# XRD, XPS, and raman data collected from 2013 to 2017 (INSPIRE Pyrite)

**Website**: https://www.bco-dmo.org/dataset/684649
**Data Type**: experimental
**Version**: 1
**Version Date**: 2017-03-13

**Project**
» INSPIRE Track 1: Microbial Sulfur Metabolism and its Potential for Transforming the Growth of Epitaxial Solar Cell Absorbers (INSPIRE_Pyrite)

| Contributors | Affiliation | Role |
|---|---|---|
| Girguis, Peter | Harvard University | Principal Investigator |
| Clarke, David | Harvard University | Co-Principal Investigator |
| Guan, Xiaofei | Harvard University | Contact |
| Ake, Hannah | Woods Hole Oceanographic Institution (WHOI BCO-DMO) | BCO-DMO Data Manager |

**Abstract**
XRD, XPS, and raman data collected from 2013 to 2017 (INSPIRE Pyrite)

## Table of Contents



## Coverage

**Temporal Extent**: 2013 - 2017

## Dataset Description

X-ray diffraction (XRD) pattern of the iron substrate sample after electrodeposition.

X-ray photoelectron spectroscopy (XPS) of the synthetic mackinawite deposit for (a) Fe 2p spectrum and (b) S 2p spectrum, confirming the deposited sulfide is mackinawite and not stoichiometric pyrite.

Raman spectrum of iron pyrite nano-particles synthesized by the hot injection method at 200 deg C.

### Methods & Sampling

**X-ray diffraction (XRD):**

An X-ray diffractometer (Bruker, D2 phaser) with a conventional Theta-2theta diffraction geometry was used to determine the crystalline phase of the deposit on an iron substrate.

**X-ray photoelectron spectroscopy (XPS):**

The elements (Fe and S) present in the thin film deposit and their chemical bonding states were identified by using XPS (K-Alpha, Thermo Scientific, MA). The spectra were collected using a 400 um spot size and 20 eV pass energy from an Al source after Ar plasma sputtering to remove any surface contamination.

**Raman spectrum data:**

The Raman spectrum of the iron pyrite nanoparticles were collected by using a LabRAM Aramis Raman system (Horiba Jobin Yvon, NJ) with laser excitation at 532 nm.

### Data Processing Description

**BCO-DMO Data Processing Notes:**

- compiled multiple spreadsheets of data into one table.
- replaced blank cells with nd.
- reformatted column names to comply with BCO-DMO standards.

[ table of contents | back to top ]

## Data Files

| File |
| --- |
| **XRD_XPS_raman.csv** (Comma Separated Values (.csv), 216.81 KB) MD5:b06f36625aef2f6e3adb1a8eda996c25<br>Primary data file for dataset ID 684649 |

[ table of contents | back to top ]

## Parameters

| Parameter | Description | Units |
| --- | --- | --- |
| data_type | Type of data described: XRD XPS or Raman1 and 2; Raman1 is the Raman spectrum of iron pyrite nano-particles; Raman2 is the Raman spectrum of an iron pyrite thin film formed on an iron pyrite substrate using the hot injection method. | unitless |
| theta2 | 2-Theta angle | degree |
| binding_energy | Binding energy of XPS | eV |
| intensity_type | Intensity measured for either Fe 2p or S 2p | unitless |
| raman_shift | Raman spectrum | centimeters |
| intensity | Raman spectrum and XRD intensity | arbitrary units |

[ table of contents | back to top ]

## Instruments

| | |
|---|---|
| **Dataset-specific Instrument Name** | LabRAM Aramis Raman system |
| **Generic Instrument Name** | Raman Microscope |
| **Dataset-specific Description** | Used to analyze Raman spectrum |
| **Generic Instrument Description** | The Raman microscope is a laser-based microscopic device used to perform Raman spectroscopy. The Raman microscope begins with a standard optical microscope, and adds an excitation laser, laser rejection filters, a spectrometer or monochromator, and an optical sensitive detector such as a charge-coupled device (CCD), or photomultiplier tube, (PMT). One example is the XploRA confocal Raman microscope (information from the manufacturer). |

| | |
|---|---|
| **Dataset-specific Instrument Name** | Microscope |
| **Generic Instrument Name** | X-Ray Microscope |
| **Dataset-specific Description** | Used to measure xray defraction |
| **Generic Instrument Description** | An X-ray microscope uses electromagnetic radiation in the soft X-ray band to produce images of very small objects. The resolution of X-ray microscopy lies between that of the optical microscope and the electron microscope. |

[ table of contents | back to top ]

---

## Deployments

**Girguis_2013**

| | |
|---|---|
| **Website** | https://www.bco-dmo.org/deployment/684563 |
| **Platform** | lab Harvard |
| **Start Date** | 2013-09-01 |
| **End Date** | 2017-08-01 |
| **Description** | Peter Girguis' lab at Harvard University |

[ table of contents | back to top ]

---

## Project Information

**INSPIRE Track 1: Microbial Sulfur Metabolism and its Potential for Transforming the Growth of Epitaxial Solar Cell Absorbers (INSPIRE_Pyrite)**

This INSPIRE award is partially funded by Biological Oceanography Program in Division of Ocean Sciences, in the Directorate of Geosciences; the Electronic and Photonic Materials Program in the Division of Materials Research, Directorate of Mathematical and Physical Sciences.

A simple idea motivates this project: By characterizing the mechanisms underlying pyrite film deposition by subsurface microbes living at hydrothermal vents, can approaches be developed to controllably grow high-purity pyrite films that could be used to produce low-cost photovoltaic solar cells? Recent in situ studies at hydrothermal vents have found "subsurface" microbes associated with the deposition of large crystalline metal sulfides (up to 1.1 millimeters), including iron pyrite. In laboratory incubations, vent microbes specifically deposited pyrite (FeS2), devoid of Zn, Cu and other metals that were abundant in the liquid media. Abiotic incubations did not exhibit this specificity. The investigators hypothesize that, in situ, microbes deposit pyrite via a number of potential processes, including a physiological process called extracellular electron transfer (EET), wherein microbes shuttle electrons to/from minerals. In situ, EET-enabled microbes may use conductive minerals to electrically access oxidants, and deposit pyrite on these surfaces. Vents are thus natural bioelectrochemical cells, which grow metal sulfides via microbial and abiotic electrochemical processes, though the details and mechanisms remain to be determined. This project is aimed at elucidating the mechanisms underlying microbial FeS2 pyrite bio-deposition, and assessing how microbes might be used to deposit epitaxial films for solar cells absorbers. FeS2 pyrite has been identified as prospective low cost solar absorbers because of their abundance, suitable band-gap (~0.95 eV) and high optical absorbance. Microbial pyrite film deposition at lower temperatures (<100 C) might offer a radically new, low cost approach to creating large area PV solar cells. Nothing is currently known about the mechanisms underlying microbial pyrite growth, though the large crystal sizes suggest epitaxial deposition is favored over re-nucleation implying that, once nucleated, epitaxial growth can occur. A series of experiments using natural vent microbial communities and isolates will be conducted to determine: A) environmental factors that influence bio-deposition; B) potential molecular mechanisms; C) the microstructural and electrical properties of these films; and D) whether bio-deposition by single species or consortia yields films of highest purity, size and homogeneity.

The project is both highly-integrated and transformative. It is relevant to our understanding of microbial sulfur cycling, as little is known about how microbes mediate crystalline pyrite formation and the degree to which this influences sulfur isotope geochemistry. Molecular studies will be used to interrogate relevant microbial metabolic processes and constrain the possible mechanisms of pyrite film growth, which is critical to advancing our ability to grow FeS2 films for device applications. Understanding the effects of substrate crystallography and electrical conductivity on the growth morphology will further inform our knowledge of microbial pyrite deposition. Notably, this research differ from existing biomimetic approaches. The studies are not focused on crystal growth via tethered peptides or synthetic extracellular matrices. Rather, they aim to advance our understanding of natural biodeposition, use the insights gained to grow pyrite materials and devices.

[ table of contents | back to top ]

## Funding

| Funding Source | Award |
|---|---|
| NSF Division of Ocean Sciences (NSF OCE) | OCE-1344241 |

[ table of contents | back to top ]