

## Structure and modification of iron-oxide surfaces during reaction with dissolved iron

T.P. TRAINOR<sup>1</sup>, C.S. ICEMAN, K.S. TANWAR<sup>1</sup>,  
S.C. PETITTO<sup>1</sup>, P.J. ENG<sup>2</sup>, S. MASON<sup>3</sup> AND A.M. CHAKA<sup>3</sup>

<sup>1</sup>Department of Chemistry and Biochemistry, University of Alaska Fairbanks, Fairbanks, AK 99775-6160, USA  
(fftp@uaf.edu, fncr@uaf.edu, ftkjt@uaf.edu, fncsp@uaf.edu)

<sup>2</sup>Consortium for Advanced Radiation Sources, University of Chicago, Chicago, IL 60637, USA  
(eng@cars.uchicago.edu)

<sup>3</sup>National Institute of Standards and Technology,  
Gaithersburg, MD 20899, USA (anne.chaka@nist.gov,  
sara.mason@nist.gov)

The structure and composition of iron (hydr)oxide surfaces is influenced by solution conditions, particularly the redox state (e.g. aqueous Fe(II)/(III) activity) of the contacting solution. The structural variations in turn may influence the overall reactivity of the mineral-water interface with respect to binding of trace dissolved constituents. The present study is focused on the structure of hematite (0001) and (1 $\bar{1}$ 02) surfaces during reaction with aqueous Fe(II) using synchrotron based crystal truncation rod (CTR) X-ray diffraction. The results show surface bound Fe occupies crystallographic lattice sites on both surfaces with average Fe-O bond lengths of surface bound Fe characteristic of Fe(III). However, the overall coordination chemistry of surface functional groups remain distinct on the different surfaces and suggest different pathways for sorption, resembling incipient growth, that are distinct based on the crystallographic orientation of the substrate. The experimental observations to date will be discussed in conjunction with the results of periodic density functional theory (DFT) calculations. Calculations have been performed on super-cells with variable degree of surface site occupancy, providing surface energies and optimized geometries that are directly compared with experimental structures. We will also discuss recent work focused on the binding of aqueous Pb(II) to the modified surfaces as a probe of surface reactivity.

## Speciation of anthropogenic radionuclides in Arctic marine environment

A. TRAVKINA AND O. STEPANETS

Arctic Basin plays a very important role in preservation of ecological equilibrium on earth. The sources of its radionuclide contamination are very different. They could be local like direct dumps including industrial pollution and operation of vehicles and global ones like Northern hemisphere fallout or trans-boundary transfer.

One of the most important sources of radioactive pollution of Russian Arctic area is the Great Siberian Rivers runoff. PO Mayak is very well-known reprocessing plant, which can be very dangerous contaminator due to connection with Kara Sea throw rivers Techa-Iset-Tobol-Ob water system. On the other hand functioning of Krasnoyarsk mining industrial plant leads to radionuclide contamination of Yenisey river and as a consequence to pollution of Arctic Basin.

In order to study geochemical behaviour of man-made radionuclides in marine environment determinations of plutonium isotopes, <sup>137</sup>Cs and <sup>90</sup>Sr activities in suspended matter and colloidal forms have been carried out. <sup>240</sup>Pu/<sup>239</sup>Pu isotopic ratios were studied to separate various sources of radioactive contamination.

Summarized the obtained results, it has shown a significant difference in behaviour and migration pathways of plutonium, caesium and strontium isotopes in the system river-estuary-adjunct part of the sea.