X-ray diffractogram data collected from 2013 to 2017 (INSPIRE Pyrite project)

Website: https://www.bco-dmo.org/dataset/684634
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
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Abstract
X-ray diffractogram data collected from 2013 to 2017 (INSPIRE Pyrite project)

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Dataset Description

X-ray diffractogram data from INSPIRE track 1.

These data are associated with the paper:

Aude Picard, Amy Gartman, David R. Clarke, Peter R. Girguis, Sulfate-reducing bacteria influence the nucleation and growth of mackinawite and greigite, In Geochimica et Cosmochimica Acta, Volume 220, 2018, Pages 367-384, ISSN 0016-7037, https://doi.org/10.1016/j.gca.2017.10.006.

Methods & Sampling

X-ray diffraction data (2-Theta angle vs. intensity).

Data Processing Description

BCO-DMO Data Processing Notes:

- compiled multiple spreadsheets of x-ray diffraction data into one table.

- replaced blank cells with nd.
- reformatted column names to comply with BCO-DMO standards.

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Data Files

File
xray_defraction.csv (Comma Separated Values (.csv), 76.29 KB) MD5:1b1edce8f7194b5b90d8e63c3eac81a8 Primary data file for dataset ID 684634

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Related Publications

Picard, A., Gartman, A., Clarke, D. R., & Girguis, P. R. (2018). Sulfate-reducing bacteria influence the nucleation and growth of mackinawite and greigite. Geochimica et Cosmochimica Acta, 220, 367–384. doi:10.1016/j.gca.2017.10.006
Results

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Parameters

Parameter	Description	Units
experiment_type	Abiotic or biotic experiment description	unitless
angle_2Theta	2-Theta angle after 1 week of incubation	unitless
intensity	Intensity after 1 week of incubation	arbitrary unit

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Instruments

Dataset-specific Instrument Name	Microscope
Generic Instrument Name	X-Ray Microscope
Dataset-specific Description	Used to measure x-ray diffraction
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.

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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

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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 ($FeS2$), 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.

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Funding

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

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