Mineral Nucleation and Growth in Nanopores and Planar Interfaces

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NANOMATERIALS, INTERFACES, AND CONFINEMENT FOR ENERGY & THE ENVIRONMENT LABORATORY

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A little about me…

- **University:** Universidad Ana G. Mendez
- **Campus:** Gurabo
- **Major:** BS Mechanical Engineering.
- **Where I come from**: Puerto Rico

- **Associations: ASME** (American Society of Mechanical Engineers), **SAME** (Society of American Military Engineers)

- Projects undergrad:
- **CHRES Program**: Mineral Nucleation and Growth in Nanopores and Planar Interfaces
- **Design and Development:** of A Bio-Inspired Unmanned Underwater Vehicle Bases of Bio- Inspired Unmanned

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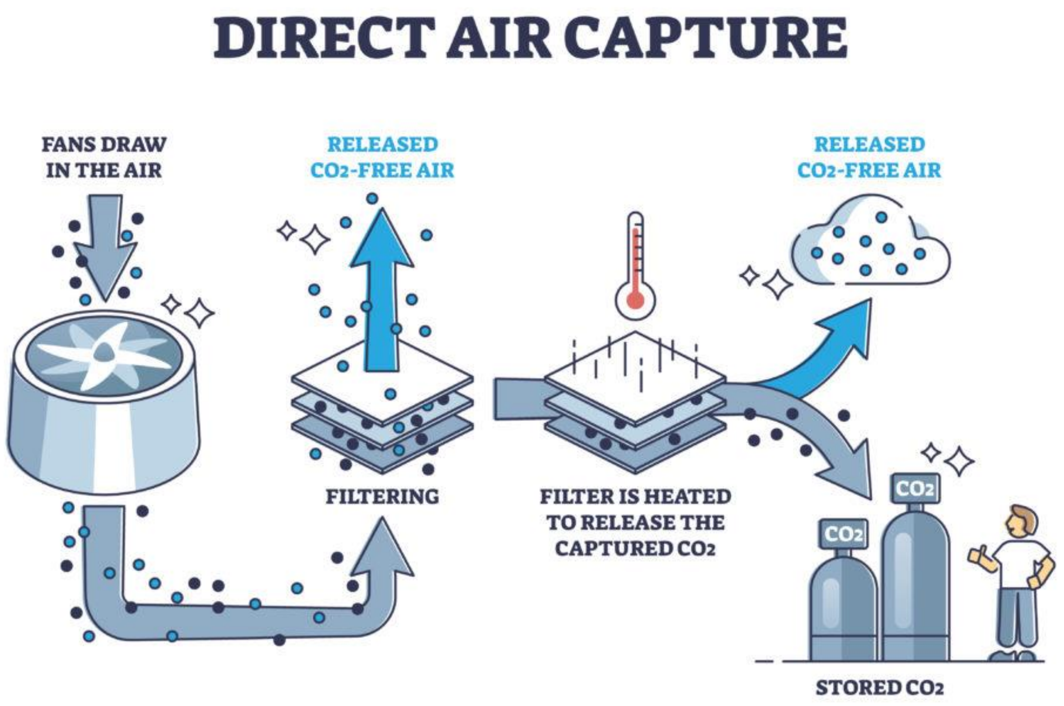
01

Background

What is Direct Air Capture (DAC)?

Direct air capture (DAC) is a technology and process that involves capturing carbon dioxide (CO2) directly from the atmosphere.

- Traditional carbon capture and storage (CCS) methods primarily target CO2 emissions at the source, like power plants or industrial facilities.
- In contrast, Direct Air Capture (DAC) technology focuses on removing CO2 directly from the ambient air.
- After capture, the CO2 can be processed and stored for later use.
- One of the storage methods includes sequestering the captured CO2 underground.
- Alternatively, captured CO2 can be utilized in various industrial processes, including the production of synthetic fuels.



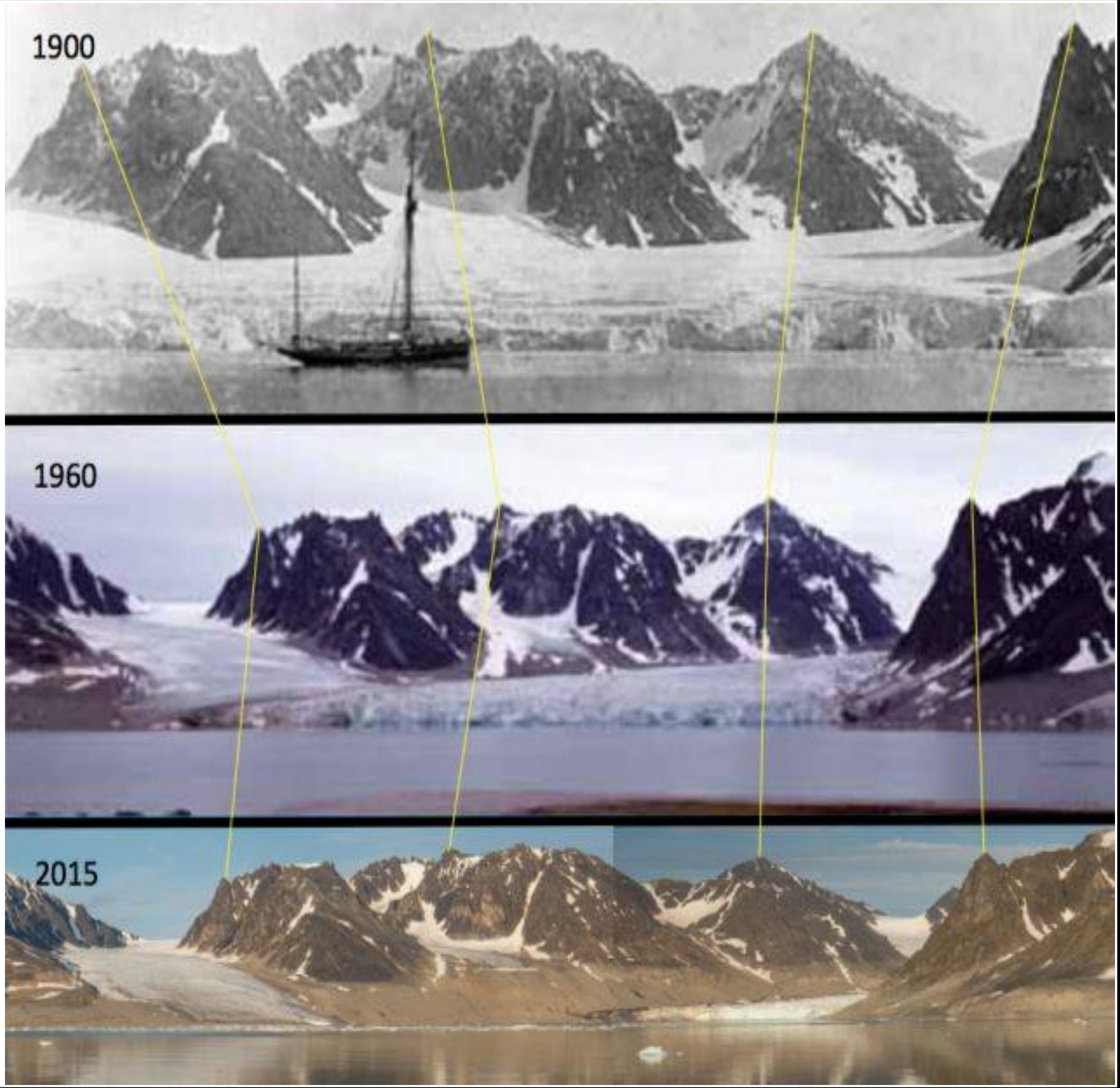
Picture: *Educational Carbon Dioxide Separation With Particle Absorption Filters Vector Illustration. Emissions Recycling Method*

Why is this project relevant?

This project revolves around Direct Air Capture methods and technologies, which is relevant due its potential to contribute addressing one of the most pressing challenges of our time - climate change mainly caused by increasing CO2 levels in the atmosphere.
Let's break down the importance of my project:

- Direct Air Capture (DAC) of CO2 using MgO
- Scale-Up and Cost-Efficiency gigaton scale at <$100/ton CO2
- Filling Knowledge Gaps in the reactivity of MgO

Photo: Andreas Weith



Waggonwaybreen glacier in Svalbard, Norway

MgO Looping for Direct Air Capture (DAC) of $CO2$

MgO looping, in the context of direct air capture (DAC) of CO2, refers to a process that involves using magnesium oxide (MgO) as a sorbent to capture CO2 from the atmosphere. The MgO sorbent is then regenerated through a calcination step to release the CO2, which can be sequestered or utilized for other purposes. The regenerated MgO is then reused in successive cycles for CO2 capture.

1. CO2 Capture

- MgO spread over ground, exposed to atmosphere
- Reacts with CO2 to form MgCO3: **MgO(s) + CO2(g) → MgCO3(s)**

2.Regeneration

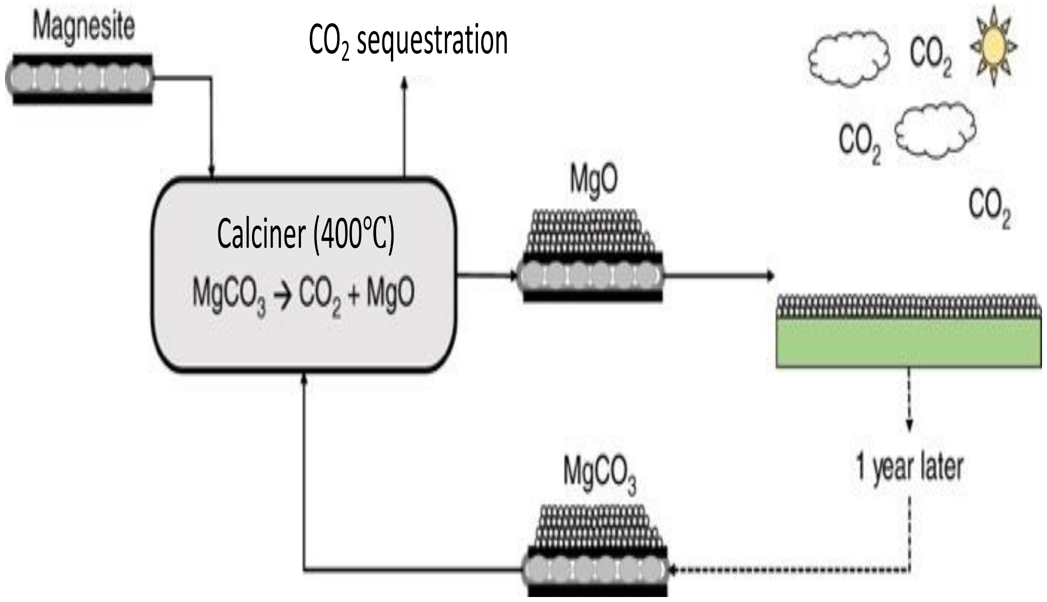
- Reacted material (MgCO3) subjected to calcination
- CO2 released, MgO regenerated: **MgCO3(s) → MgO(s) + CO2(g)**

3.CO2 Sequestration

- Separated CO2 sequestered or used for other purposes

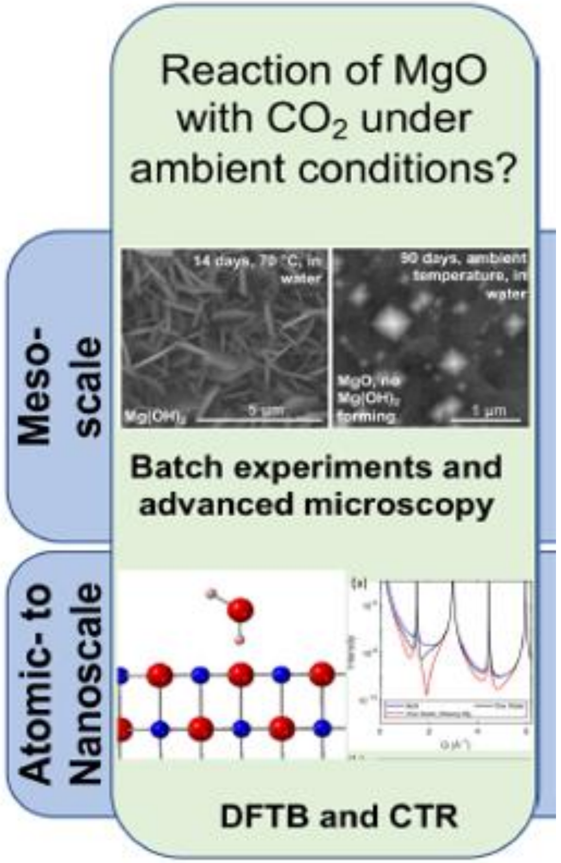
4.Reuse

- Regenerated MgO cycled back for CO2 capture



Picture: Envisioned MgO-based mineral looping process for direct air capture of CO_2 modified from McQueen et al., 2020, Nat. Commun.)

Overall Goal



Picture: Weber, Fundamental Mechanisms Driving Efficiency of CO2 Capture Using Mineral Looping

The goal of this project is to understand and control the chemical reactions that govern hydroxylation and carbonation processes during Direct Air Capture (DAC) of CO_2 using magnesium oxide (MgO).

- Understand MgO-CO2 reactions at ambient conditions and varying humidity.
- What are the mechanisms of reaction-induced fracturing during MgO hydroxylation?

Proposition: Oak Ridge National Laboratory

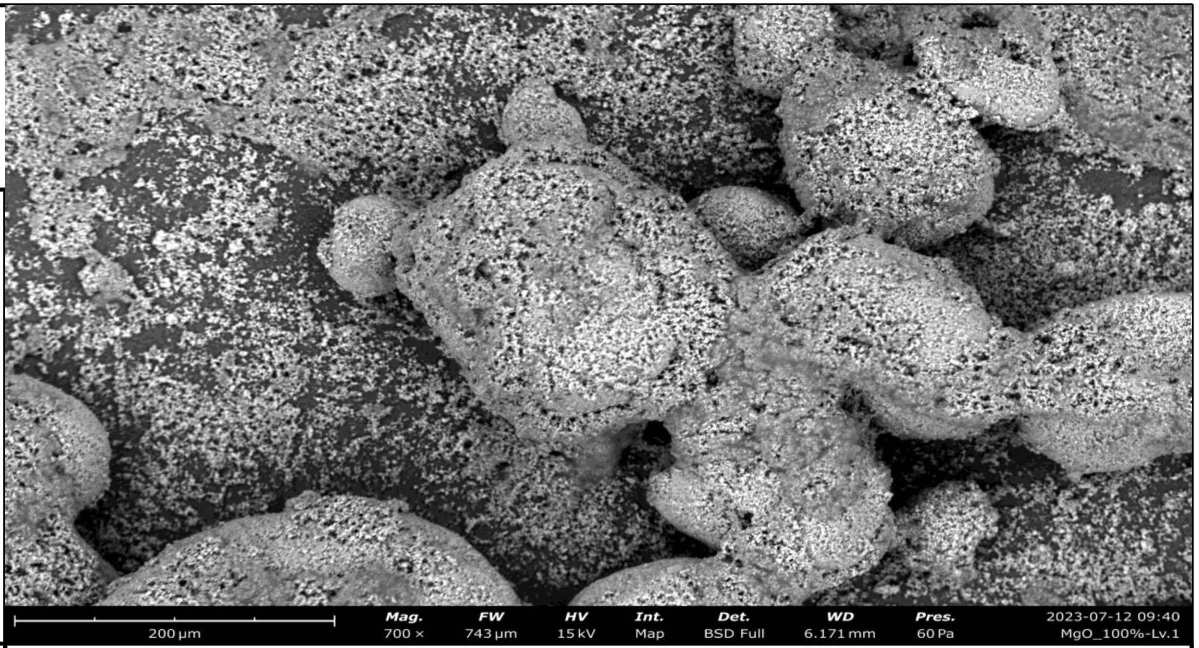
Principal Investigator: Administrative Point of Contact: Juliane Weber, Associate R&D Staff

02

Methodology

My project main focus is:

The focus of this project is to use x-ray scattering techniques to investigate how relative humidity (R.H.) influences the behavior of MgO



Aims to understand

How varying humidity levels affect three key aspects of MgO:

- Mass uptake
- Inter-grain pore structures
- Formation of crystalline phases

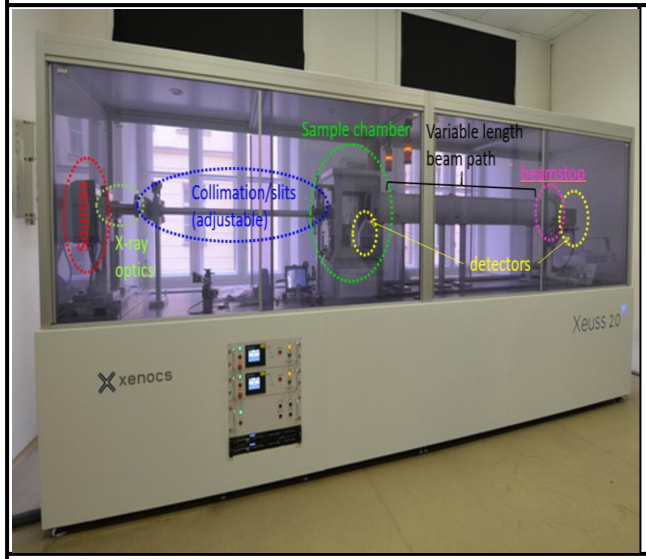
Variations of MgO Substrate

- Alfa Aesar
- BTC
- SKY

Specific surface area of MgO:

$321.3 \ \frac{m^2}{g^{-1}}$

Techniques

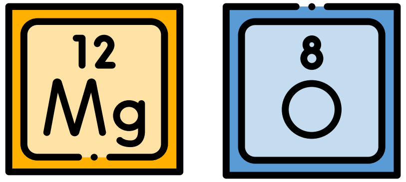


What is XEUSS ?

Xeuss is an X-ray scattering system. Is used for a variety of scientific and industrial applications, such as studying the properties of polymers, biological materials, and nanomaterials.

Why is it so important ?

The Xeuss systems, through their SAXS and WAXS capabilities, allows to examine the structural changes in Magnesium Oxide (MgO) under different humidity levels, which is crucial for optimizing its efficiency in carbon dioxide (CO2) capture.

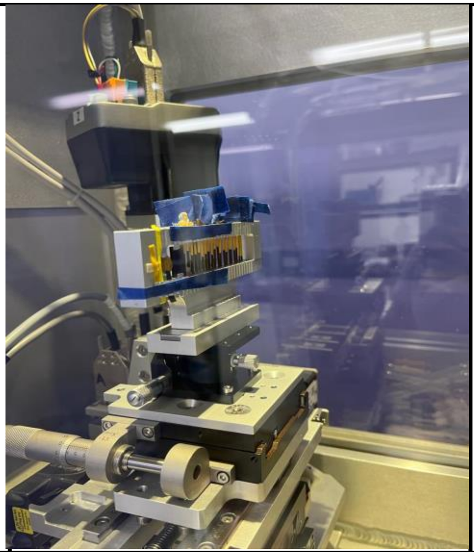


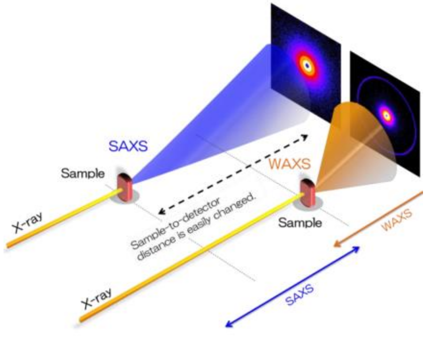
Picture: Xenocs Xeuss 2.0. (n.d.). Materials Growth & Measurement Laboratory. https://mgml.eu/assets/images/instruments/xeuss-main.jpg

Thechniques

SAXS

Used to probe the larger scale structure of materials (from about 1 nm to 100 nm). Ideal for studying features such as inter-grain pore structures.



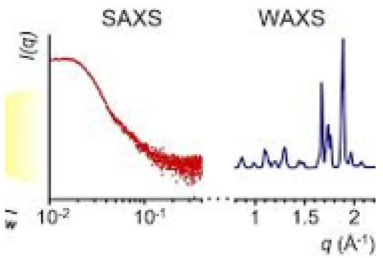


WAXS

A technique for analyzing smaller scale structures of materials (about 0.1 nm to 2 nm). Perfect for observing changes in crystalline structures.

How SAXS is applied in experiment

Used to examine the effect of R.H. on the inter-grain pore structures of MgO

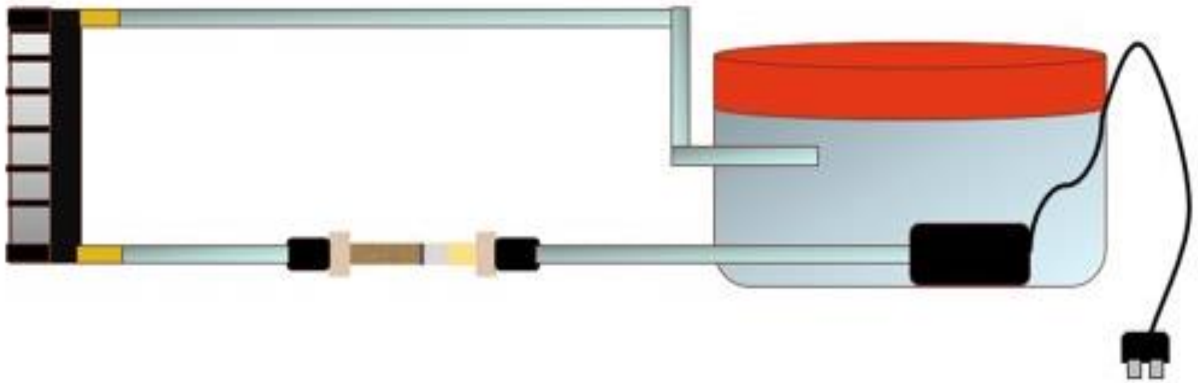


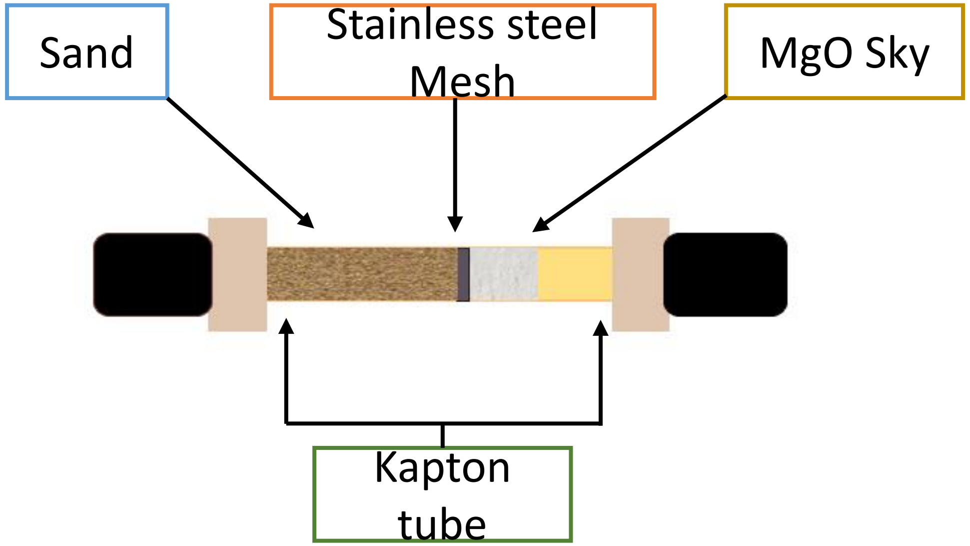
How WAXS is applied in the MgO study.

Used to observe the formation of different crystalline phases within MgO at varying levels of humidity

Picture: *Industrial SAXS / WAXS*. (n.d.). Rigaku. https://www.rigaku.com/sites/default/files/2018-11/isaxs.jpg

Set up for Insitu Experiment





During this experiment, we controlled the airflow by pumping it through the sample Kapton tube, which was filled with sand and a small stainless-steel mesh, to prevent the MgO from moving, which goes at the end.

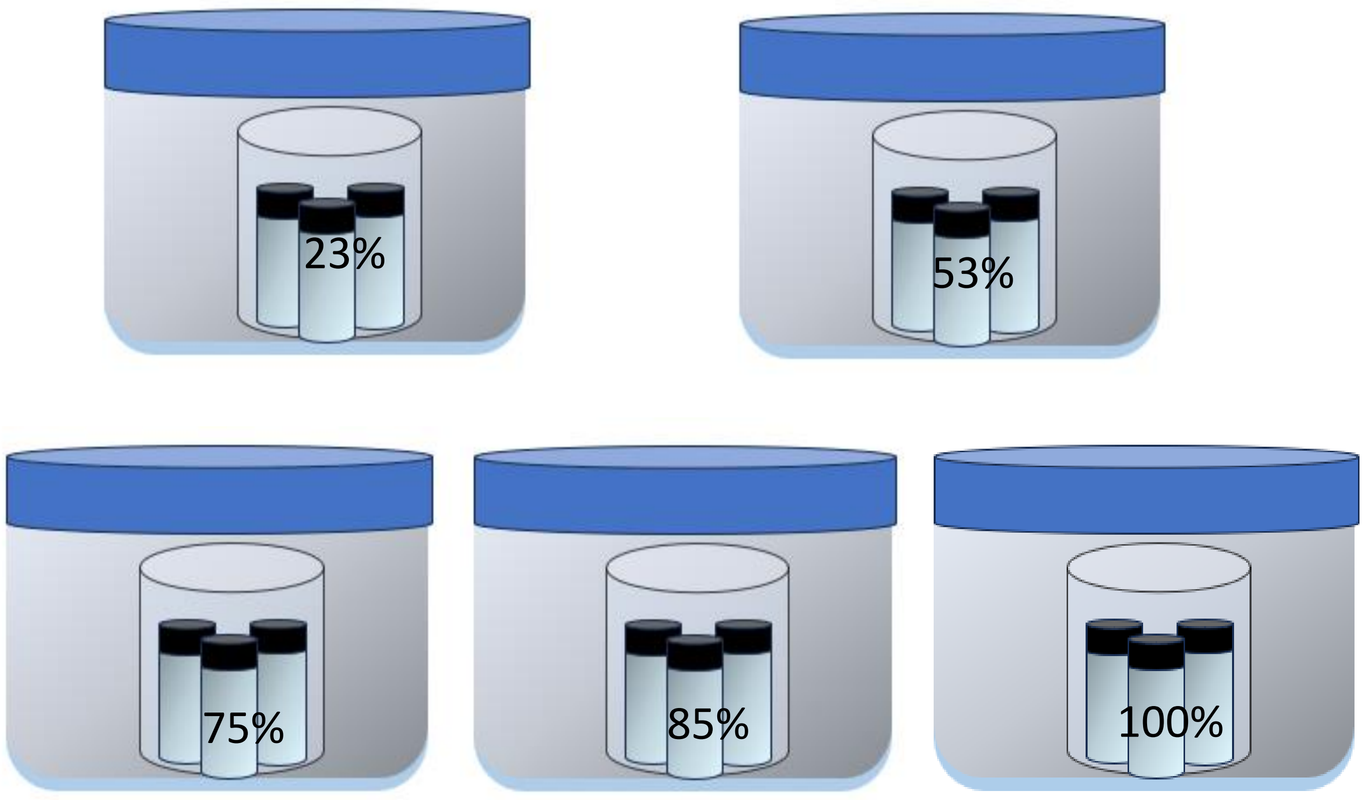
The used was Sky MgO was exposed to 100% humidity overnight and the expand of two for a duration of two weeks.

Humidity Control

The purpose of this setup was to ensuring Uniform Exposure:

By maintaining a constant airflow through the MgO-filled Kapton tube, you ensure that the MgO is uniformly exposed to the humid air. This is critical to ensure that all parts of the MgO sample experience the same conditions, allowing for consistent and reliable experimental results.

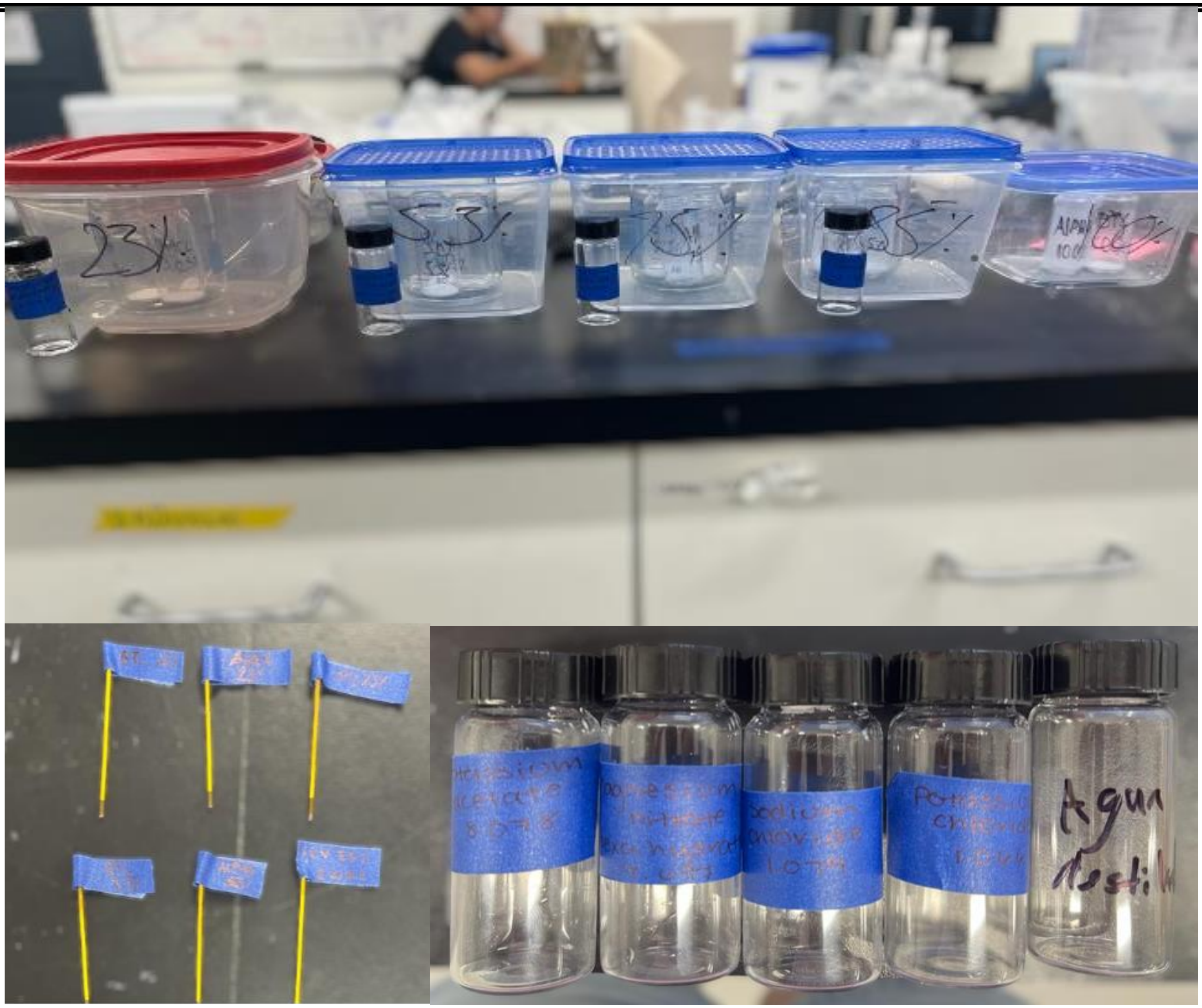
Set up for Exsitu Experiment



In this experiment, three distinct types of Magnesium Oxide (MgO) were systematically exposed to a variety of relative humidity conditions within a Tupperware container. These conditions were facilitated by five specific salt solutions, each inducing a distinct level of relative humidity.

- Potassium Acetone 23%
- Magnesium Nitrate 53%
- Sodium Chloride 75%
- Potassium Chloride 85%
- Deionized Water 100 %
- 0.3g of MgO in each container

Humidity Control



Purpose of Using a Container for MgO Exposure:

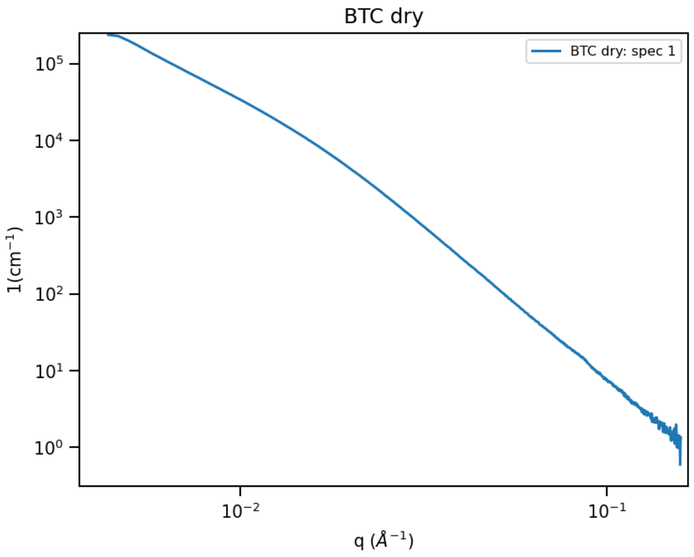
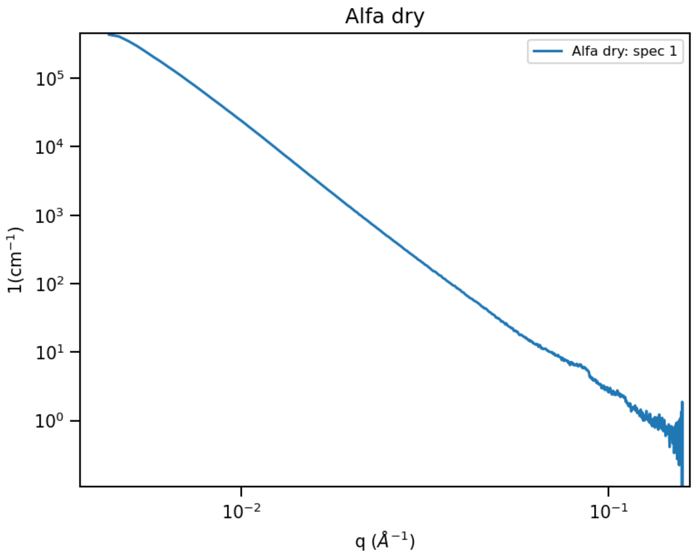
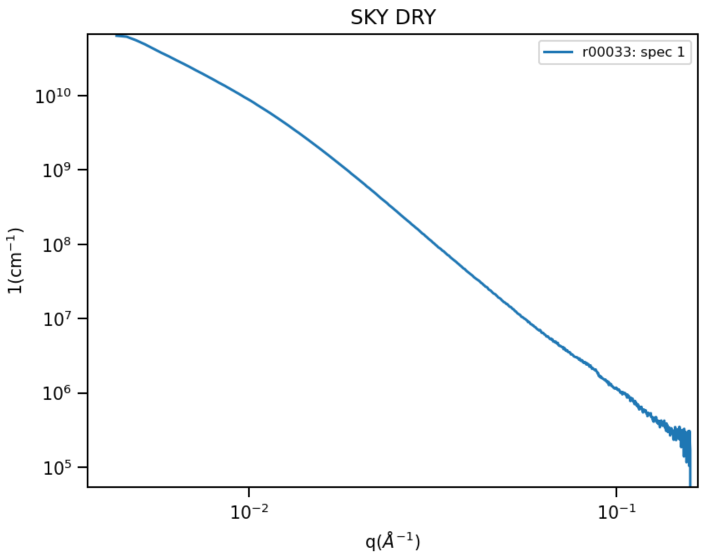
Controlled Environment: The container provides a controlled setting where MgO samples are exposed to specific relative humidity conditions, ensuring reproducibility and consistency in the experiment.

Systematic Exposure: The container enables systematic exposure of MgO to varying relative humidity levels induced by distinct salt solutions, facilitating organized comparison and analysis.

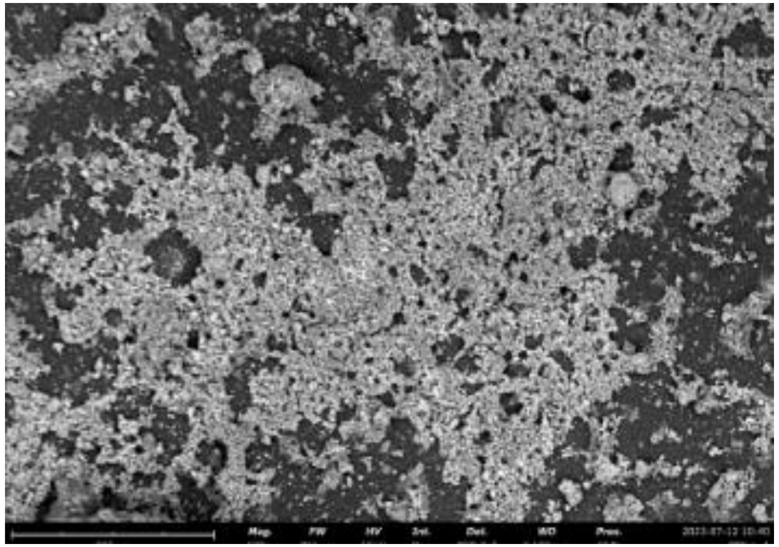
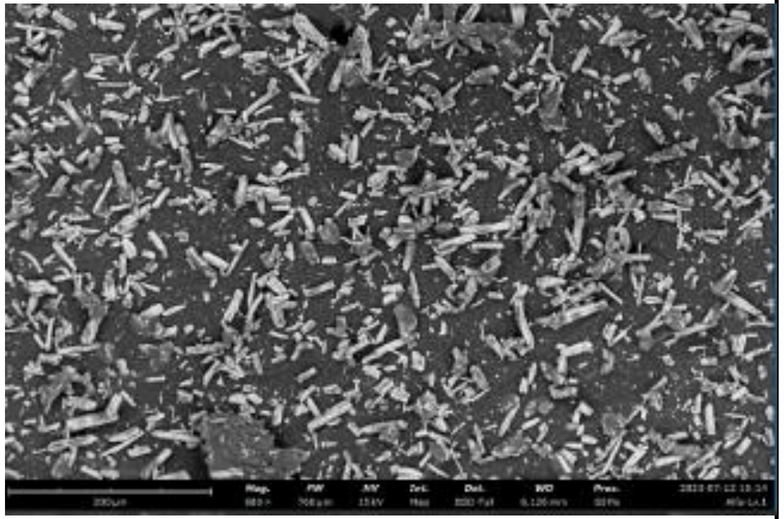
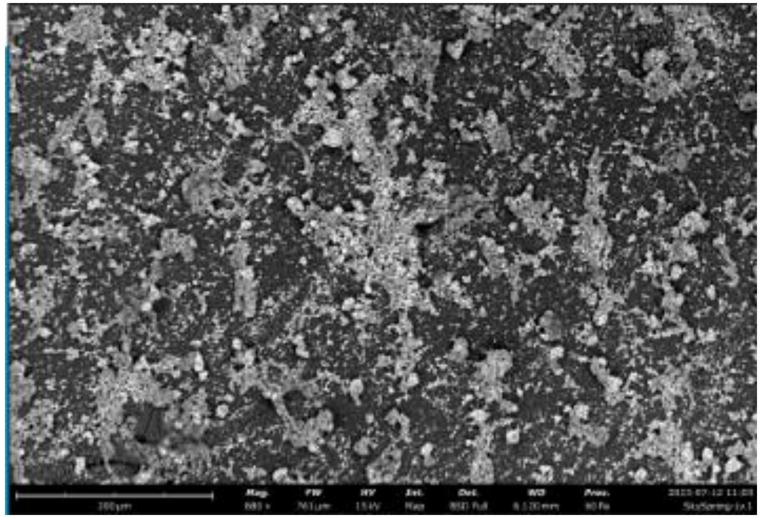
03

Graphs

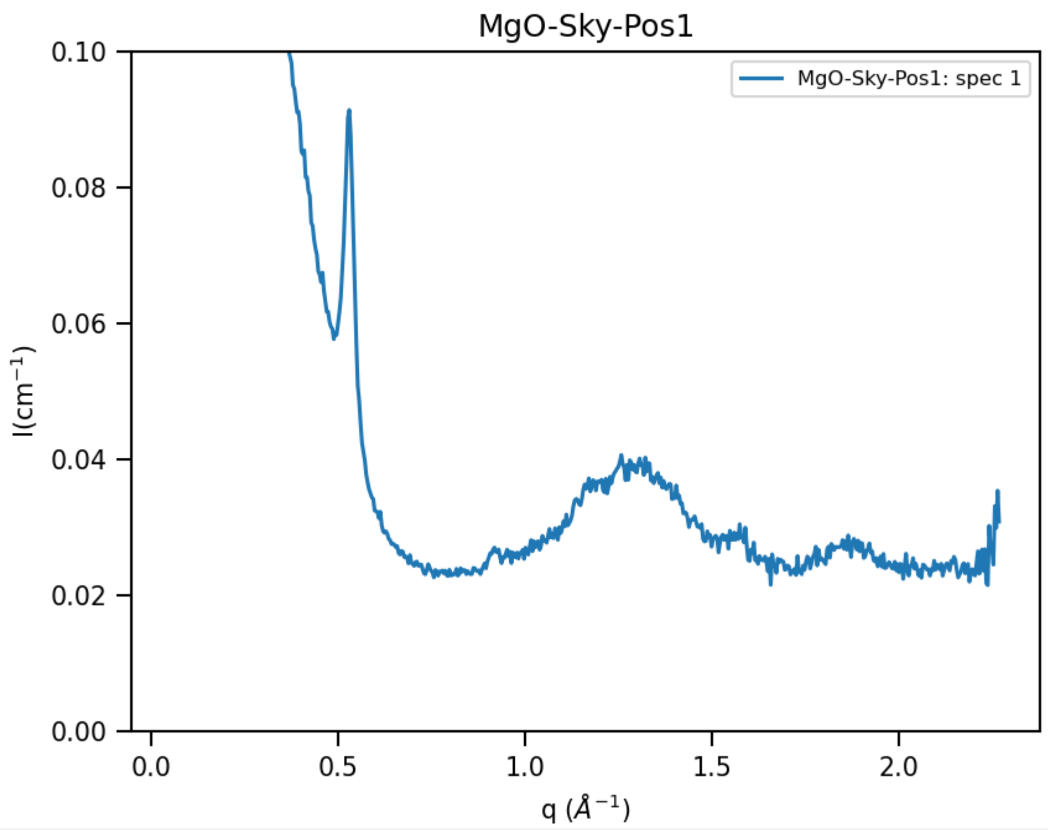
Graphs of all 3 Dry MgO

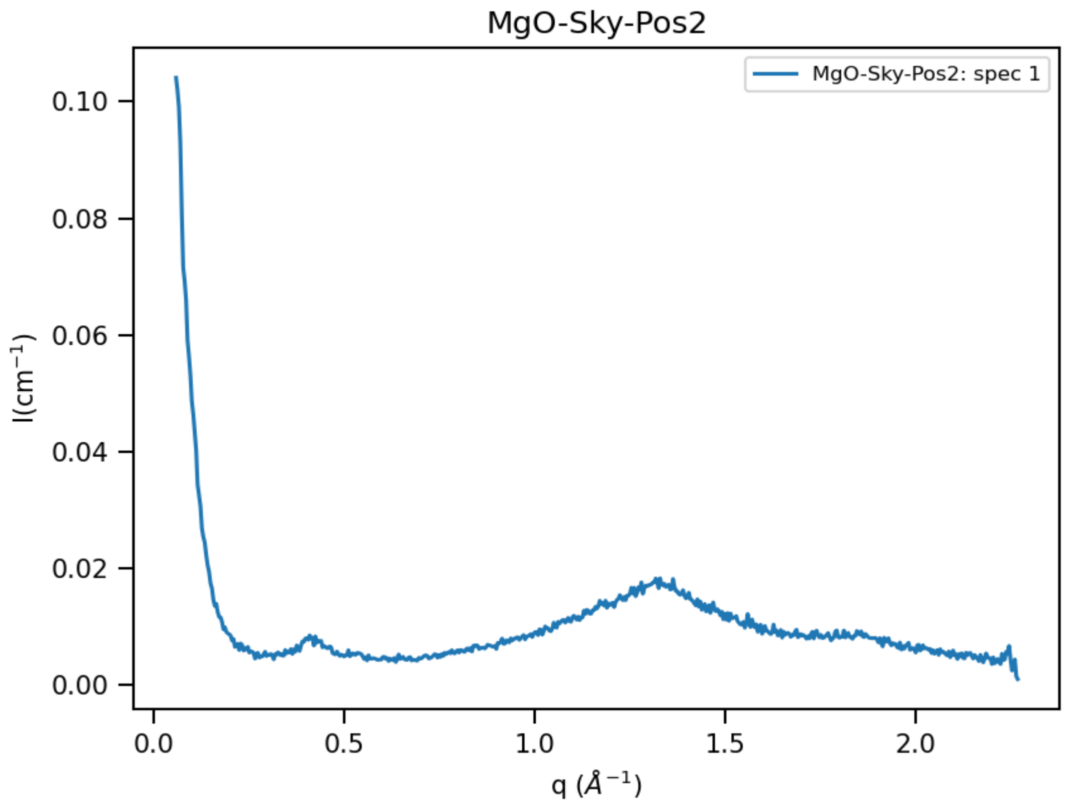
BTC	Alfa	SKY
		

Graphs of all 3 Dry MgO

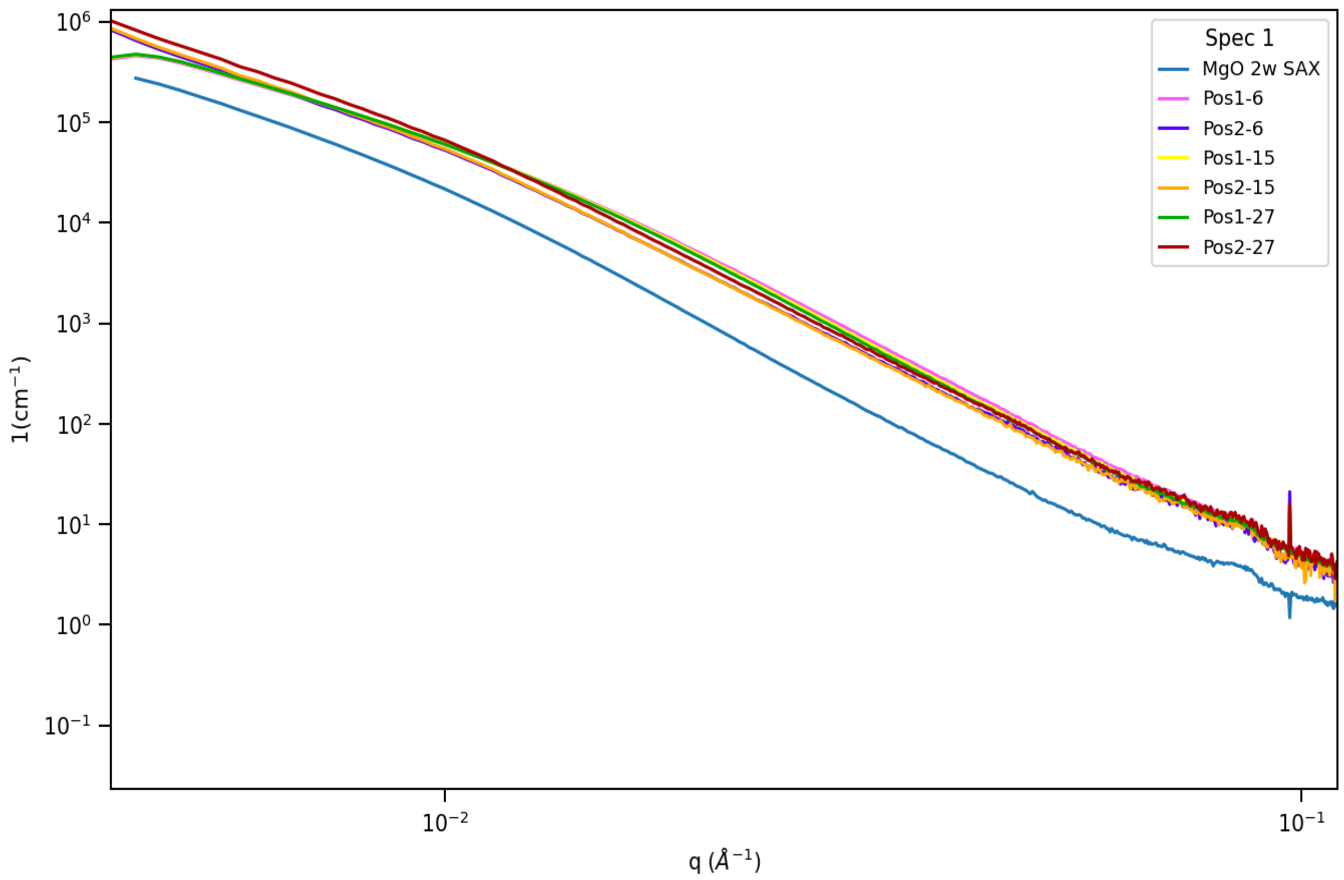
BTC	Alfa	SKY
		
Seems to be accrued over specific areas, giving certain perspective of height and deep inside relatively narrow spaces.	The magnesium isn't gathered as spots and strays of powders but as dispersed microscopic rods like geometrical prisms	Like BTC seems to be accrued over specific areas

MgO SKY 2Weeks Exposure In-situ WAXS Scans



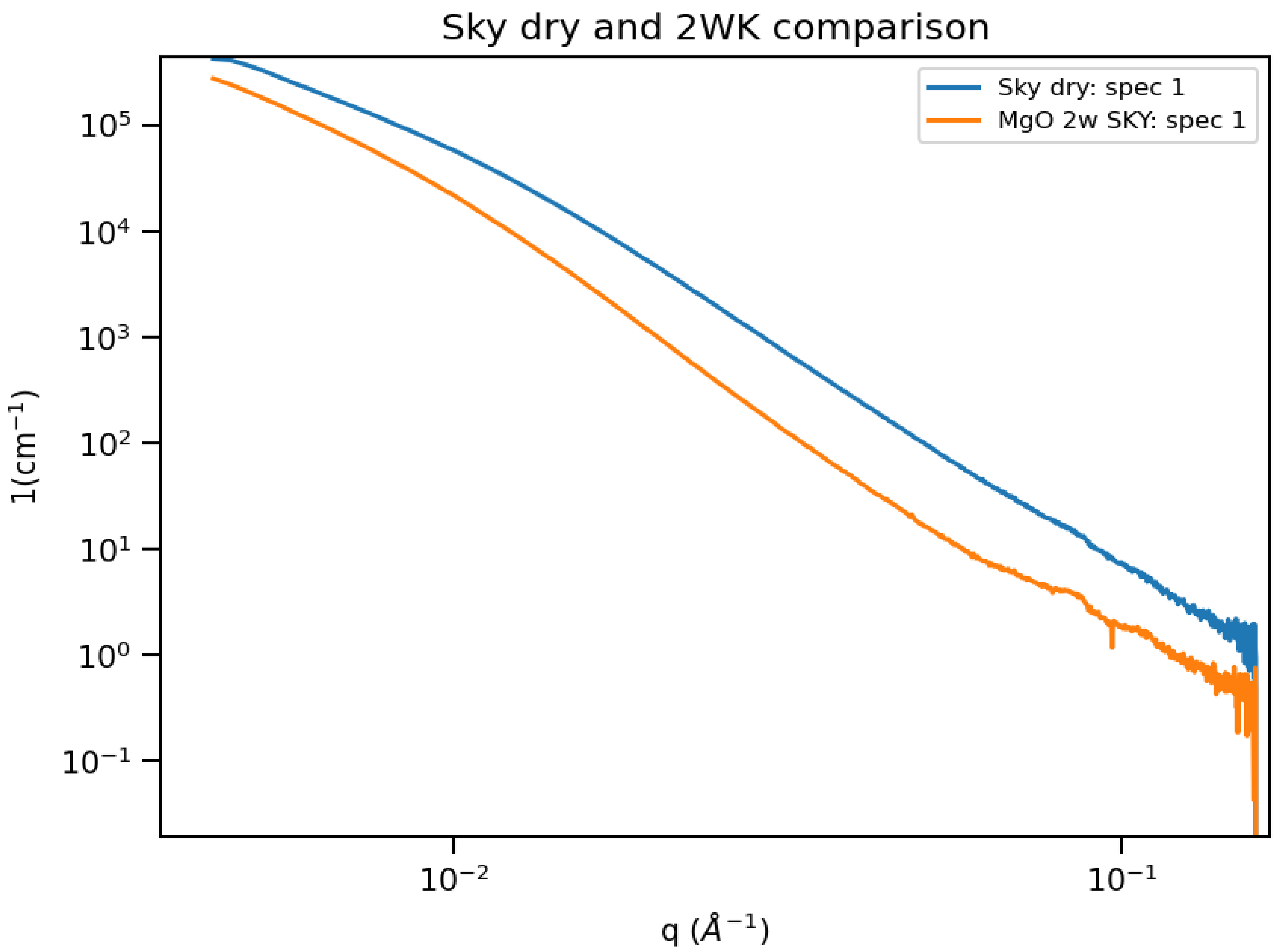


Comparison MgO SKY Overnight Exposure and 2Week Exposure SAXS



You can notice that MgO Sky has a lower intensity after two weeks of exposure.

Comparison MgO SKY Dry and 2Week Exposure SAXS



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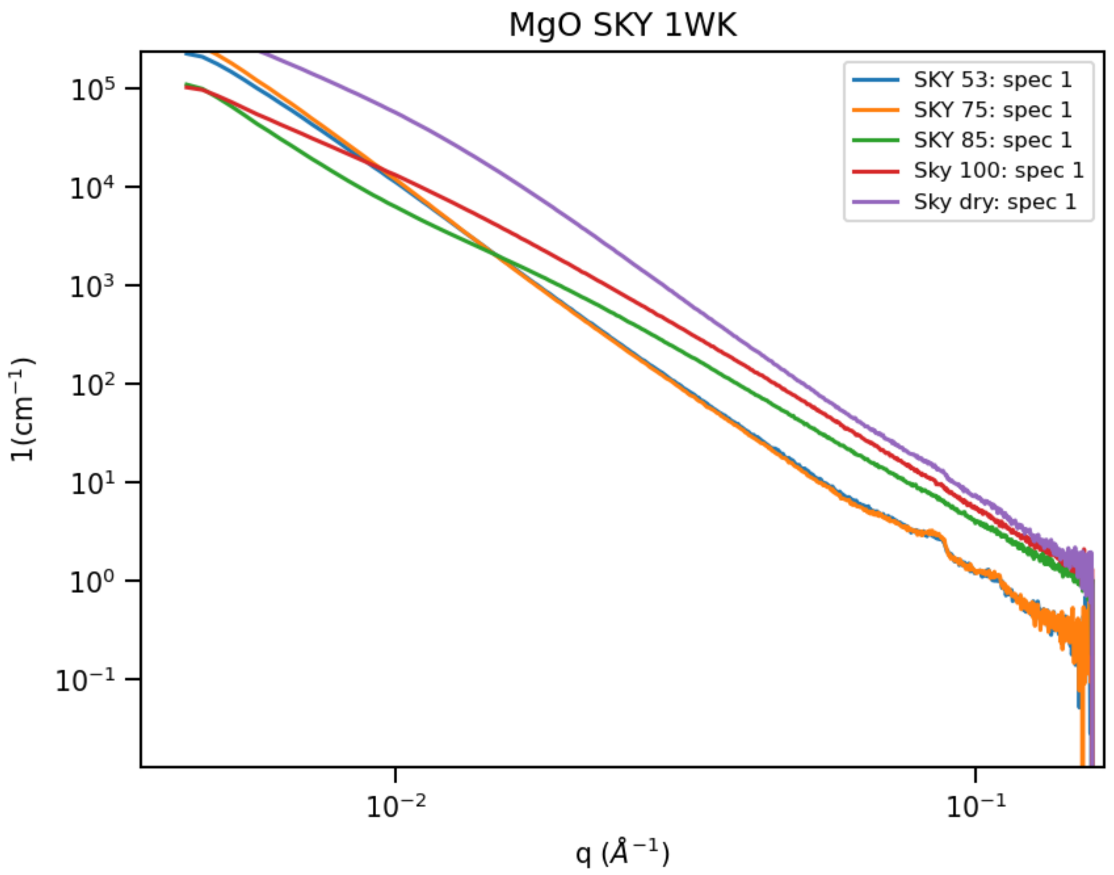
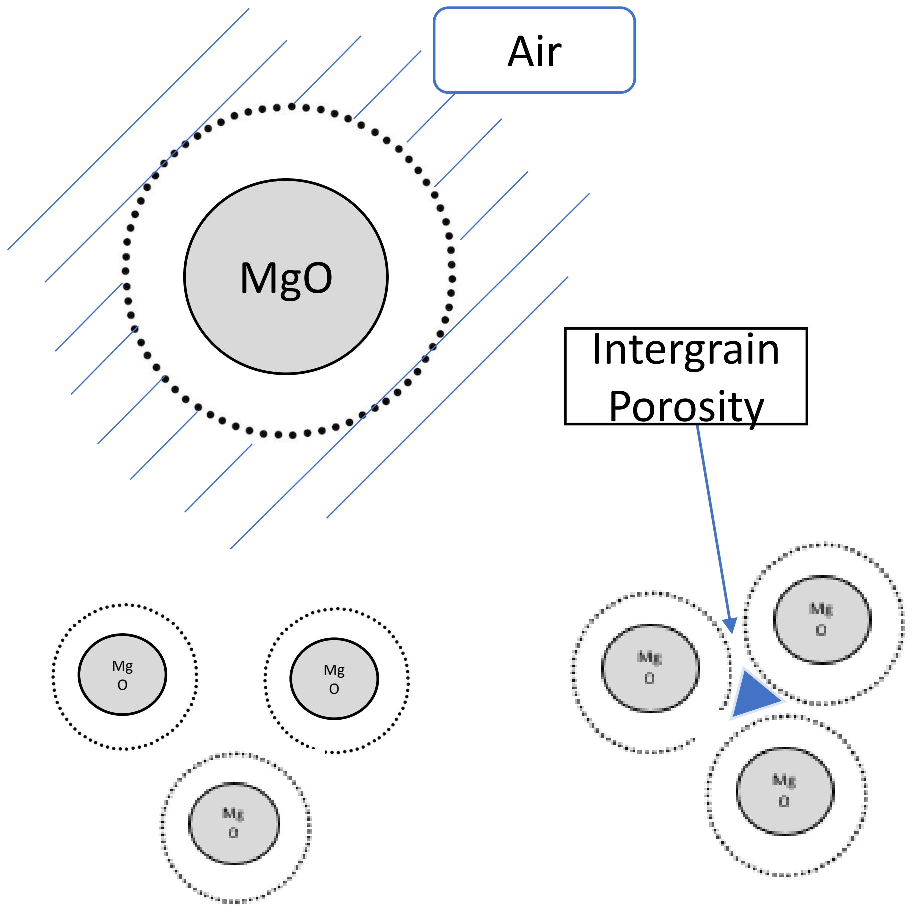
MgO 1 Week Exposure Ex-situ SAXS Scans

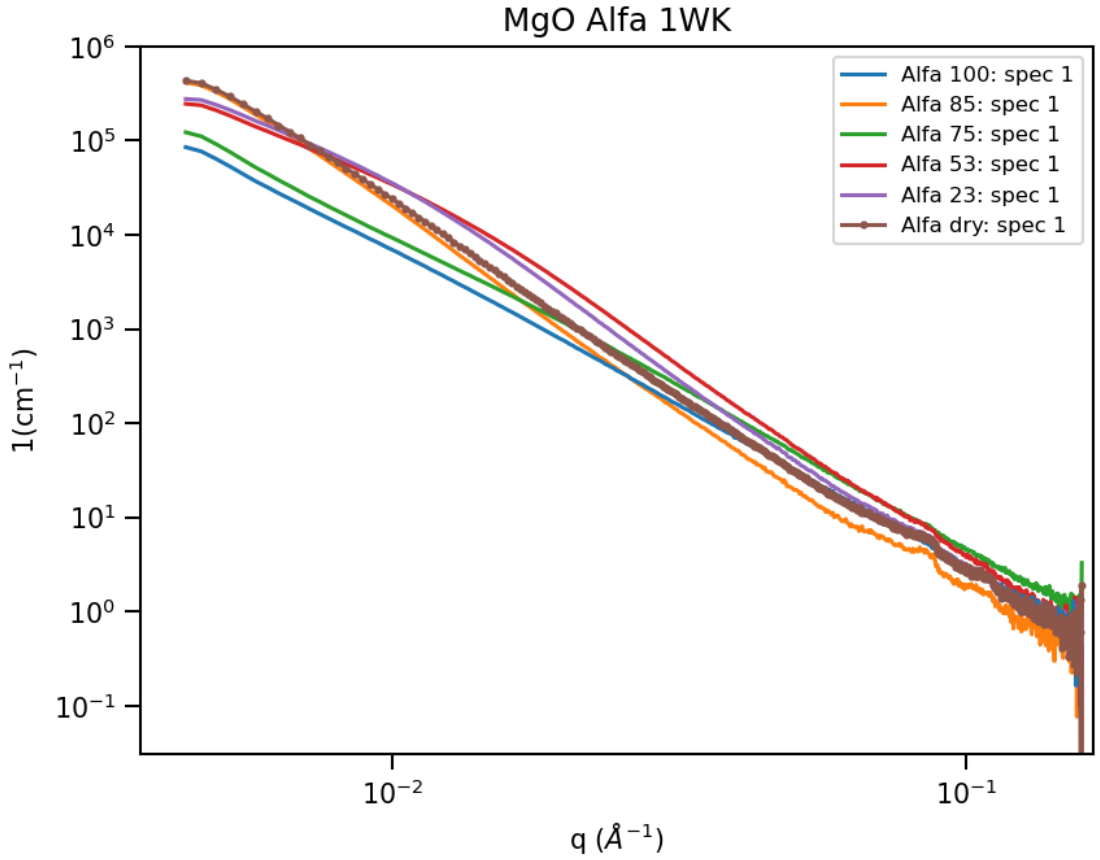
MgO SKY

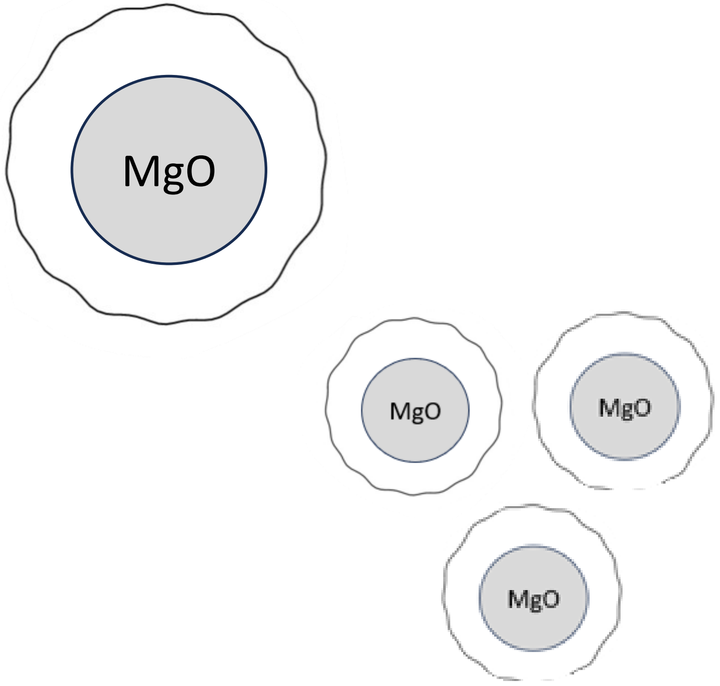




In this graph 53% and 75% you can see particle growth through brucite formation. Meaning a more homogenous formation.

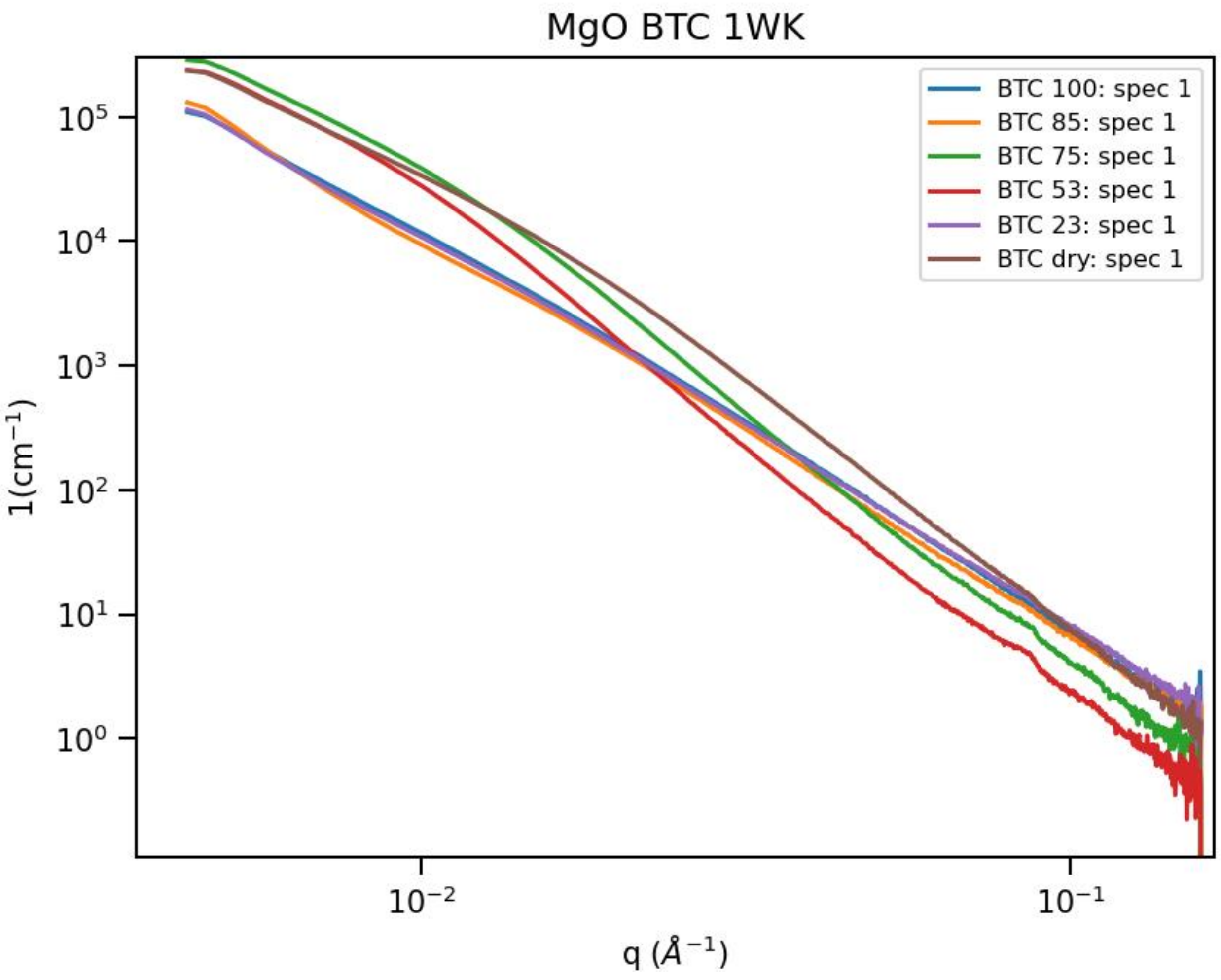
MgO Alfa





23% and 53% you can se growth on the high side. Meaning smaller structures are forming. Also has a more heterogenies growth compared to Sky.   Also 85% and 100 % show sign Mass fractal Scattering.

MgO BTC



MgO BTC 1WK
BTC 100: spec 1
BTC 85: spec 1
BTC 75: spec 1
BTC 53: spec 1
BTC 23: spec 1
BTC dry: spec 1
1(cm⁻¹)
q (Å⁻¹)

04

Results and conclusion

Summary of the results

The data revealed the behavior of MgO under varying humidity levels. Findings include significant growth in smaller structures at 23% and 53% humidity, evident mass fractal scattering at 85% and 100%, and particle growth via brucite formation at 53% and 75%. These insights reveal complex changes in MgO's physical structure under different humidity conditions

References

1. Integrated CO2 Capture, Conversion, and Storage to Produce Calcium Carbonate Using an Amine Looping Strategy, https://doi.org/10.1021/acs.energyfuels.8b02803.s001.
2. Satow, 82199-Richard L. “Aero Electronic Component Obsolescence.” Boeing, 15 June 2000, www.boeing.com/commercial/aeromagazine/aero_15/overhead_story.html.
3. Zhu, Qiancheng, et al. “A Model to Stabilize Co2 Uptake Capacity during Carbonation–Calcination Cycles and Its Case of CAO–MgO.” Environmental Science & Technology, vol. 51, no. 1, 2016, pp. 552–559, https://doi.org/10.1021/acs.est.6b04100.

THANKS

Do you have any questions?

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