Investigation of the Pyrite (100) Surface Structure in Dry Ambient Conditions with GIXRD

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Pyrite (FeS_2) surface reactions play an important role in many geological and environmental processes, e.g. acid mine drainage, contaminant sorption or heterogeneous catalysis. The most exposed surface of pyrite, the (100) surface, was object of previous investigations with various experimental techniques, mostly carried out in UHV-conditions, such as STM and LEED (Rosso et al. 1999) or XPS (von Oertzen et al. 2005). These experiments reported a stable, unreconstructed and bulk-terminated surface structure of the clean (100) surface. Experimental studies of the pyrite surface in environmental conditions are scarce, an AFM investigation of lipid layers on the (100) pyrite surface was reported previously (Zhang et al. 2006). However, recent investigations of calcite and fluorapatite surfaces at ambient conditions with grazing incidence X-ray diffraction (GIXRD) showed that GIXRD is a useful method for the analysis of mineral surfaces and mineral-organic interfaces in environment conditions (Magdans et al. 2006, Pareek et al. 2007). Here we report about a GIXRD experiment on the pyrite (100) surface in dry N_2-atmosphere at room temperature and normal pressure, carried out at the beamline ID03 at the ESRF, Grenoble, France. The analysis of site occupation factors for the topmost surface atom species shows a S-deficiency for the upper S-atom of the disulfide ions protruding from the surface. The site occupancies for the surface Fe- and the lower S-atoms were refined to full occupancy. The analysis of the surface relaxation is still in progress. The experimental data yield no evidence for a surface reconstruction.

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