

# 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
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## Abstract

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

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## Coverage

**Temporal Extent:** 2013 - 2017

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## 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.

## Acquisition Description

### **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.

## 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.

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## 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

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## Instruments

<b>Dataset-specific Instrument Name</b>	LabRAM Aramis Raman system
<b>Generic Instrument Name</b>	Raman Microscope
<b>Dataset-specific Description</b>	Used to analyze Raman spectrum
<b>Generic Instrument Description</b>	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).

<b>Dataset-specific Instrument Name</b>	Microscope
<b>Generic Instrument Name</b>	X-Ray Microscope
<b>Dataset-specific Description</b>	Used to measure xray defraction
<b>Generic Instrument Description</b>	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.

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## Deployments

### Girguis\_2013

<b>Website</b>	<a href="https://www.bco-dmo.org/deployment/684563">https://www.bco-dmo.org/deployment/684563</a>
<b>Platform</b>	lab Harvard
<b>Start Date</b>	2013-09-01
<b>End Date</b>	2017-08-01
<b>Description</b>	Peter Girguis' lab at Harvard University

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## 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 (FeS<sub>2</sub>), 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 FeS<sub>2</sub> pyrite bio-deposition, and assessing how microbes might be used to deposit epitaxial films for solar cells absorbers. FeS<sub>2</sub> 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 (

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### Funding

Funding Source	Award
<a href="#">NSF Division of Ocean Sciences (NSF OCE)</a>	<a href="#">OCE-1344241</a>

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