENOK AND A.E. MASHUKOVA

Siberian Federal University, Krasnoyarsk, Russia (*correspondence: AVMashukov@sfu-kras.ru)

There was studied the dependence of the goethite content on the sulphur-iron ratio in the pyrrhotine samples after being synthesized at 1273 K and kept in the atmosphere at room temperature for 29 years. The phase and chemical composition was monitored by using the methods of X-ray diffraction.

In the samples, which were kept, the pyrite content increased and pyrrhotine content decreased, as compared to the original ones. It may be supposed that in the atmosphere conditions there was going on the isothermal transition of pyrrhotines into goethite and pyrite as for this process hydrogen and oxygen are required.

The influence of sulphur-iron ratio on the content of the formed goethite was considered on the basis of calculating the thermodynamic potentials using the Pauli quantum statistics. The theoretical calculations were compared with X-ray phase analysis data (Table 1).

S/Fe ratio	Goethite percentage	
	X-ray	As calculated
1.710	1.14	1.150
1.684	1.27	1.226
1.660	2.10	1.303
1.580	1.99	1.604
1.571	2.93	1.643
1.567	1.89	1.661
1.490	2.05	2.054
1.382	2.03	2.819
1.380	3.73	2.836
1.158	3.65	5.937
1.134	8.34	6.484
1.105	6.62	7.232
1.039	11.13	9.373

Table 1. The goethite percentage in the samples

As it is shown in the table, tendency to increasing of goethite content with decreasing S/Fe ratio is observed both X-ray data and the theoretical calculation results.

Mobility of natural and engineered nanoparticles in aquatic media

A. MASION^{1,2}, C. LEVARD^{1,2,3}, N. SOLOVITCH^{1,2}, M.A. DIOT^{1,2}, M. AUFFAN^{1,2}, C. BOTTA¹, J. LABILLE^{1,2}, J. ROSE^{1,2}, P. CHAURAND^{1,2}, D. BORSCHNECK^{1,2}, E. DOELSCH⁴, F. ZIARELLI⁵, A. THILL^{2,6} AND J.Y. BOTTERO^{1,2}

¹CEREGE, Aix Marseille University CNRS IRD CdF, Europole de l'Arbois, BP80, 13545 Aix en Provence, France (masion@cerege.fr)

- ²International Consortium for the Environmental Implications of Nanotechnology iCEINT, Europole de l'Arbois, 13545 Aix-en-Provence, France
- ³Geological & Environmental Sciences, Green Earth Sciences, 367 Panama Street, Stanford University, Stanford, CA 94305-2115, USA
- ⁴CIRAD, UPR Recyclage et risque, 34398 Montpellier, France
- ⁵Fédération de Recherche des Sciences Chimiques de Marseille, ave Escadrille Normandie Niemen 13397 Marseille, France.
- ⁶CEA Saclay, IRAMIS, LIONS, 91191 Gif sur Yvette, France.

The extent to which nanoparticles may impact the environment is largely dependent on their mobility in soils and in surface and groundwater systems. Size and aggregation/dispersion state are obvious parameters, whose determination (and prediction) requires a detailed knowledge of the surface chemistry of the nanophases and their reactivity with a variety of organic and inorganic nutrients and pollutants, taking into account possible competition between ligands. Hydrophobicity is another important parameter to take into consideration. The hydrophobicity can be either intrinsic (e.g. fullerene) or acquired (intentional coating during manufacturing or reaction with natural organics), and this hydrophobic quality may evolve during transport in the environment. Here we examine the mechanisms by which even minor changes in the physico-chemical conditions may results in drastic modifications of the ability of nanoparticles to be transported in environmental systems. The present work will focus on commercially available products, viz. C₆₀, TiO₂ and CeO₂ based nanomaterials, as well as naturally occurring nanostructured alumino-silicates. The transformations at the surface of this nanomaterials and the structure and mobility of the resulting phases have been examined by several analytical tools (TEM, X-ray absorption and scattering, NMR...) so as to obtain an observation scale spanning over at least three orders of magnitude. The results underline the difficulty to obtain a global view of the phenomena due to competing mechanisms.