

The Material Engineering Diffractometer BEER at ESS

What we have and what we envision

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Software Workshop on Engineering Diffraction



Outlook

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Introduction

Operation modes

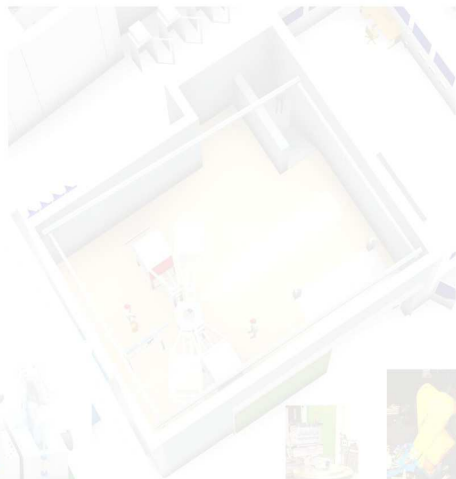
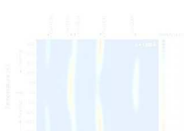
Full pattern

Single peak

1 Introduction
Operation modes

2 Full pattern fitting example

3 Single peak fitting example





Operation modes

Modes classification by Intensity and Resolution

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Introduction

Operation modes

Full pattern

Single peak

IR modes	Neutron flux ($\lambda = 0.8 \dots 2.5 \text{ \AA}$) $[n \cdot s^{-1} \cdot cm^{-2}]$	$\Delta d/d$ [%]
high flux (HF)	$0.8 \cdot 10^9$	1.2
medium resolution (MR)	$0.7 \cdot 10^8$	0.36
high resolution (HR)	$0.4 \cdot 10^7$	0.15
multiplexing (MHR)	$0.3 \cdot 10^8$	0.11
multiplexing (MLR)	$0.2 \cdot 10^9$	0.33

Wavelength selection options

- basic wavelength bandwidth 1.7 Å
- single frame × double frame (3.4 Å)
- alternating frames → diffraction and SANS



Operation modes

Modes classification by Experimental method

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Operation modes

Full pattern

Single peak

• Diffraction

- only diffraction data are needed
- all IR modes available
- all wavelength selection options

• Diffraction and SANS

- Diffraction and SANS data collection
- all IR modes available
- alternating frame selection
- double frame only with multiplexing

• Diffraction and imaging

- not truly simultaneous
- fast beam adaptation for each method
- no multiplexing



Operation modes

Modes classification by Sample environment

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Operation modes

Full pattern

Single peak

- mechanical or thermo-mechanical experiments
 - deformation rigs with furnaces or cryogenic system
 - dilatometers
 - multi-axial deformation rigs
 - Gleeble[®]
- heating or cooling experiments
 - furnaces
 - cryostats
 - cryo-furnaces
- sample scanning experiments - strain scanning, texture
 - hexapod
 - robot
 - cybaman
- in-operando experiments
 - welding or forging machines
 - corrosion chambers
 - user sample environment, ...
- ...



Operation modes

Modes classification by Experiment control

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Operation modes

Full pattern

Single peak

- **standard experiment flow**
 - set SE parameter and wait till stabilization
 - collect scattering data
 - set SE parameter to another point
 - collect scattering data
 - ...
- **advanced experiment flow**
 - set SE procedure as independent process
 - start SE procedure
 - collect scattering data continuously
 - not stop SE procedure when beam is unavailable
- **active feedback experiment**
 - set SE parameter and wait until predefined condition is fulfilled
 - collect scattering data continuously
 - condition based on real-time data analysis
 - adapt SE procedure and continue



Operation modes

Modes classification by Data analysis

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Operation modes

Full pattern

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- Full pattern fitting
 - Rietveld refinement of full pattern
 - patterns linked with SE status
 - need for phase transformation analysis
 - sequential refinement of multiple datasets
- Single peak fitting
 - fitting of individual reflection separately
 - peak parameters linked with SE status
 - automatic peak search and indexing routine
 - used in strain scanning, profile analysis or deformation experiments
 - possible complex and/or user defined profile functions
- Texture measurement
 - partial or full PF data analysis
 - full texture measurement with rotation
 - *in-situ* texture evolution

Full pattern fitting

Phase transformation analysis experiment example

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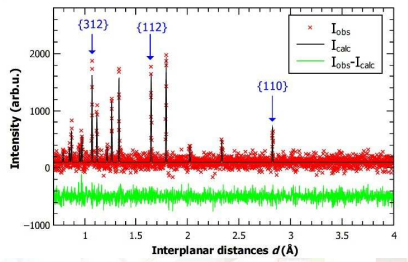
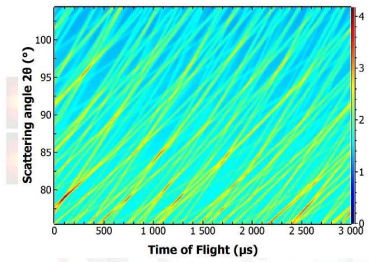
Introduction

Operation modes

Full pattern

Single peak

- Visualisation
 - Live visualisation of 1D $I(Q)$, $I(d)$ and 2D $I(\text{ToF}, \text{angle})$



Full pattern fitting

Phase transformation analysis experiment example

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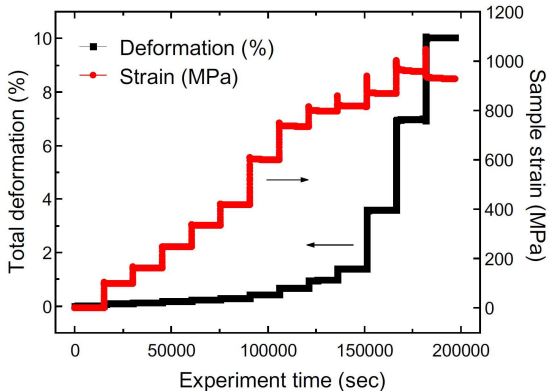
Operation modes

Full pattern

Single peak

- Visualisation

- Live visualisation of 1D I(Q), I(d) and 2D I(ToF, angle)
- Live view of SE parameters and their evolution



Full pattern fitting

Phase transformation analysis experiment example

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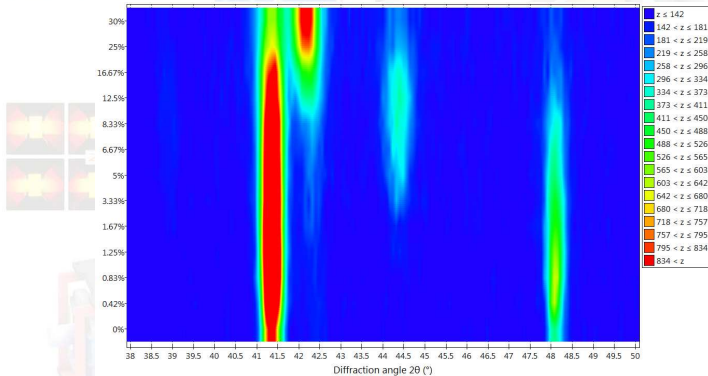
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- Live visualisation of 1D I(Q), I(d) and 2D I(ToF, angle)
- Live view of SE parameters and their evolution
- 2D colour maps of 1D patterns vs. SE status





Full pattern fitting

Phase transformation analysis experiment example

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- Live view of SE parameters and their evolution
- 2D colour maps of 1D patterns vs. SE status

- Data analysis

- Rietveld refinement of 1D pattern (FullProf, GSAS, Maud, ...)
- Refinement of 2D data (POLDI, POWTEX)
- Micro-structural models (size/strain) of isotropic/anisotropic peak broadening (FullProf but only for constant wavelength data)



Full pattern fitting

Phase transformation analysis experiment example

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- Final output

- Phase evolution as a function of SE parameter
- Evolution of micro-structural parameters for each phase

Single peak fitting

Deformation experiment example

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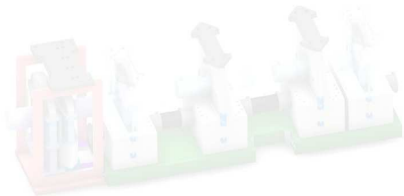
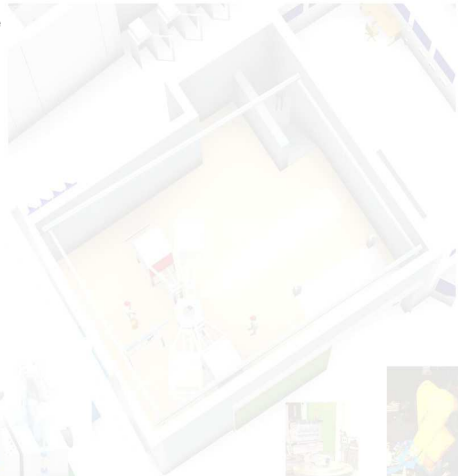
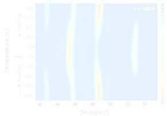
Introduction

Operation modes

Full pattern

Single peak

- **Visualisation** - same as before



Single peak fitting

Deformation experiment example

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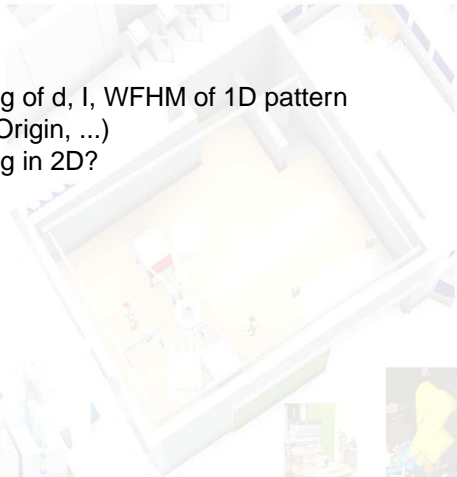
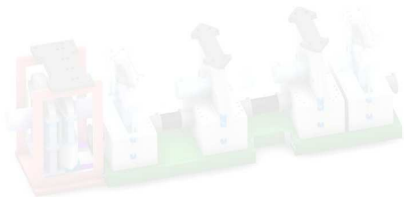
Introduction

Operation modes

Full pattern

Single peak

- Visualisation - same as before
- Data analysis
 - Individual peak fitting of d , l , WFHM of 1D pattern (WinPlotr, PeakFit, Origin, ...)
 - Individual peak fitting in 2D?





Single peak fitting

Deformation experiment example

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Operation mode

Full pattern

Single peak

- Visualisation - same as before
- Data analysis
 - Individual peak fitting of d , I , WFHM of 1D pattern (WinPlotr, PeakFit, Origin, ...)
 - Individual peak fitting in 2D?
- Final output
 - Evolution d , I , FWHM as a function of SE parameter

