Introduction:

Chemical reactions at the (100)-pyrite surface play an important role in many environmental, geological and chemical processes. To understand these processes it is of essential importance to understand the adsorption properties of pyrite to organic molecules and water. 

In this study the adsorption model of water at the (100)-pyrite surface near iron and sulphur defect sites is presented and compared to experimental results. We present molecular dynamic simulations using the forcefield COMPASS. The simulations were carried out with the program package Materials Studio 5.0, particularly the program “Forcite”, from Accelrys Inc. A surface cell, that was determined from GIXRD previously, was used as a start model for the simulations.

Methods:

- Materials Studio 5.0
- Forcite
- Forcefield simulations [COMPASS]
- Molecular dynamic (MD) and mechanic (MM) simulations
- Dynamic calculations for H$_2$O-molecules at defect sites

- iron defect sites
- sulphur defect sites
- three layer defect at the surface slab

Previous GIXRD-results:

CTB-scans (crystal truncation rod) were carried out at the ESRF (2003) using GIXD (see Fig.2). The (100)-pyrite-water interface was determined using the program Studio. The cell is bulk terminated and shows only small relaxations, no reconstruction and an increasing amount of adsorption on the surface from the bottom to the topmost layer of the surface slab.

Surface structure of pyrite

Fe & S defect surface structure

Adsorption model for H$_2$O

dynamic H$_2$O-adsorption system

The dynamic H$_2$O adsorption process at a three layer defect surface

1. Sulphur defect sites
2. Iron defect sites
3. Multiple layer defects

The combination of GIXRD and forcefield simulations is a powerful method to determine mineral-water interfaces and periodical ordered dynamic systems.

Outlook:

- adsorption model of different organic molecules in aqueous solution at the (100) pyrite surface
- adsorption models at different pyrite surfaces
- adsorption near surface steps

Dynamic behaviour of H$_2$O-molecules at a three layer defect surface

The video shows the dynamic behaviour of H$_2$O-molecules at a three layer defect surface.

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