Frequently asked questions (FAQ) for the XRD-lab

General

How do I get instrument training for XRD?

Please follow the instructions on this wiki-page.

How do I get access to the data and the XRD software?

After you have participated in the instrument training session, you get an email with some information and passwords etc (Subject: Getting started with XRD analysis). You can also follow the descriptions here.

How do I use the database?

There are currently 2 options which can be built into EVA Search and Match:

1) PDF (Powder Diffraction File): On the lab PCs we have licenses for the ICDD-4+PDF-database (https://www.icdd.com/pdf-4/). A quick demo of this database can be viewed here: https://www.youtube.com/user/TheICDD. The database entries can be referenced using the PDF number in the text (PDF xx-xxx-xxxx), and a reference to "International Centre for Diffraction Data (ICDD), Powder Diffraction File PDF-4+ database" in the reference list

2) COD (Crystallography Open Database): http://www.crystallography.net/cod/. This database can be installed on your own computer, and you can implement it in EVA for Search/Match. "Tools" "Settings" "Database", and select "Crystallography Open Database".

You can use the databases directly (e.g. before measuring) to seach for patterns, however, they are also implemented in the DIFFRAC.EVA-software. First you have to download the "cod-for-diffraceva_vxx.exe" (see the "Getting started with XRD analysis-email descriped above for details), and install the .exe-file on your computer. Then open EVA, and click "Tool" "Search / Match". For more details, please see the "EVA-How to" booklet in the lab.

Another option: (not included in EVA Search and Match)

Cambridge Structural Database: https://www.ccdc.cam.ac.uk/structures/

Routine powder diffractometer (DaVinci1)

I measure some small peaks that I can't identify. What can it be?

- If the small peaks are at slightly smaller 2-theta-angle than the main peaks (and measured at the routine diffractometer (DaVinci1)), it is perhaps W-La or Cu-Kbeta contamination from the X-ray source. For explanation, please log on to the odin server, and select " /useful_documents/d8_davinci_1/Explanation of the peaks due to different wavelengths.pdf" .
- How to match the contamination-peaks in EVA: please log on to the odin server, and select "/useful_documents/d8_davinci_1/Identifying peaks due to different wavelength.pdf" .

Have my samples been measured? I came to the lab to check, however, I didn’t find the new files in my folder.

Check if the files have been saved to the default directory: C:\ProgramData\Bruker AXS\Results

9-position sample holder powder diffractometer (D8-Focus)

I get an "error" when I try to start my measurements: "some drives need to be initialized. Check for crashing possibilities". What should I do?

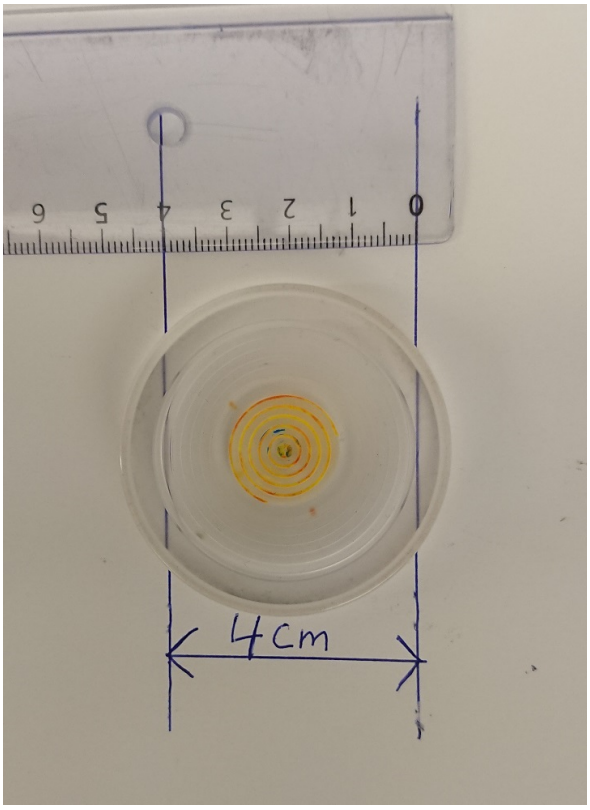
It is not really an error, just a warning. Simply click "OK", and watch the diffractometer arms/sample changer as the motors move.

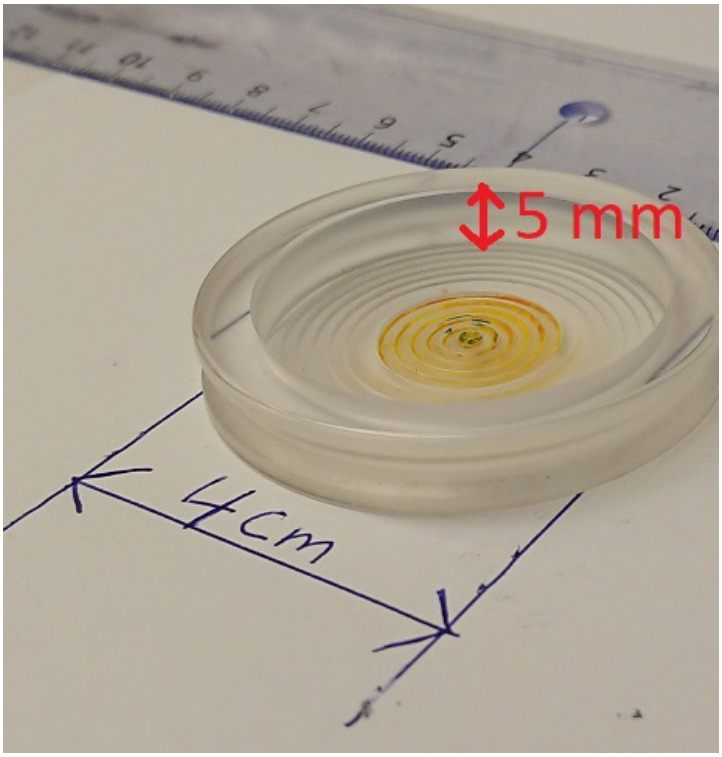
Sample holders

What is the maximum size a sample can be for standard deep sample holders?

The sample has to fit within the sample holder that is 5 mm deep, and 40 mm diameter, as shown is these photos. It is recommended that the sample is maximum 4 mm in height, so that we have space for fastening it with modelling clay.

Top view	Side view


4cm


5 mm
4cm