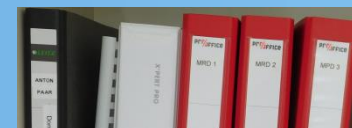


X-ray CoreLab @ HZB

- Data format
- Data storage
- Data security



Michael Tovar, lab responsible LMC
Data seminar 11.06.2019

Key points of the X-ray CoreLab

- X-ray CoreLab anchors lab-scale X-ray diffraction methods on an institutional and cross-cutting level
- Various and **complementary X-ray diffraction method** for internal and external users
- Over **100 registered internal and external users** from academic and industrial institutions
- Expert scientists for keeping the **lab up-to-date and sharing knowledge** and experience
- **Central management** of scientific databases and user support with evaluation software
- Annual X-ray school



Mission statement

The X-ray CoreLab is supervised by a **Steering Committee**

Susan Schorr, chair (EM-ASD)

Christoph Genzel (EM-AME)

Roel van de Krol (EE-IF)

Bella Lake (EM-AQM)



LMC
Michael Tovar,



René Gunder



WCRC

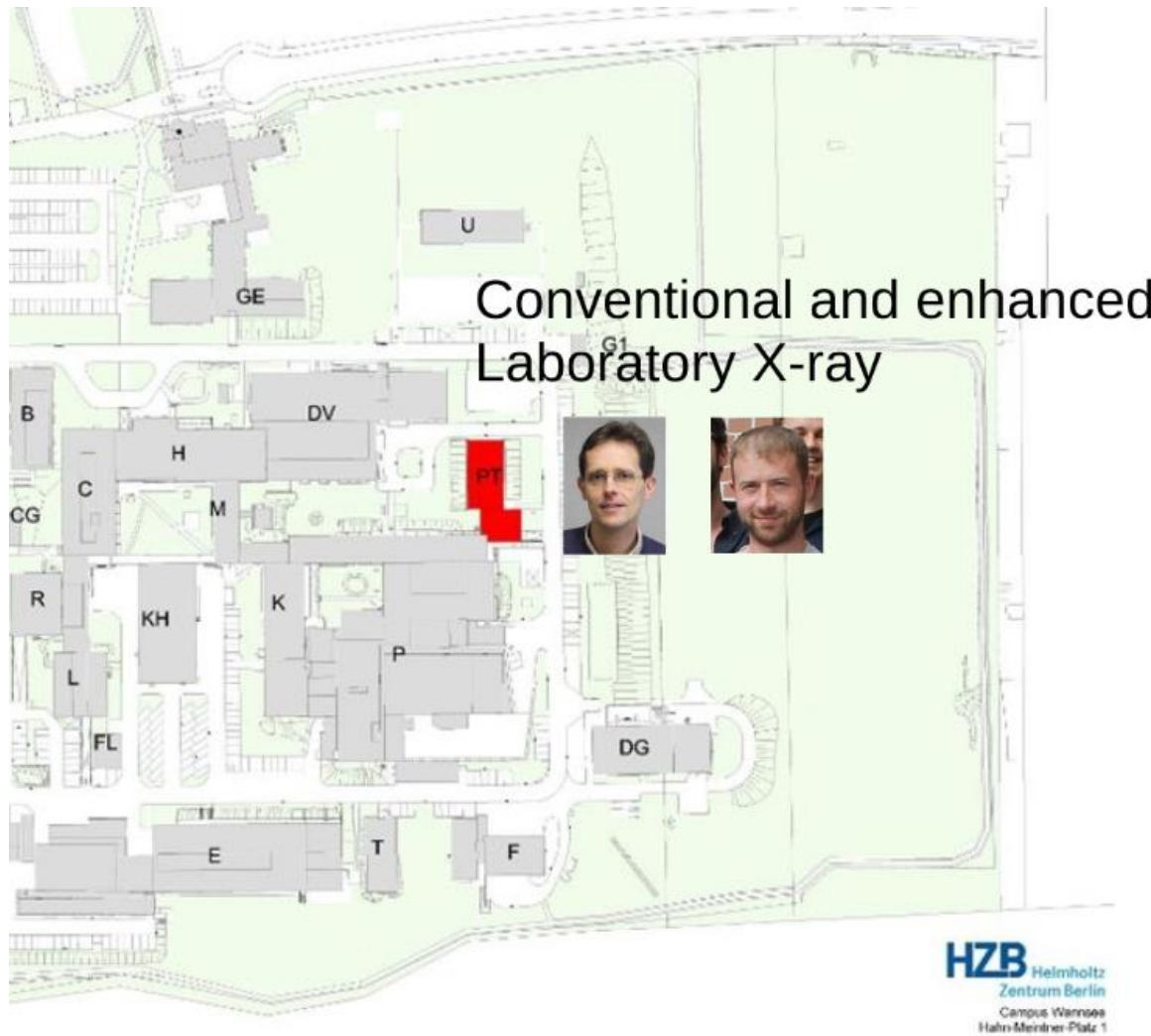
Christoph Genzel

Manuela Klaus

Roland Mainz

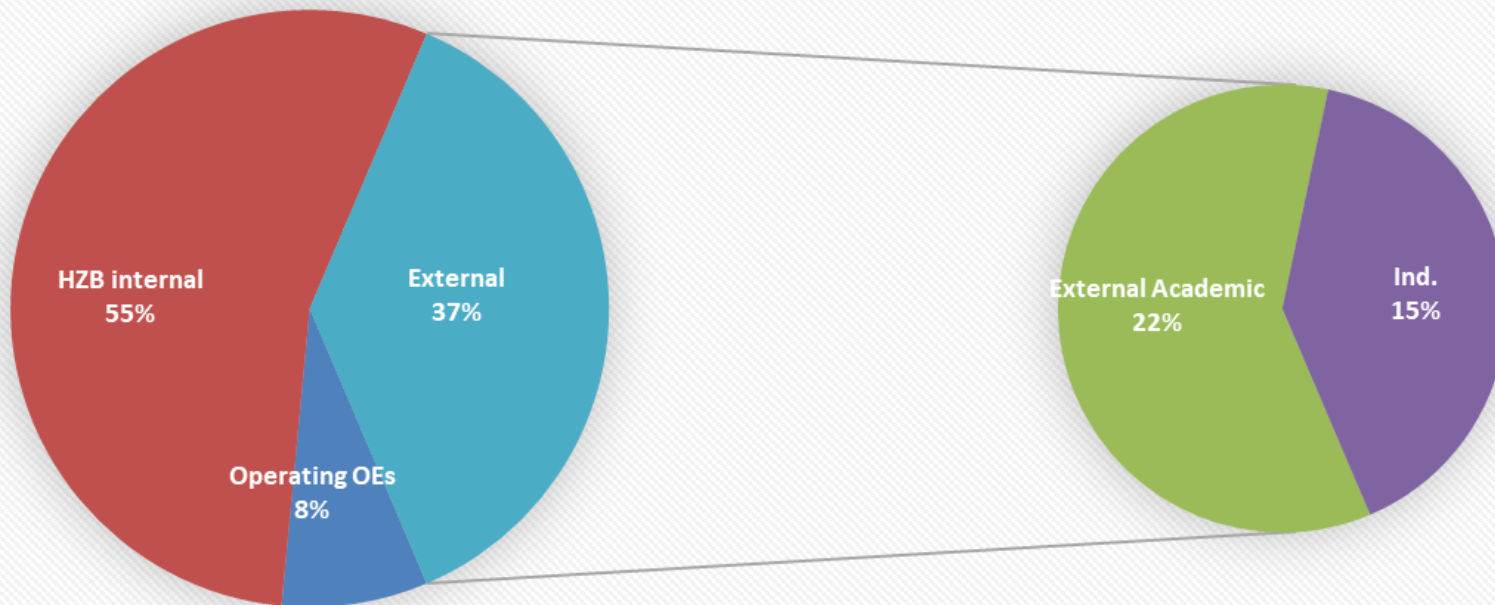
Katherine Ann Mazzio

X-ray CoreLab Lise-Meitner Campus



User Allocation internal/external (2018-II)

X-Ray CoreLab User (Jul - Dec 2018)

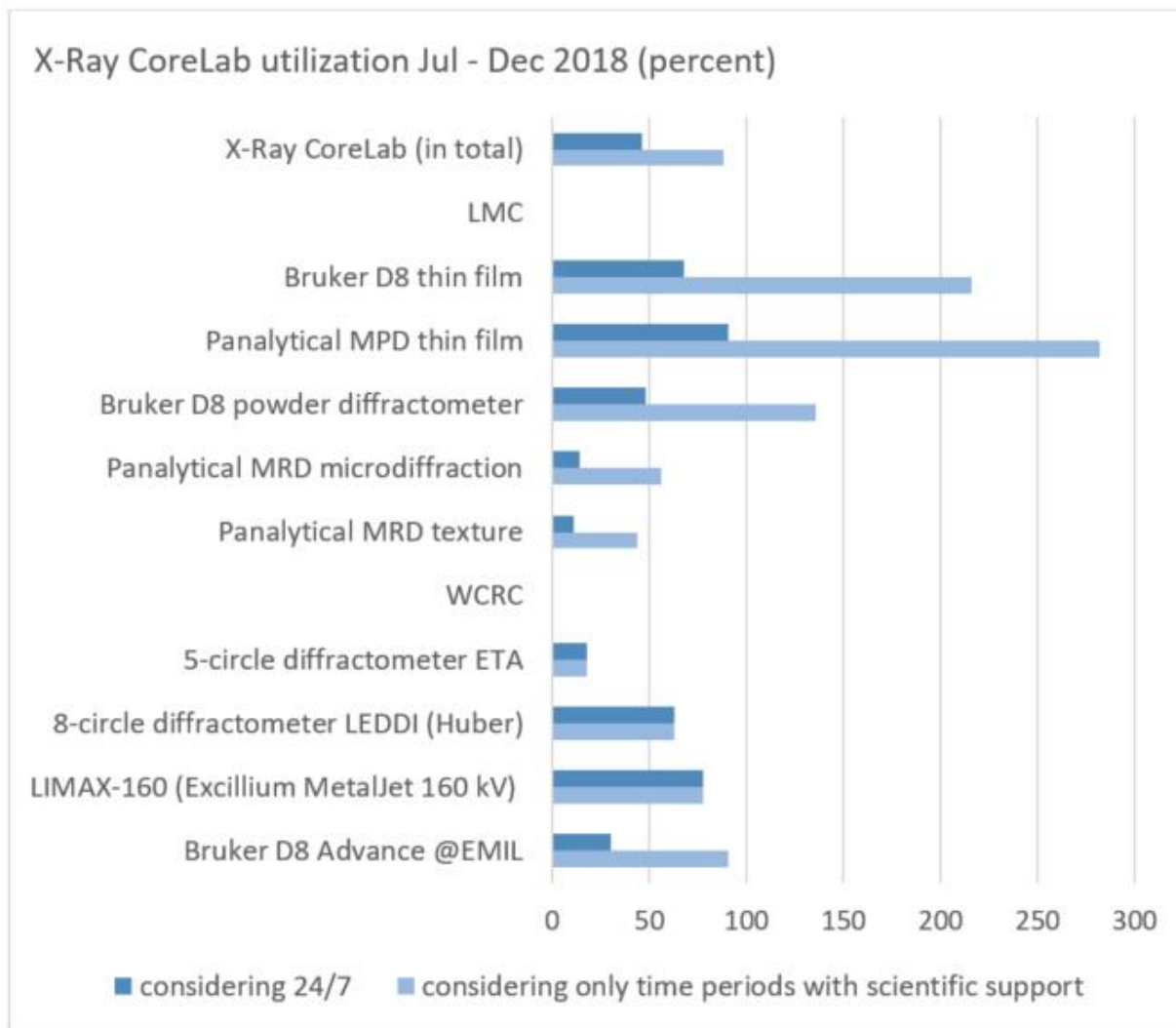


Theses and Publications (reporting period)

X-Ray CoreLab obtained data are part of:

- 5 Bachelor Theses
- 6 Master Theses
- 22 PhD Theses

X-Ray CoreLab utilization July – December 2018



Booking calendar IGAMA

Booking calendar

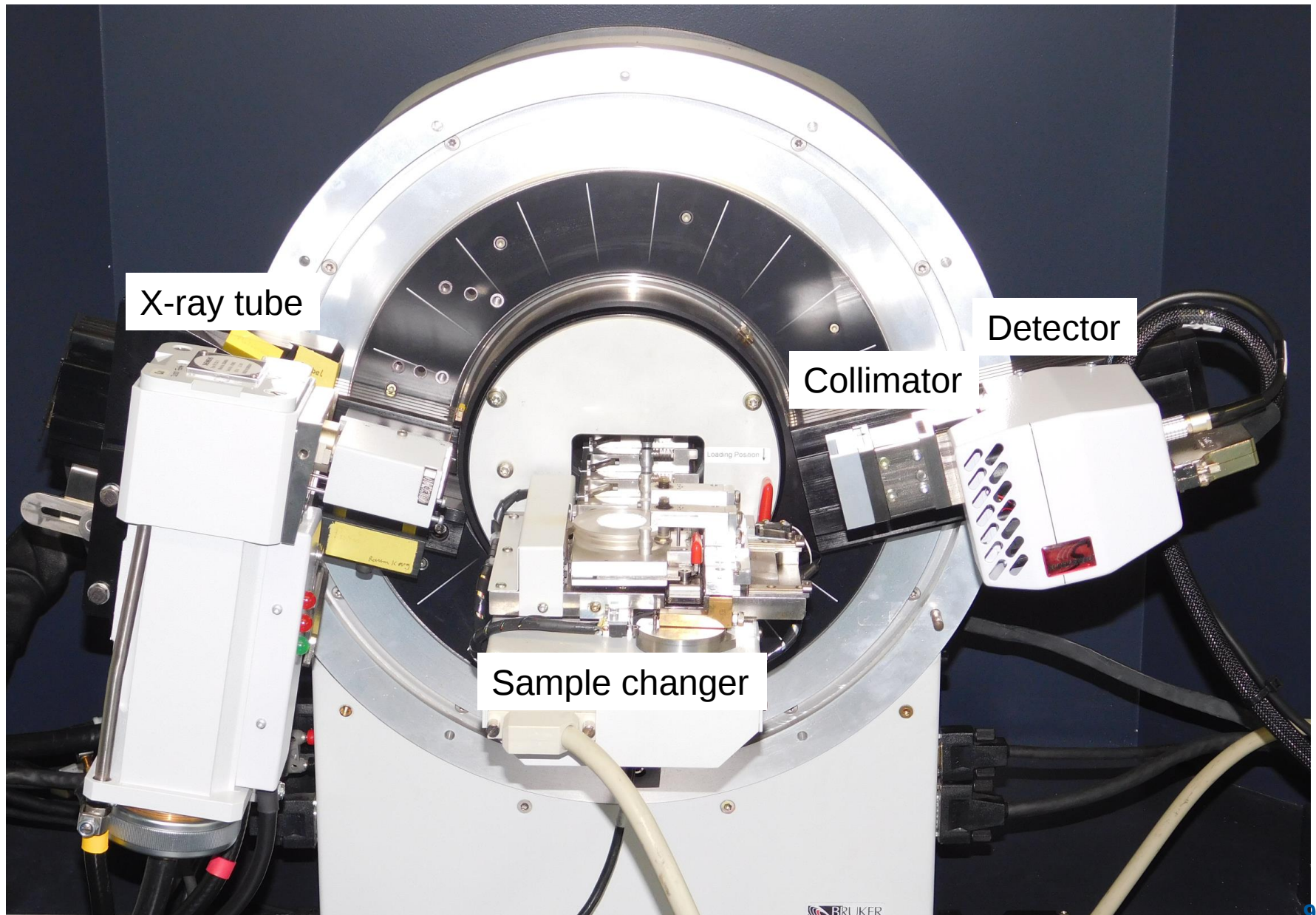
◀ June 2019 ▶

Date	01	02	03	04	05	06	07	08	09	10	11	12	13
Day	Sat	Sun	Mon	Tue	Wed	Thu	Fri	Sat	Sun	Mon	Tue	Wed	Thu
PANalytical MPD for thin film analysis (LMC)	+	+	+	+	15:00–23:59: Alexander Steigert +	09:00–16:00: Dr. Galina Gurieva +	10:30–18:00: Hasan Arif Yetkin +	+	+	+	+	+	+
PANalytical MRD for texture analysis (LMC)	+	+	+	+	Dr. Ruslan Muydinov	Dr. Galina Gurieva				+	+	+	+
PANalytical MRD for epitaxy analysis (LMC)	+	+	+	+	+	+	+	+	+	+	+	+	+
Bruker D8 Advance for thin film analysis (LMC)	12:00–23:59: Sebastian Pischel +	+	09:00–23:59: Dr. Ronen Gottesman +	09:00–23:59: David Kérinec +	11:30–21:30: Maryam Nabil Shaker +	09:00–16:30: Moritz Kölbach 16:31–23:59: Raphael Präg +	09:00–23:59: Hasan Arif Yetkin +	00:00–00:00: Hasan Arif Yetkin +	+	+	09:00–16:30: Moritz Kölbach 16:31–23:59: Raphael Präg +	+	+
Bruker D8 for powder diffraction (LMC)	00:00–00:00: De Ning +		09:30–11:59: Sebastian Pischel 12:00–12:59: Fatma Avci 14:00–14:59: Fatma Avci 18:00–23:59: Yaolin Xu +	09:30–13:30: Dipl.–Ing. Zhenyu Wang 17:00–23:59: PhD student Ting Quan +	13:30–16:59: Jan–Ekkehard Hoffmann 17:00–23:59: PhD student Ting Quan +	17:00–23:59: PhD student Ting Quan +	09:00–23:59: Hasan Arif Yetkin +	00:00–23:59: Hasan Arif Yetkin +		17:00–23:59: PhD student Ting Quan +	12:15–16:59: Jan–Ekkehard Hoffmann 17:00–23:59: PhD student Ting Quan +	17:00–23:59: PhD student Ting Quan +	

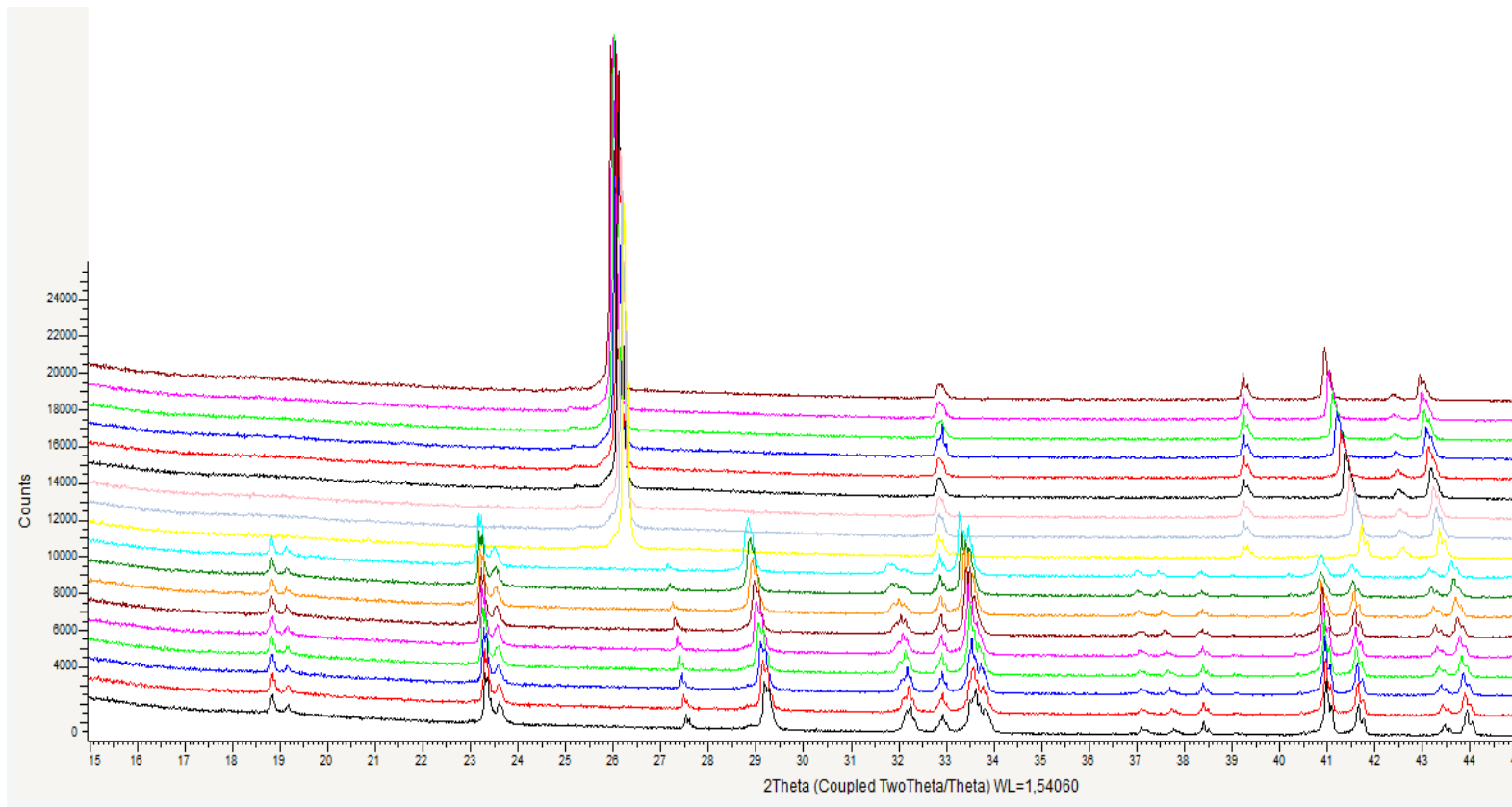
Bruker D8 Advance for analysis of thin films and powder diffraction



Bruker D8 for X-ray powder diffraction



Waterfall plot of temperature induced phase transition of KNO_3



Data format

Main data format is commercial

Bruker: .raw-binary file, with converter-Software to xy-file

Panalytical: -xrdml-ASCII-file, conversion to xy-file

```

Datei Bearbeiten Format Ansicht ?
<?xml version="1.0" encoding="UTF-8"?>
<xrdMeasurements xmlns="http://www.xrdml.com/XRDMeasurement/1.5" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://www.xrdml.com/XRDMeasurement/1.5 http://www.xrdml.com/XRDMeasurement/1.5/XRDMeasurement.xsd"
status="Completed">
  <comment>
    <entry>Configuration=Sample Spinner, Owner=User-1, Creation date=03-Apr-08 12:48:00 PM
    <entry>Goniometer=PW3050/60 (Theta/Theta); Minimum step size 2Theta:0.001; Minimum step size Phi:0
    <entry>Sample stage=Reflection-Transmission Spinner PW3064/60; Minimum step size Phi:0
    <entry>Diffractometer system=XPERT-PRO</entry>
    <entry>Measurement program=D:\user\Tovar\BB-measurement.xrdmp, Identifier={99370B4D-3A1
  </comment>
  <sample type="To be analyzed">
    <id></id>
    <name></name>
    <preparedBy></preparedBy>
  </sample>
  <xrdMeasurement measurementType="Scan" status="Completed" sampleMode="Reflection">
    <comment>
      <entry>Bragg-Brentano-Messfile</entry>
      <entry>PHD Lower Level = 7.56 (keV), PHD Upper Level = 12.87 (keV)</entry>
    </comment>
    <usedWavelength intended="K-Alpha">
      <KAlpha1 unit="Angstrom">1.540598</KAlpha1>

```



Datei	Bearbeiten	Format	A
15.003565140		115.0	
15.016695423		154.0	
15.029825705		125.0	
15.042955988		137.0	
15.056086271		107.0	
15.069216553		128.0	
15.082346836		136.0	
15.095477119		111.0	
15.108607401		122.0	
15.121737684		120.0	
15.134867967		123.0	
15.147998249		122.0	
15.161128532		134.0	
15.174258815		124.0	
15.187389097		125.0	
15.200519380		144.0	
15.213649663		127.0	
15.226779946		126.0	
15.239910778		120.0	

Problems:

- Data format depends on measuring method /instrument)
- Header (meta data) is lost during conversion process

Data are stored on hard drives on individual instrument PC in user folders:

The good:

- Uncomplicated system
- Web access via intranet
- No USB-Stick needed



The bad:

- Open structure: user can see data from other users
- Delocalised data
- No access from outside of HZB

Netzwerk
BIFEYER2
BLACKBOX6
CHEMLABPC1
CHEMLABPC2
DANTE
EMBRACE
EQEPC
FELIX
GDOES
GUESTEAKV
KIRMES
KIRU2
LENS
MIE92
NBHHGLAB
NOKRIST12
NOKRIST13
NOKRIST3
NOKRIST4
NONAMBIENT
NOTE37
PAULE
PETRO07
PVDPRACK
TA1
TOMOPC10
TOMOPC8
ULTRAFAST
VSMSQUID
XFMR01

Miriam Kegue
Monika
Moritz Kölbach
Moritz Lehmann
Natalia
Nga_Phung
Peng
Pepe
Philipp_Ortner
Prince
Radu
Raphael
Rehermann
Robin
Ronen
Ronneberg
Rowshanak
Ruslan
Sara
Saurabh
Schnell
Sean
Sebastián
Sergiu
Shanshan
Shargaieva
Suchan
Tim
Tockhorn
Tovar
Veronika
Weiwei
Yajie
z_height_adjustment
Zhang
Zhang

Regular and automatized data backup via net-backup

```
=====
CLIENT: xlabmpd3          POLICY: xlabmpd3.User-Data SCHEDULE: Full
=====
Backup started:      Thu Feb 21 19:02:42 2019
Backup type:         Server initiated Full Backup
Backup files:        D:\user
Backup ended:        Thu Feb 21 19:06:19 2019
Backup period:       217 seconds = 00:03:37
Backup tries:        1
Backup status:       0
- the requested operation was successfully completed
- No problems were detected with the requested operation.
Backup volume:       9,238 files; 449,898 KB
Backup throughput:   42.57 files/sec; 2,073.26 KB/sec
Retention period:    6 months
```

The good:

- Unkompliated management (set-it-and-forget-it)

The bad:

- Who is really responsible for the data? DV, Lab responsables, Users?

Open issues:

- Individual and secure data environment:
Users should only be able to see the own data but not data from other users
- Users should see all own data from all instruments
- Data access independent from hardware (cloud)
- **Meta data** should not get lost
- Responsibility for data storage and access

What will be needed to be done...

Open issues:

How to do this and who is going to do it? 😊

Thank you for your attention.