BRAGG2D

Illuminating the Sample Preparation Challenge

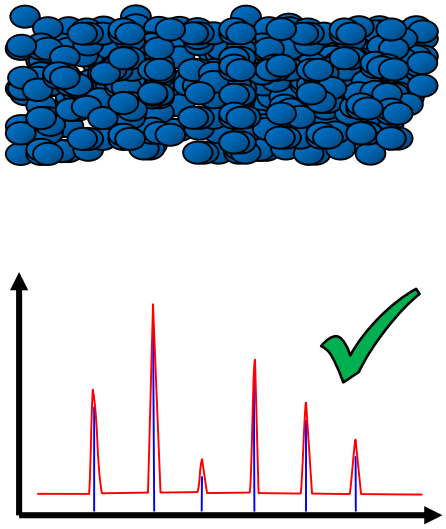
November 13, 2018

Jon Giencke

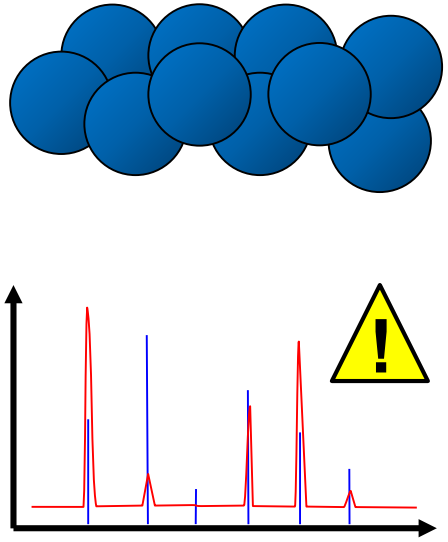
BRAGG2D: Illuminating Sample Prep

What is a perfect powder sample?

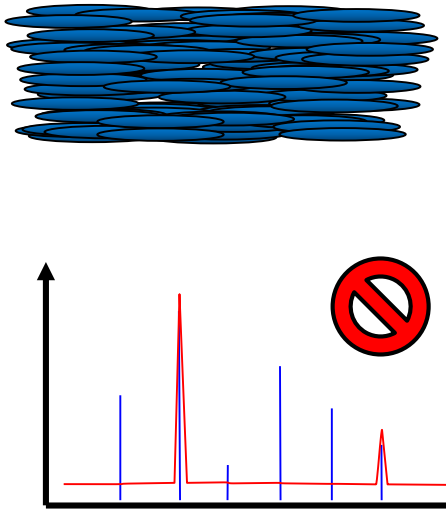
Ideal Powder



Large Crystallite Size



Preferred Orientation



How can sample preparation quickly be qualified?

2D Diffraction!

BRAGG2D: Illuminating Sample Prep

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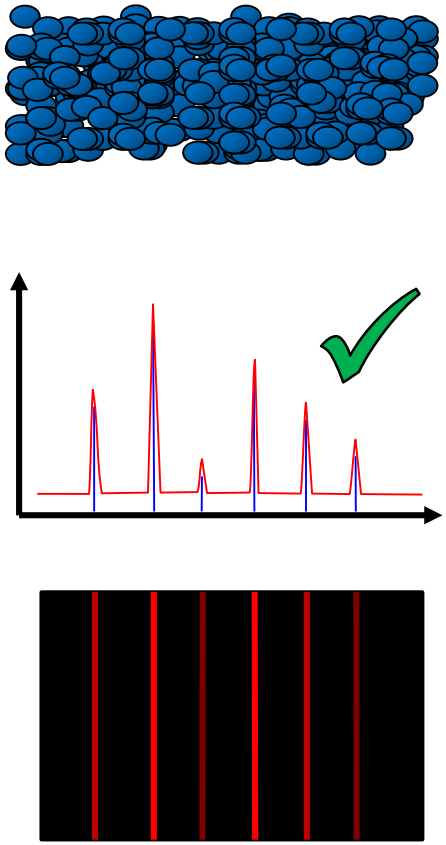
Ideal Powder



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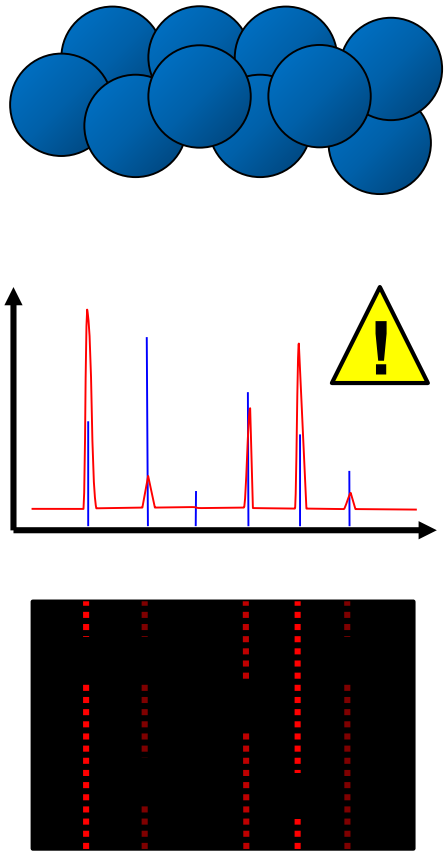

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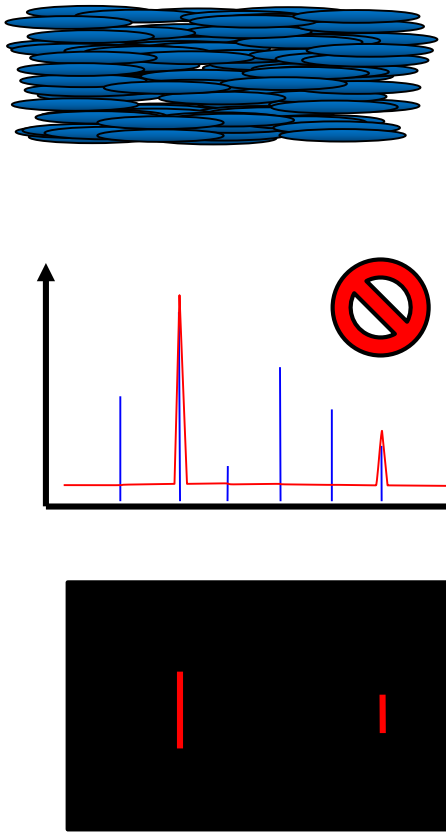
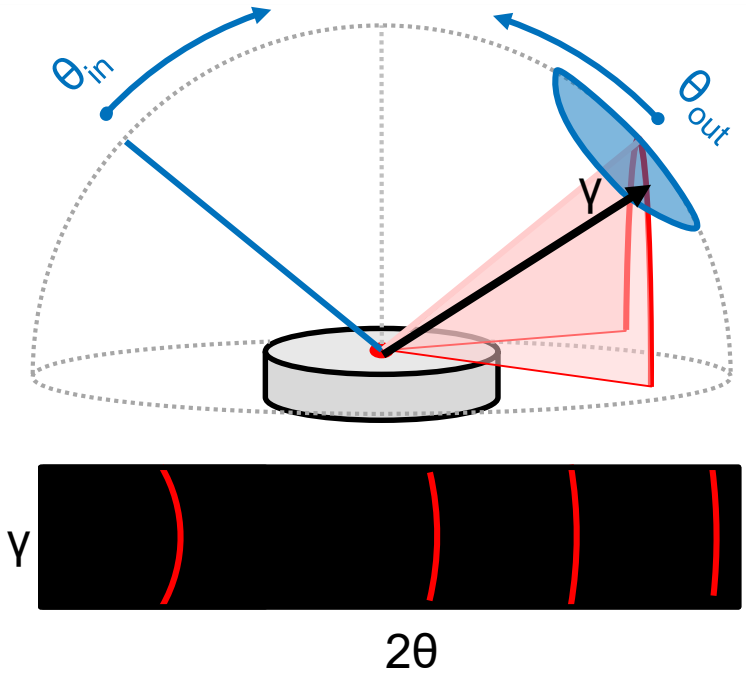
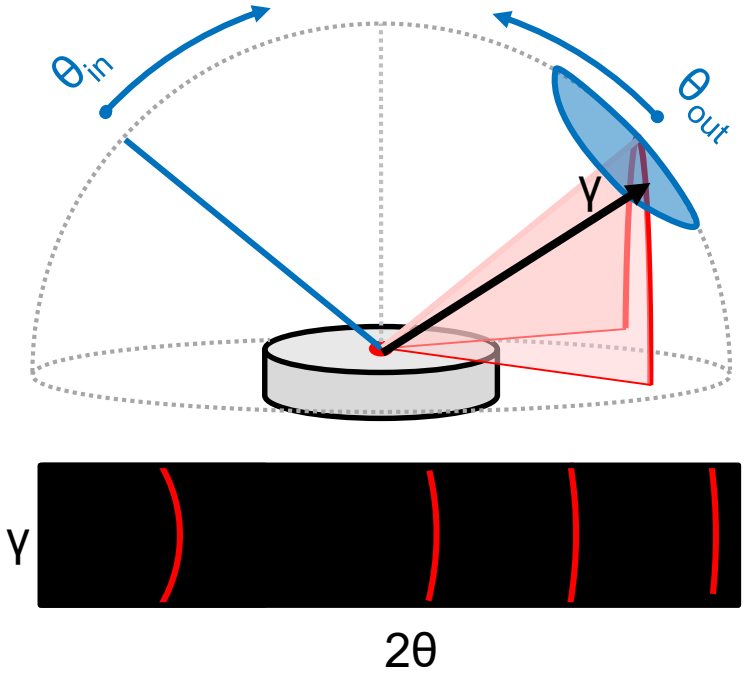


BRAGG2D: Illuminating Sample Prep
Traditional XRD²



BRAGG2D: Illuminating Sample Prep
Traditional XRD²



Benefits of Traditional XRD²

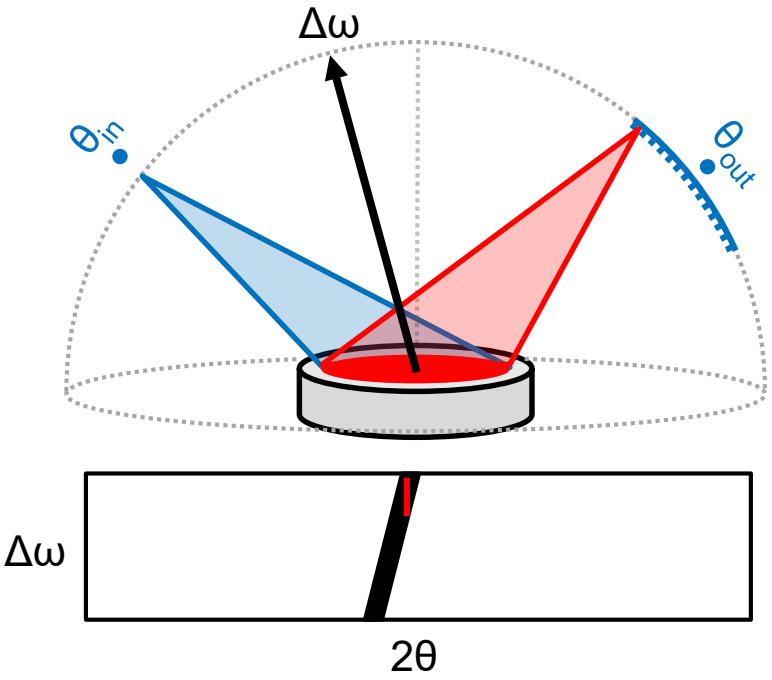
- Superior Microdiffraction
- Fast Texture and Residual Stress

Drawbacks for Sample Prep Qualification

- Low Integrated Intensity
- Local information only

XRD² is ideal for the D8 ADVANCE and D8 DISCOVER with spot focus optics, positioning stages and large 2D detectors

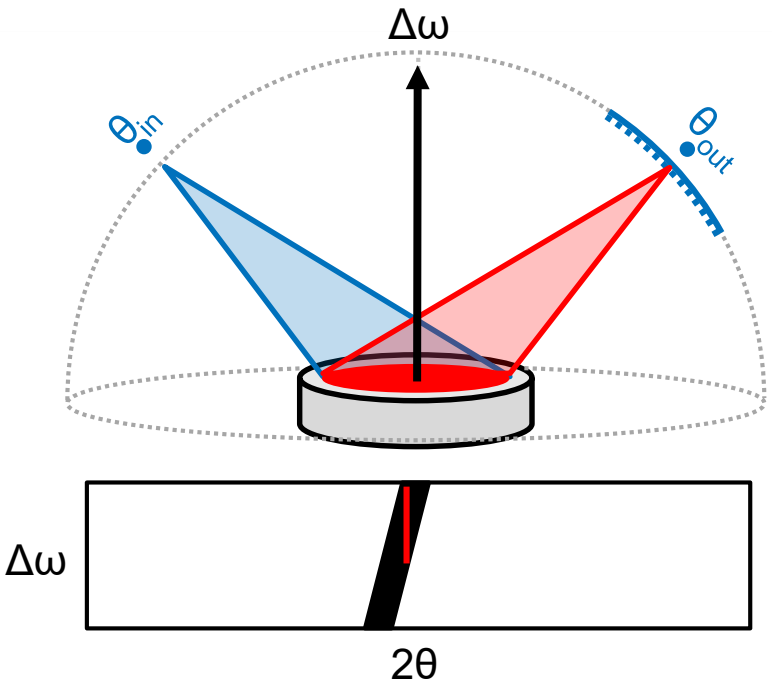
BRAGG2D: Illuminating Sample Prep
Divergent Beam 2D XRD



$$\Delta\omega = \frac{2\theta}{2} - \theta_{in}$$

$$2\theta = \theta_{in} + \theta_{out} + Channel\ Offset$$

BRAGG2D: Illuminating Sample Prep
Divergent Beam 2D XRD



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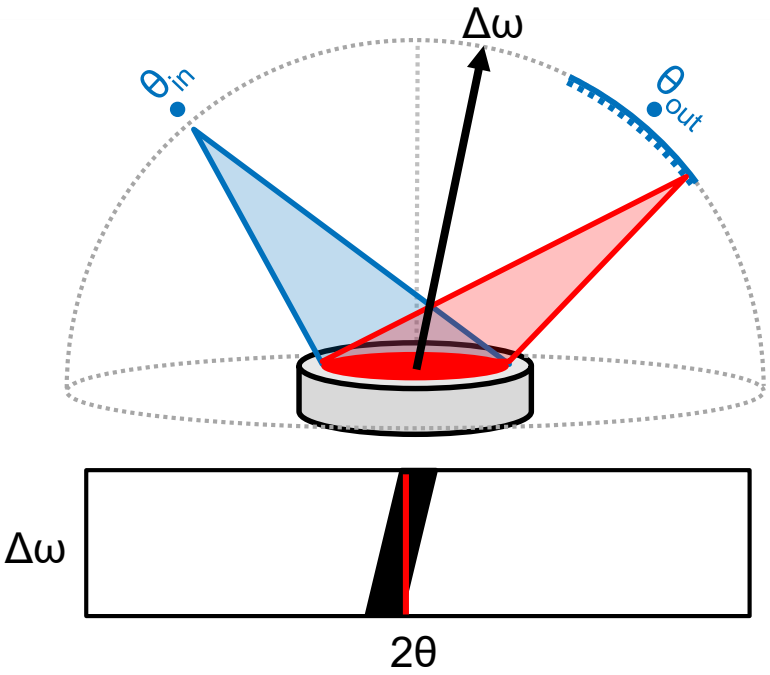
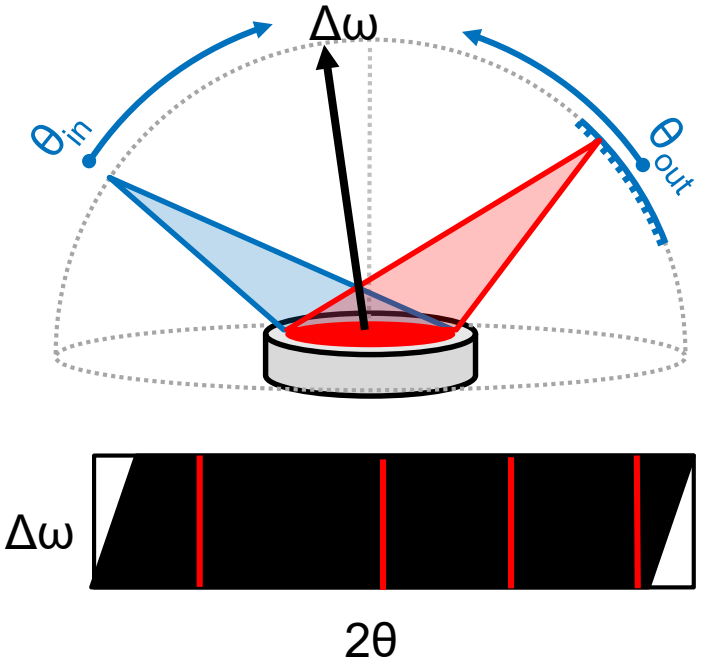
BRAGG2D: Illuminating Sample Prep
Divergent Beam 2D XRD



$$\Delta\omega = \frac{2\theta}{2} - \theta_{in}$$

$$2\theta = \theta_{in} + \theta_{out} + Channel\ Offset$$

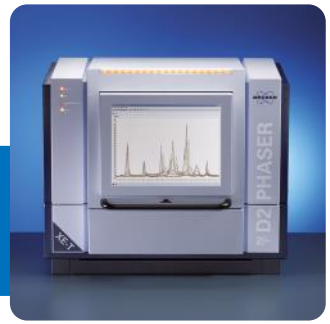
BRAGG2D: Illuminating Sample Prep
BRAGG + 2D = BRAGG2D



Benefits of BRAGG2D

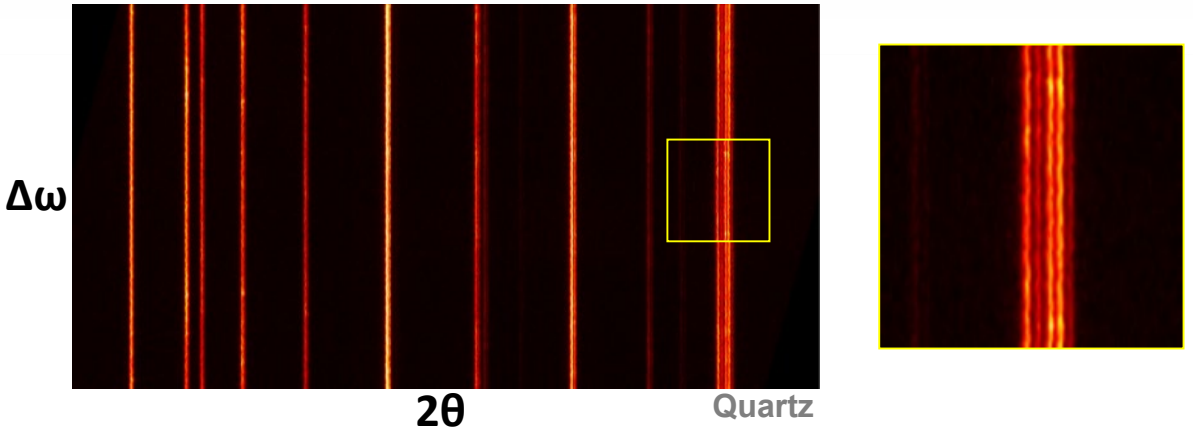
- Sample Preparation Visualization
- Full X-ray Beam Utilization
- Same setup as conventional 1D scans
  - Requires a 1D detector
  - No need for additional hardware
  - Only requirement is EVA V5

BRAGG2D is ideal for the D2 PHASER with Large sample footprint and maximum beam utilization

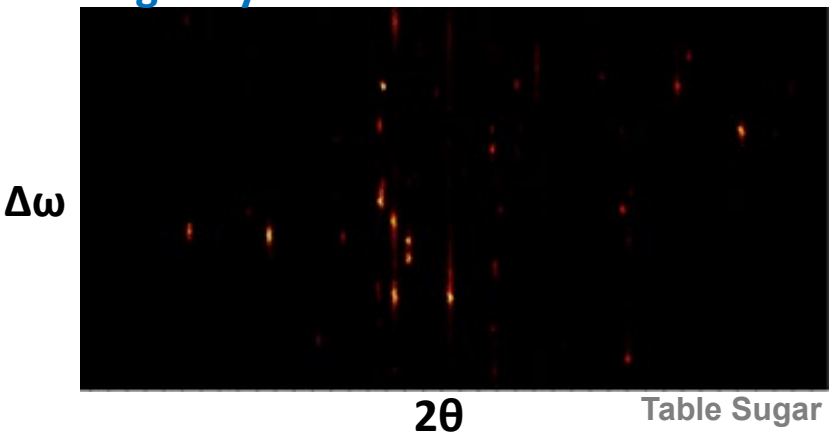


BRAGG2D: Illuminating Sample Prep
Various Sample Morphologies

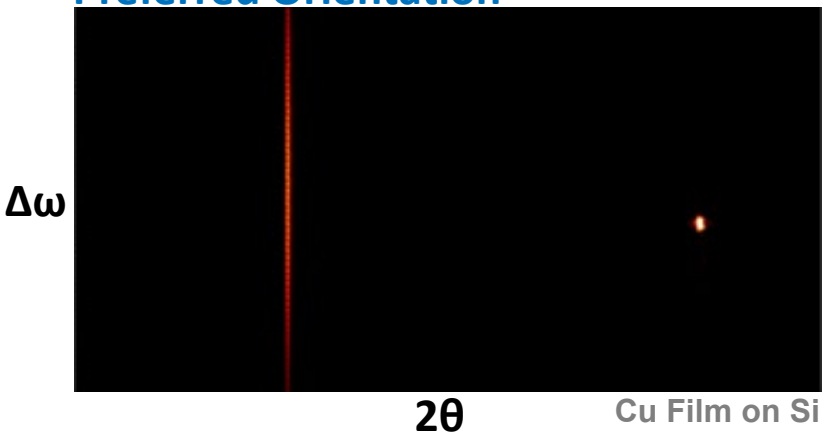
Ideal Powder



Large Crystallite Size

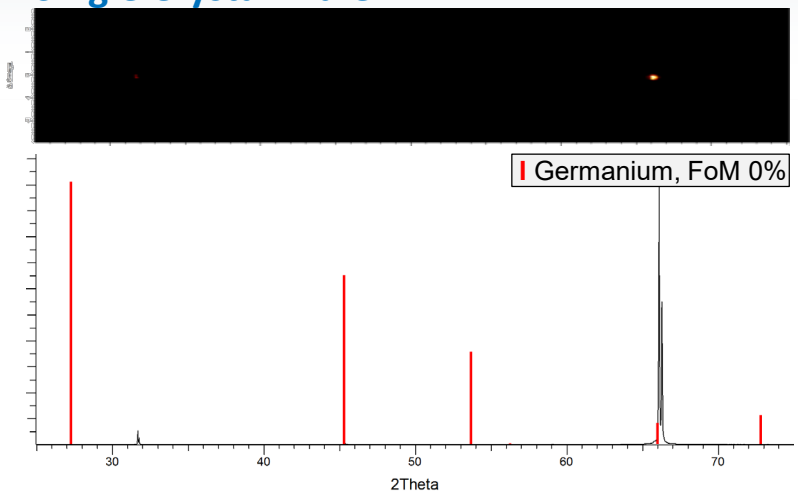


Preferred Orientation

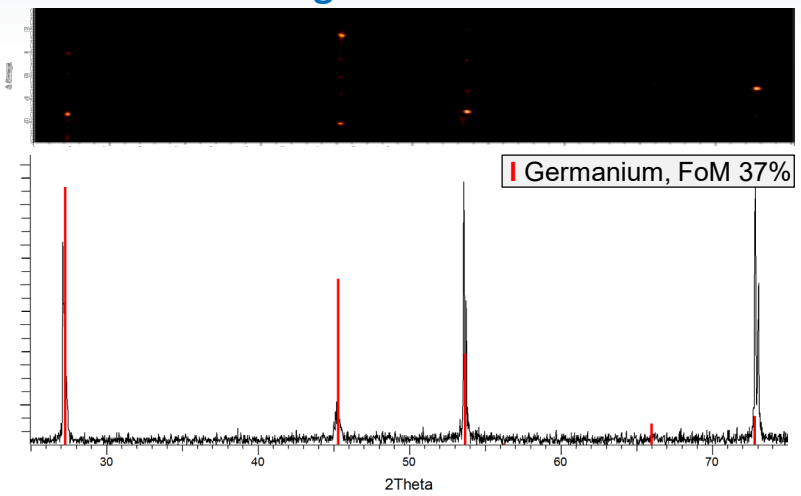


BRAGG2D: Illuminating Sample Prep
Monitoring Sample Preparation

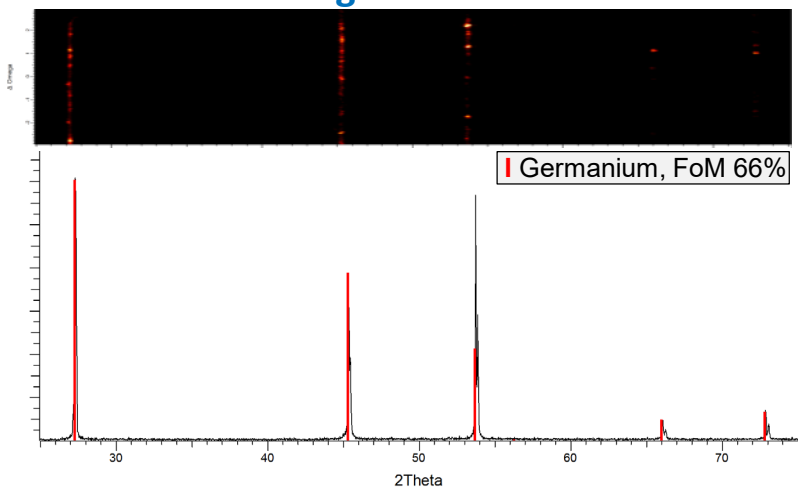
Single Crystal Wafer



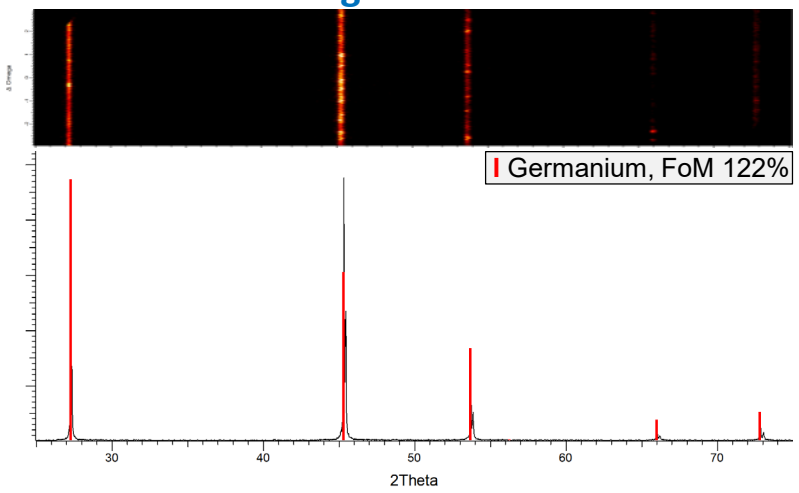
1 min of Grinding



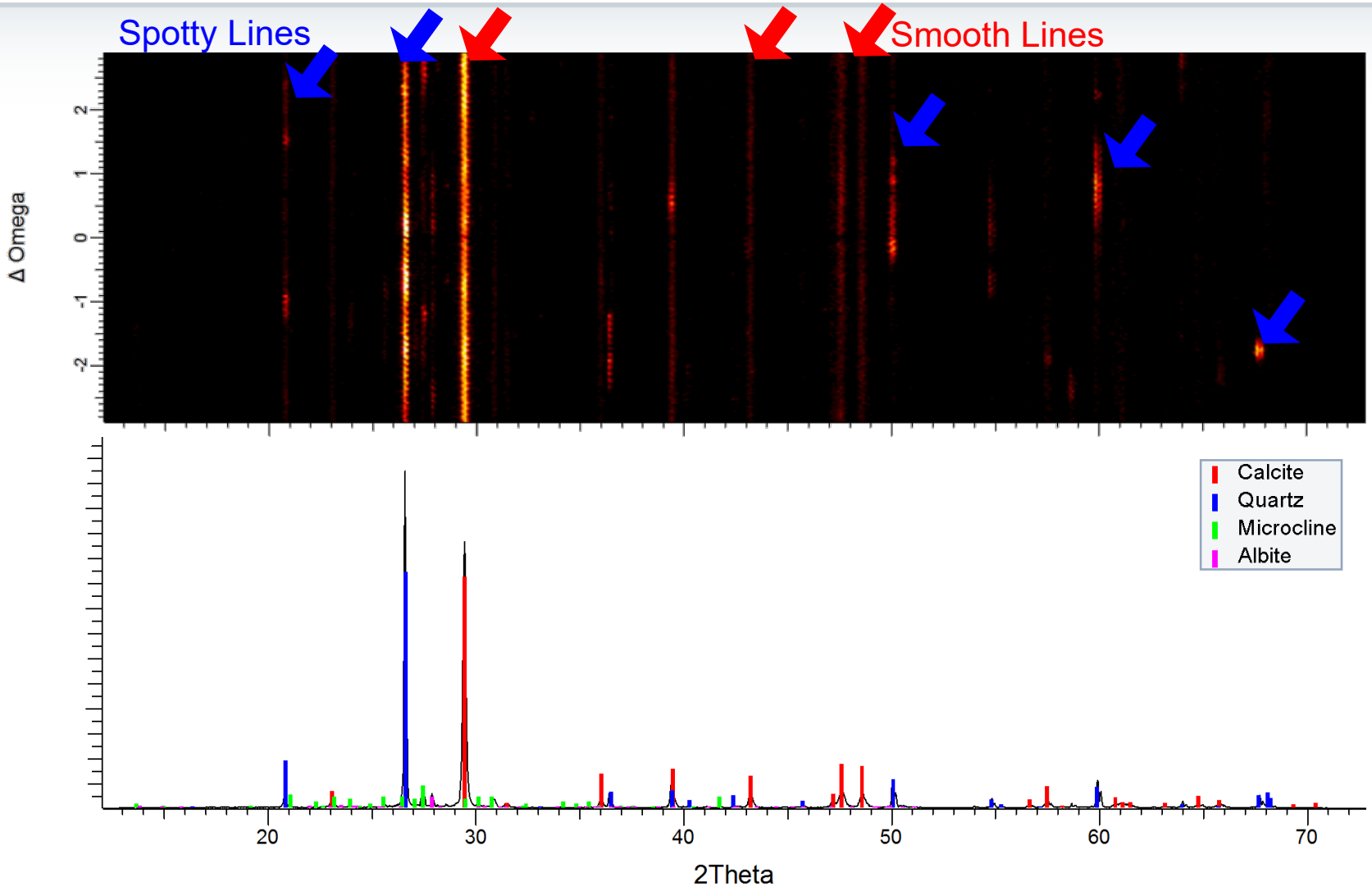
10 min of Grinding



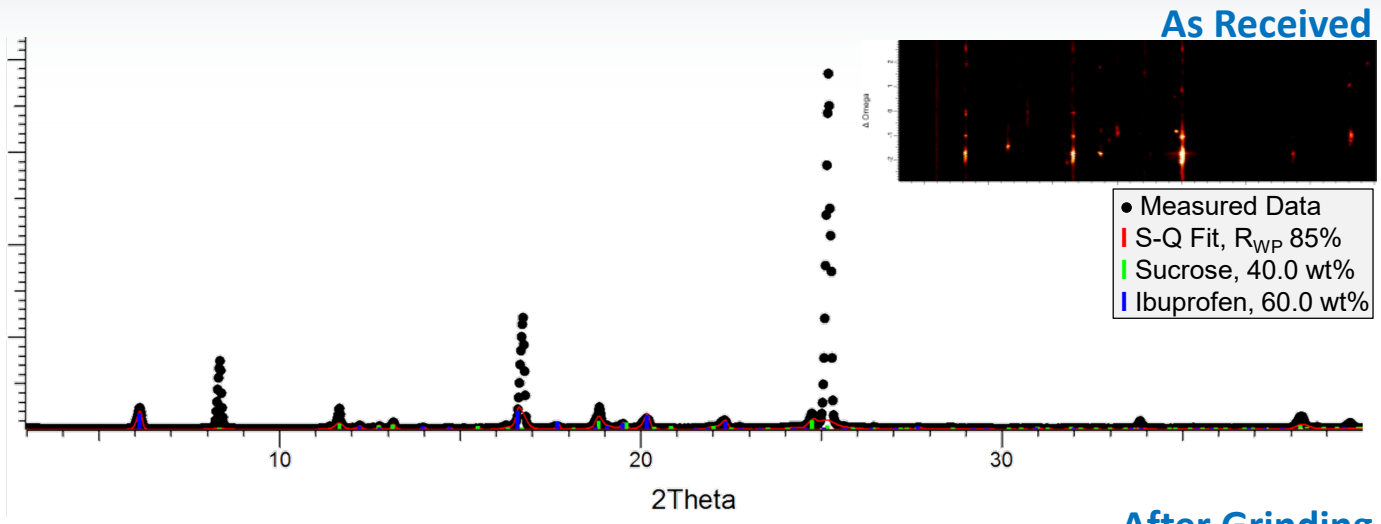
30 min of Grinding



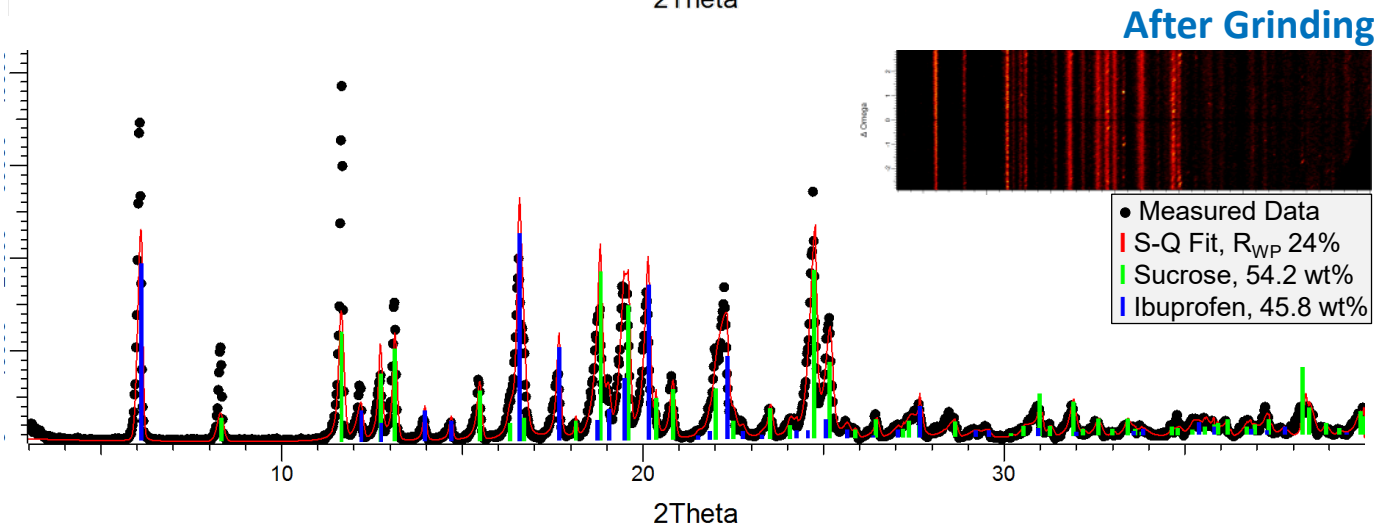
BRAGG2D: Illuminating Sample Prep
Enhanced Phase Identification



BRAGG2D: Illuminating Sample Prep
Semi-Quant Pattern Fit Analysis



Large Spots ↓ Poor Fit

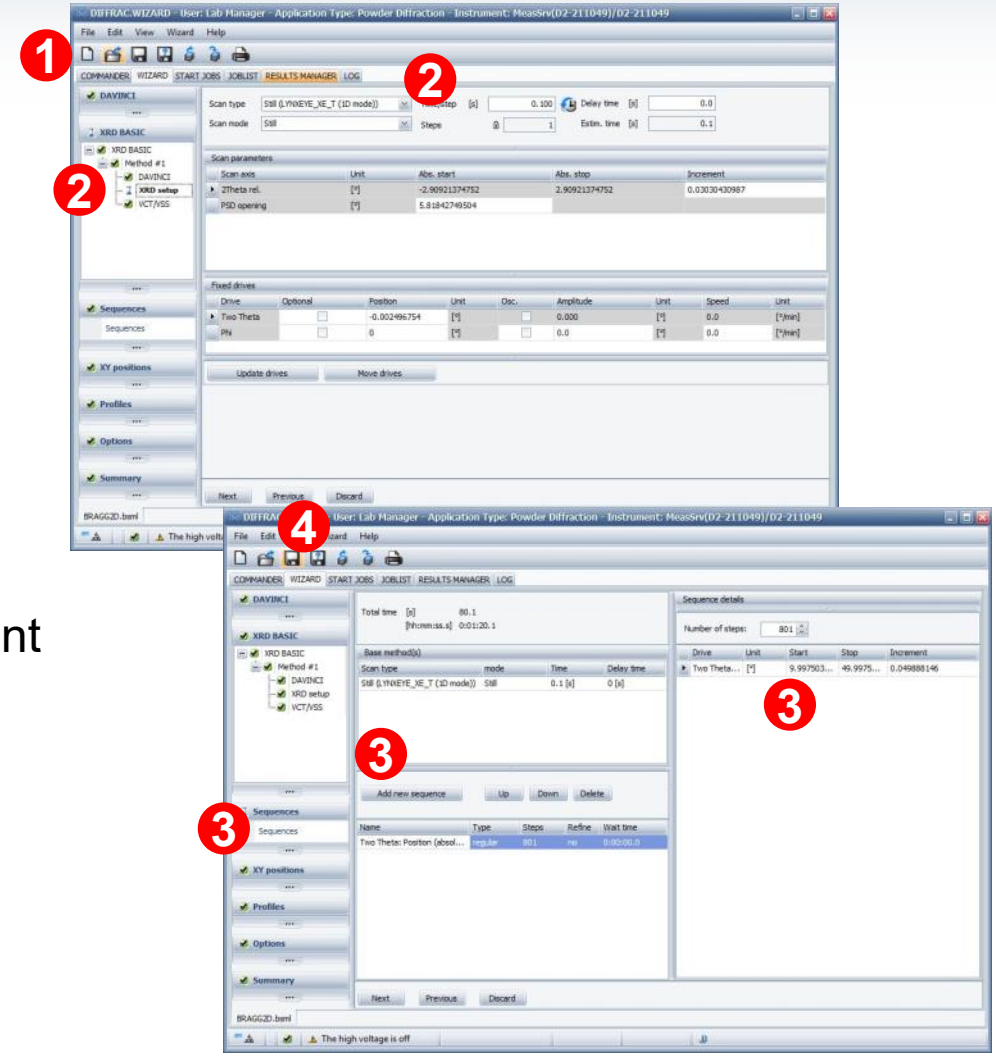


Smooth Rings ↓ Good Fit

BRAGG2D: Illuminating Sample Prep
DIFFRAC.SUITE Workflow for BRAGG2D

PLAN in DIFFRAC.WIZARD

1. Create a new XRD method
2. Under XRD setup choose scan type **Still (LYNXEYE 1D Mode)**
3. Under Sequences insert a Two Theta sequence with start, stop and increment
4. Save the method



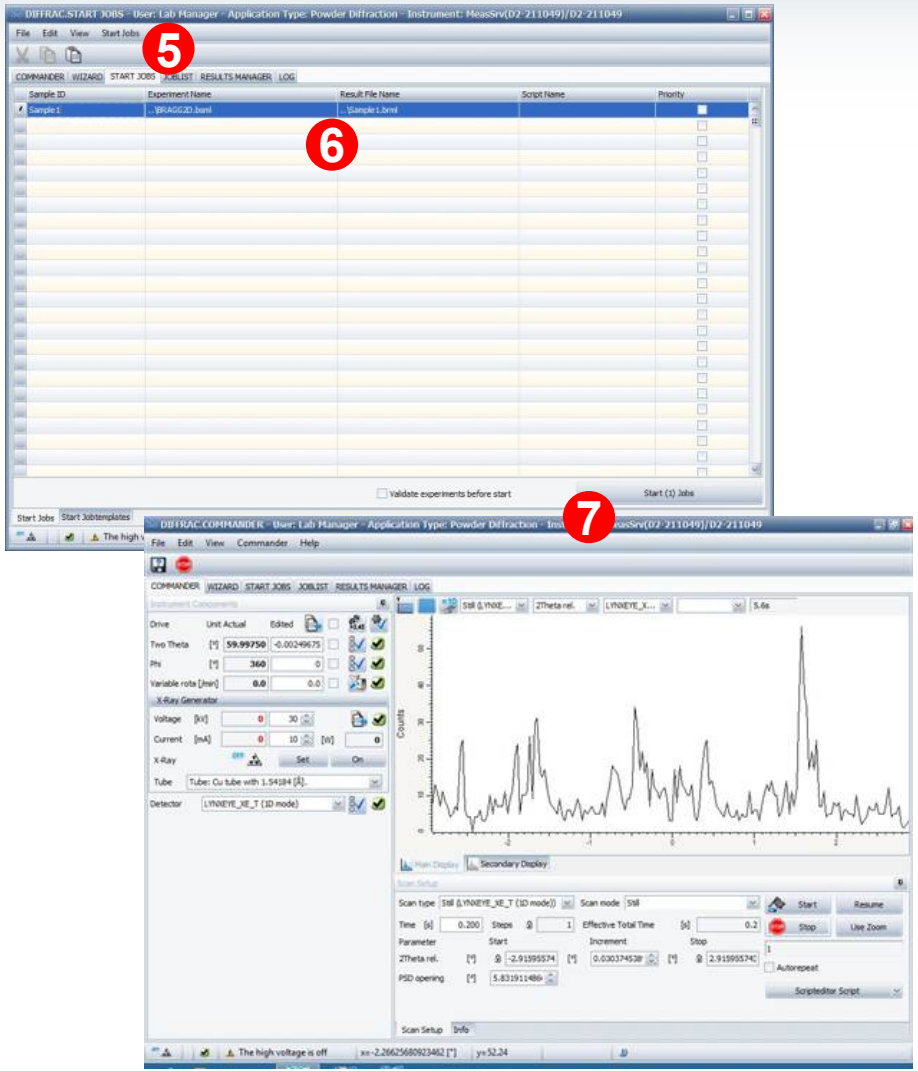
BRAGG2D: Illuminating Sample Prep
DIFFRAC.SUITE Workflow for BRAGG2D

MEASURE in **DIFFRAC.COMMANDER**

5. Click on the START JOBS Tab

6. Choose the method created in step 4 and set the desired result file location

7. Click Start and Monitor progress in COMMANDER



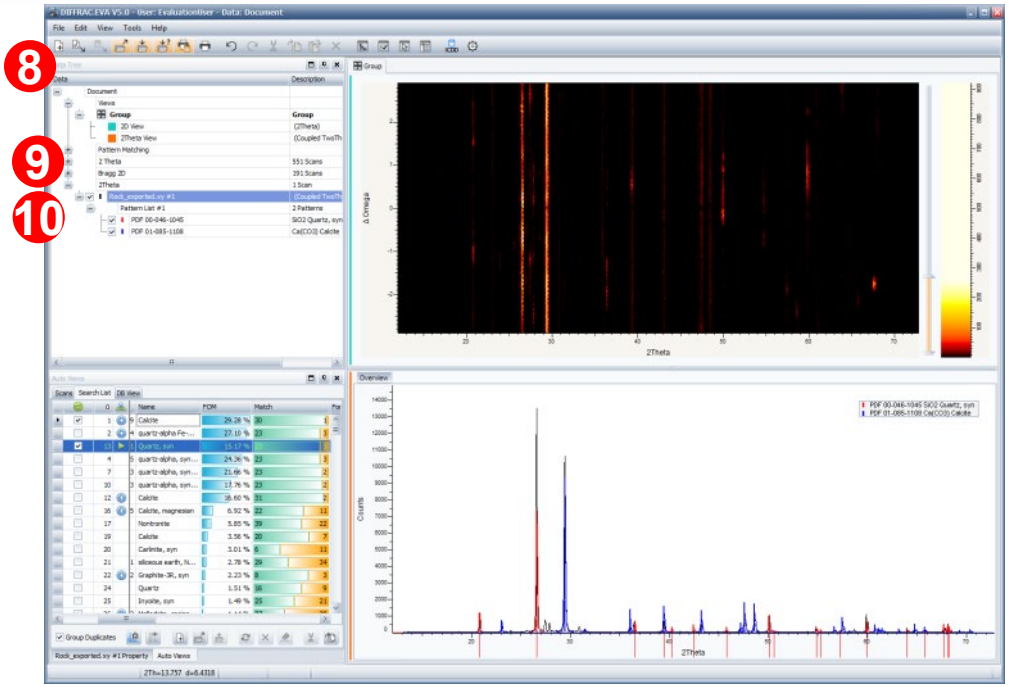
BRAGG2D: Illuminating Sample Prep
DIFFRAC.SUITE Workflow for BRAGG2D

ANALYZE in **DIFFRAC.EVA V5**

8. Open DIFFRAC.EVA and import the result file

9. Right click on the 2Theta node and choose
   Tool → BRAGG2D View Realignment

10. Right click on the BRAGG2D node and choose
    Create → 2D View



BRAGG2D: Illuminating Sample Prep
Summary

What is BRAGG2D?

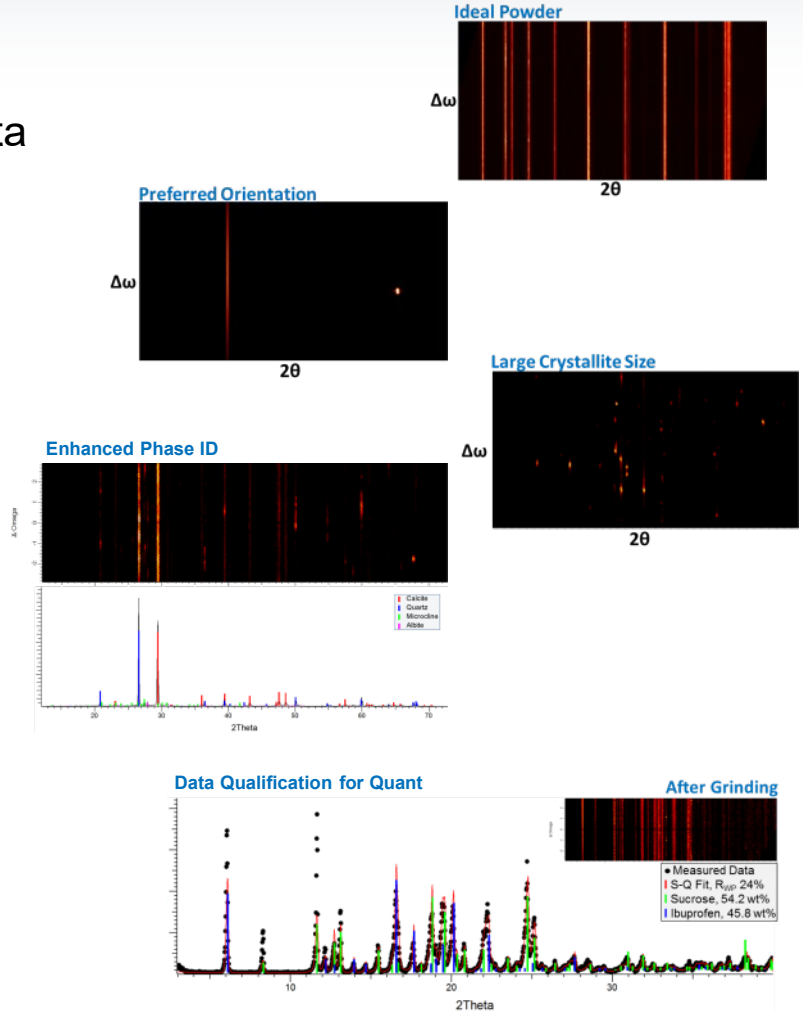
- A patent pending method for collecting 2D XRD data with a divergent primary beam

Why use BRAGG2D?

- Ideal method for assessing the quality of sample preparation for powder analysis

What is required for BRAGG2D?

- D2 PHASER with 1D detector
  - SSD160, LYNXEYE or LYNXEYE XE-T
- Standard 1D optics
- EVA V5



Questions and Answers

Any questions?

Please type any questions you may have for our speakers in the Q&A panel and click Send.

Thank you!

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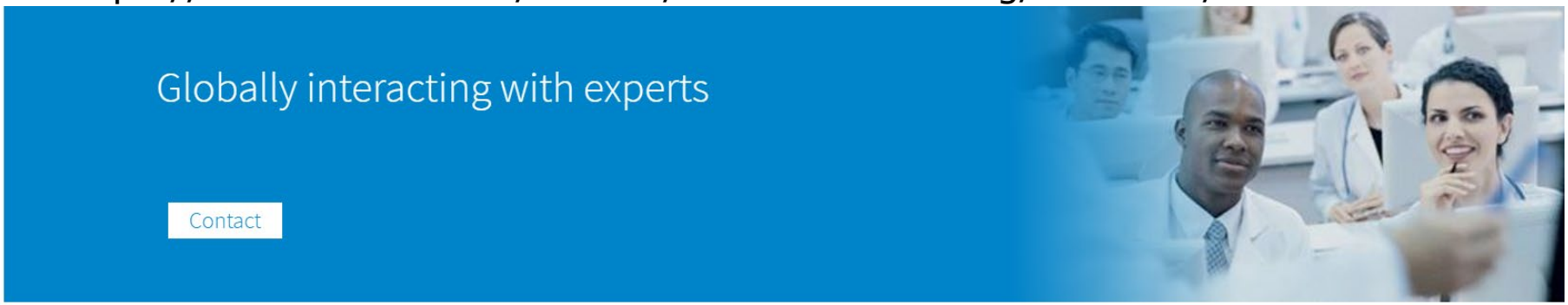

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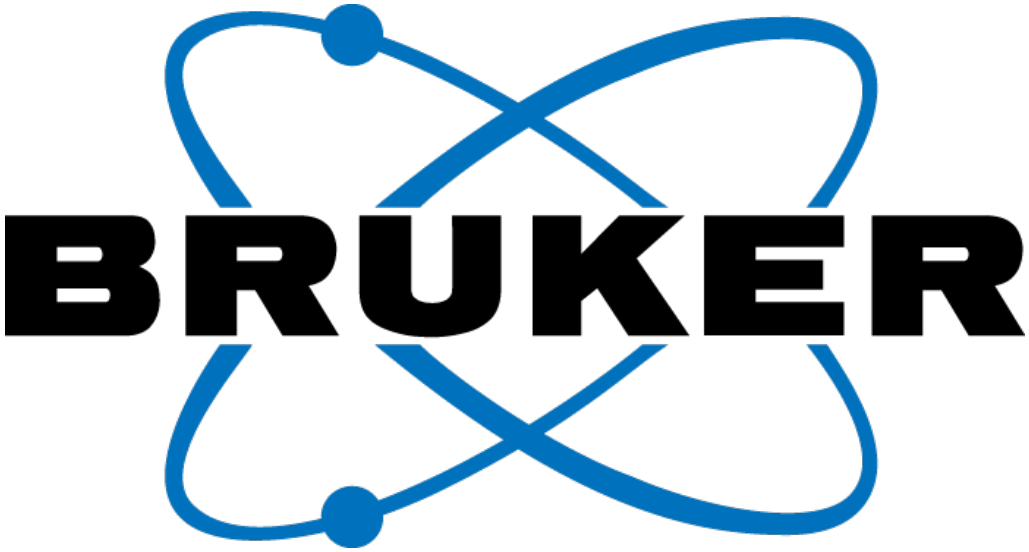
Webinar	Content
Nov 13, 2018 **BRAGG2D: Illuminating the XRD Sample Preparation Challenge**	In this 15-minute webinar, BRAGG2D, a patent-pending technique that identifies sample preparation issues and enhances phase identification and quantification, will be presented. BRAGG2D helps ensure that the specimen in a powder X-ray diffraction experiment approaches the ideal powder condition, i.e. consists of randomly oriented crystallites of appropriate dimensions. Using parafocusing beam geometry with a new two-dimensional data processing algorithm, BRAGG2D is able to illuminate a large specimen area with the full X-ray beam, thereby overcoming the small-spot limitation of traditional XRD2. Register Now



Innovation with Integrity

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