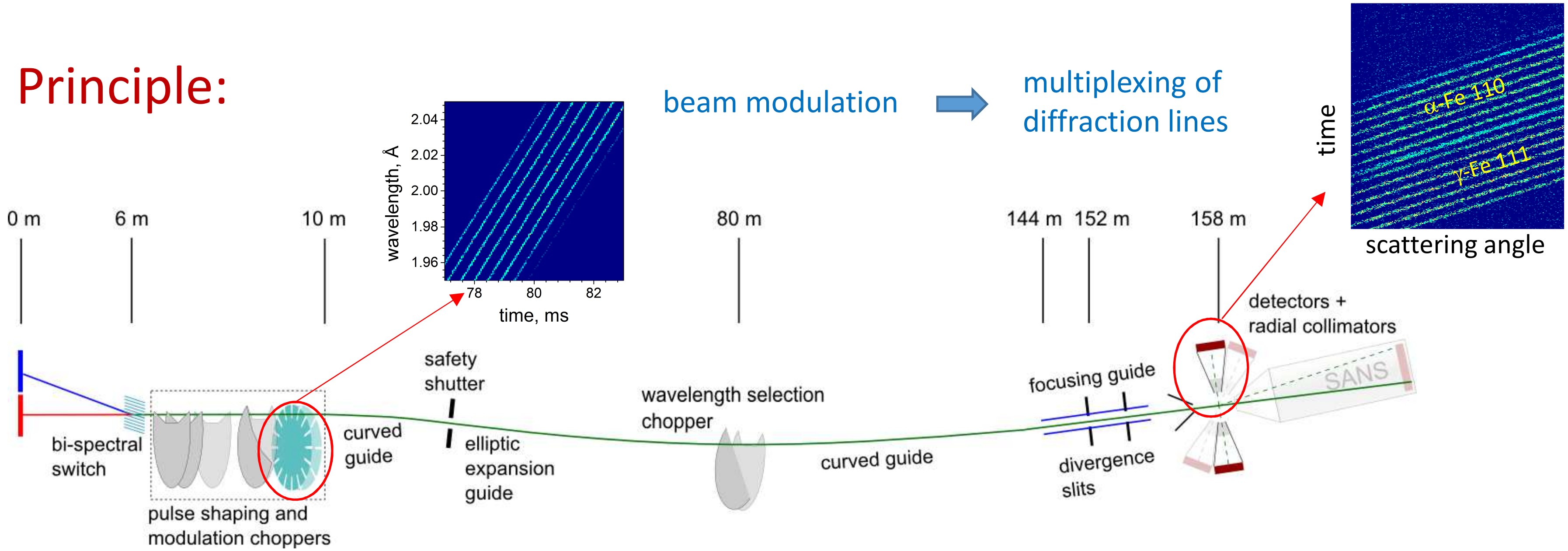
BEER multiplexing mode: data reduction

Přemysl Beran, Jan Šaroun
Nuclear Physics Institute CAS, Czech Republic

Jochen Fenske, Gregor Nowak, Mustapha Rouijaa
Helmholtz-Zentrum Geesthacht, Germany

- Multiplexing mode is specific to BEER
- Development of data reduction SW is required
- Proof of principle and validation on simulated data have been done

Principle:



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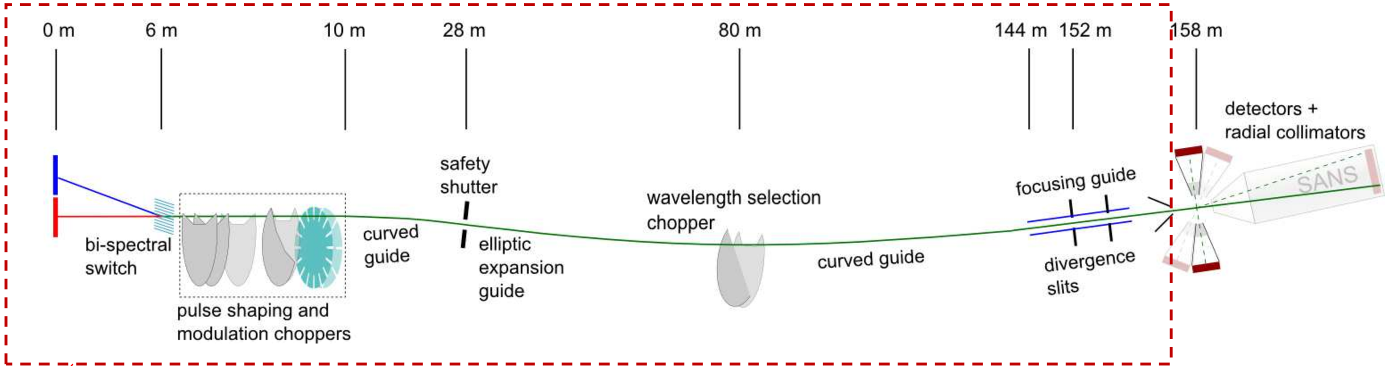
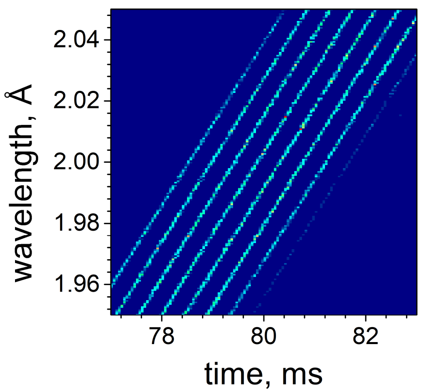


Validation:
using simulated data

Primary diffractometer
ray-tracing simulation with **Simres**

Beam structure at the sample produced by the modulation chopper
280 Hz, 8 slits x 4° (*), input slit 1 x 2 mm²

(*) Considered replacement for the original proposal 4 x 4°.



primary neutrons exported to MCPL ⇒ MCPL file ⇒ imported to a **McStas** model of the secondary diffractometer

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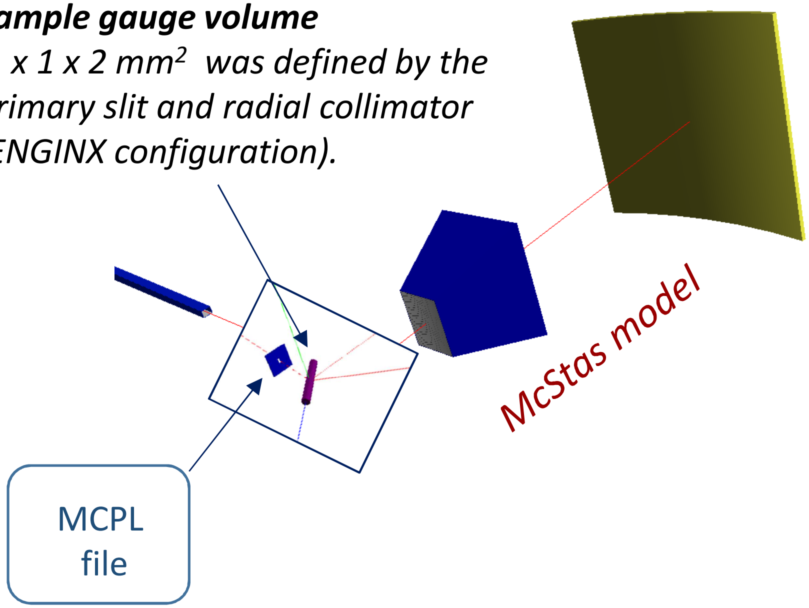
Secondary diffractometer:

ray-tracing simulation with **McStas**

Sample gauge volume

1 x 1 x 2 mm² was defined by the primary slit and radial collimator (ENGINX configuration).

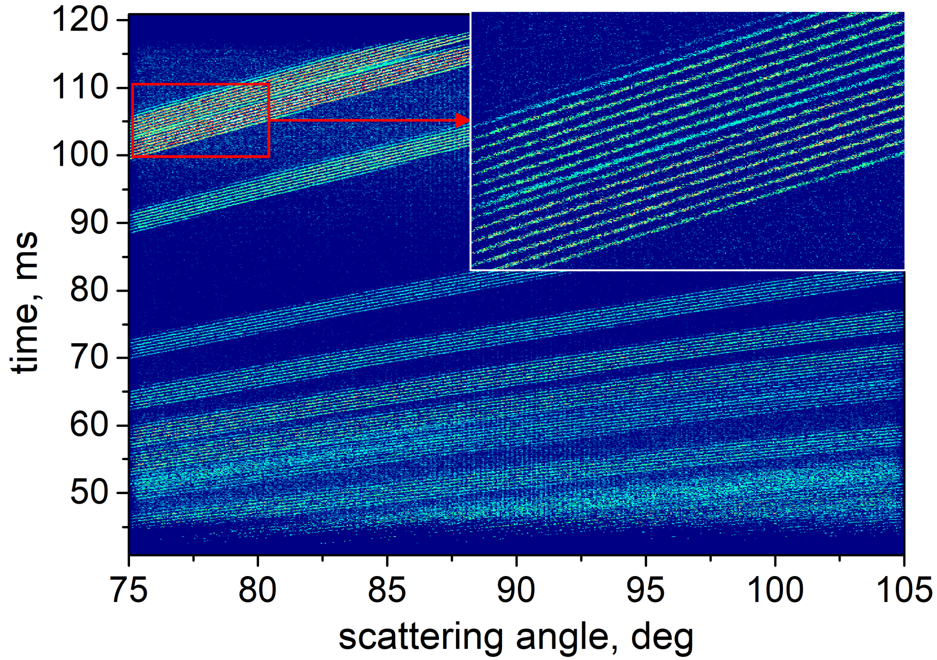


Sample: *duplex steel*

The components *SampleN.comp* and *Incoherent.comp* were used to model dia=7 mm duplex steel rod in 45° orientation.

Detector parameters:

- resolution (h x v) = 2 x 5 mm²
- L_{free} = 1 cm Å
- area 1 m²

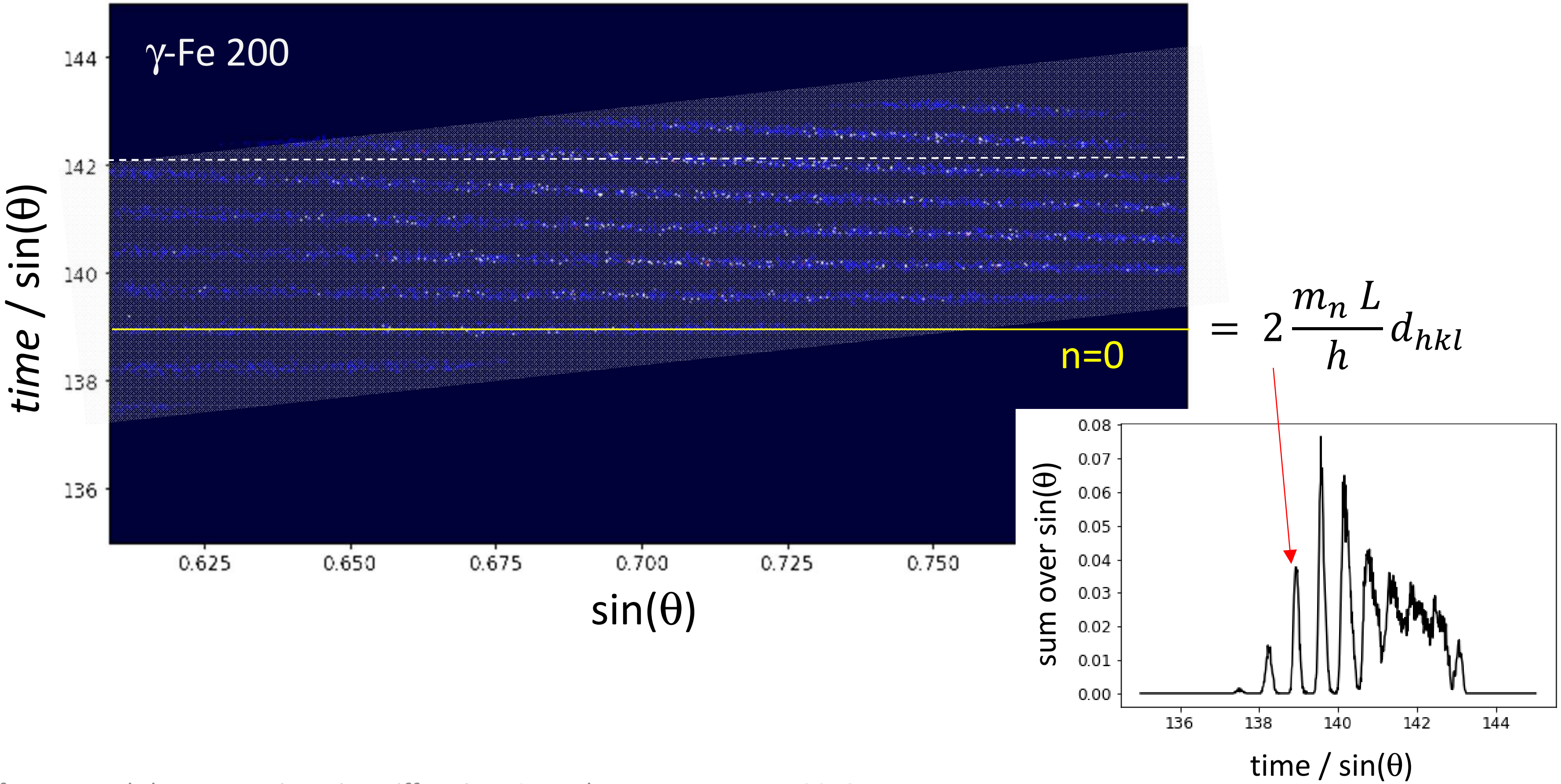


New component (`tof_dhkl_detector.comp`) has been written to perform **event based data reduction in modulation regime.**

ToF from the chopper

$$\frac{time}{\sin\theta} = 2\frac{m_n L}{h} d_{hkl}$$

The chopper phase is adjusted for a certain "master" slit (*n*=0) corresponding to *time* = 0.



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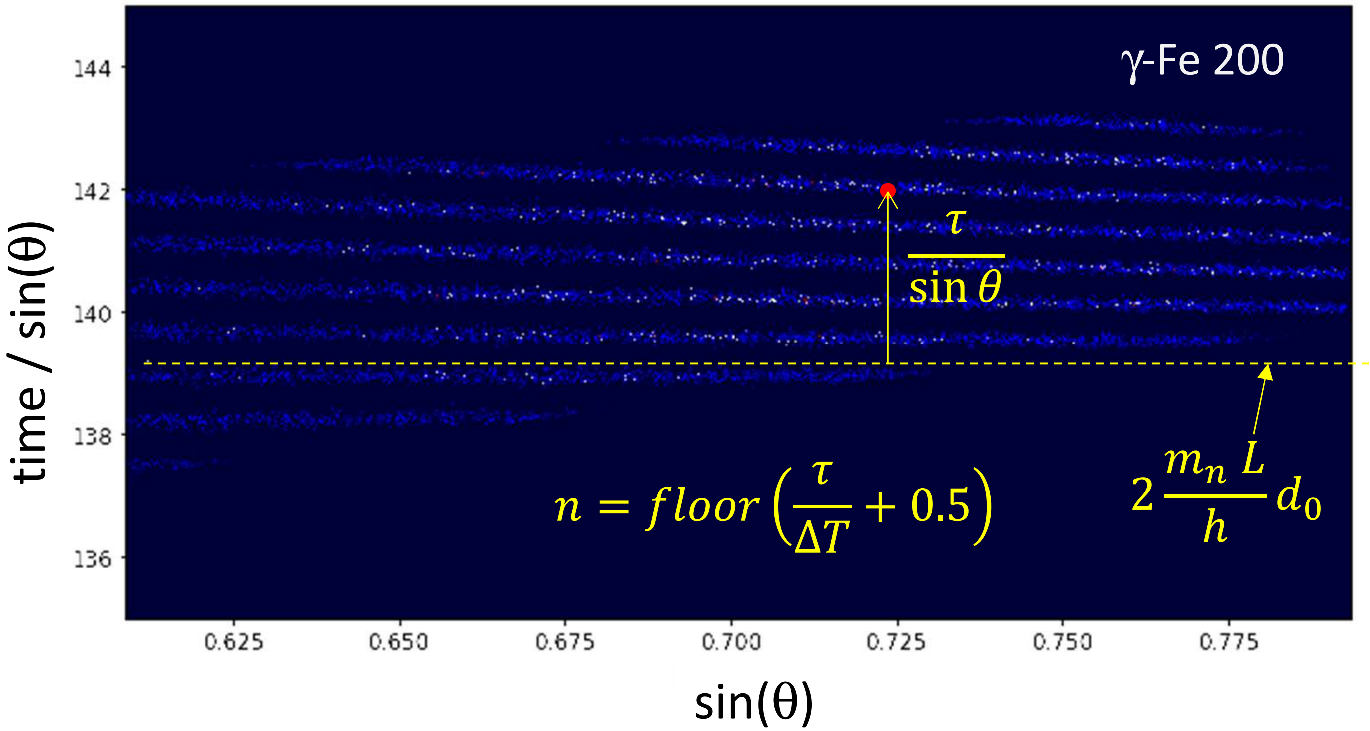
How to find the "master" line with n=0 ?

1. Guess d_0 and find the nearest line, or
2. Pick the $I(t/\sin\theta)$ line with the smallest FWHM.

Option 1 tested:



For each event (t, θ) calculate $d_{hkl} = \frac{h(t - n\,\Delta T)}{2m_n\,L\sin\theta}$ and sort into a d_{hkl} histogram.

Required accuracy of d_0 estimate: $\delta d_0 < \approx \frac{\Delta T}{t} d_0$

For this example: $\frac{\delta d_0}{d_0} < 0.005$

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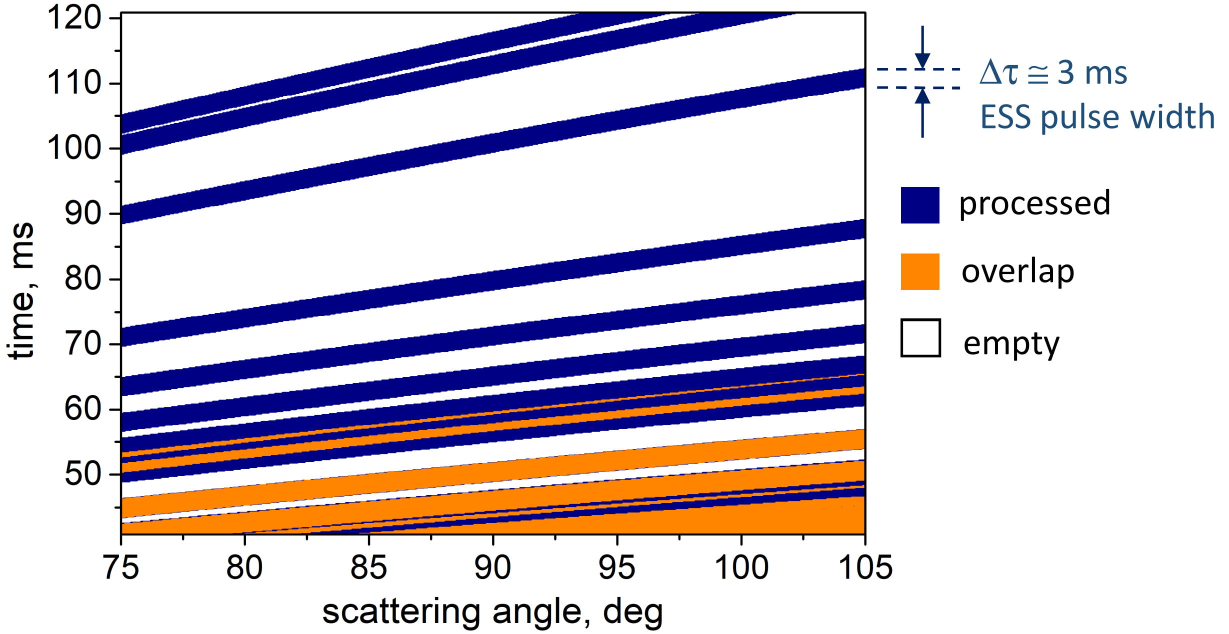
McStas detector component `tof_dhkl_detector.comp`

- Accounts for spatial and time resolution of the detector
- Performs conversion of detection events (x, y, z, time) → (2θ, time) → d_{hkl}

Handling of multiplexed data:

– Requires a list of d_{hkl} estimates.
– Estimates the index of the nearest t_0 chopper window and corrects for its phase.
– Excludes overlapping lines. Only (2θ, time) – events along the expected lines are processed.

Data mask



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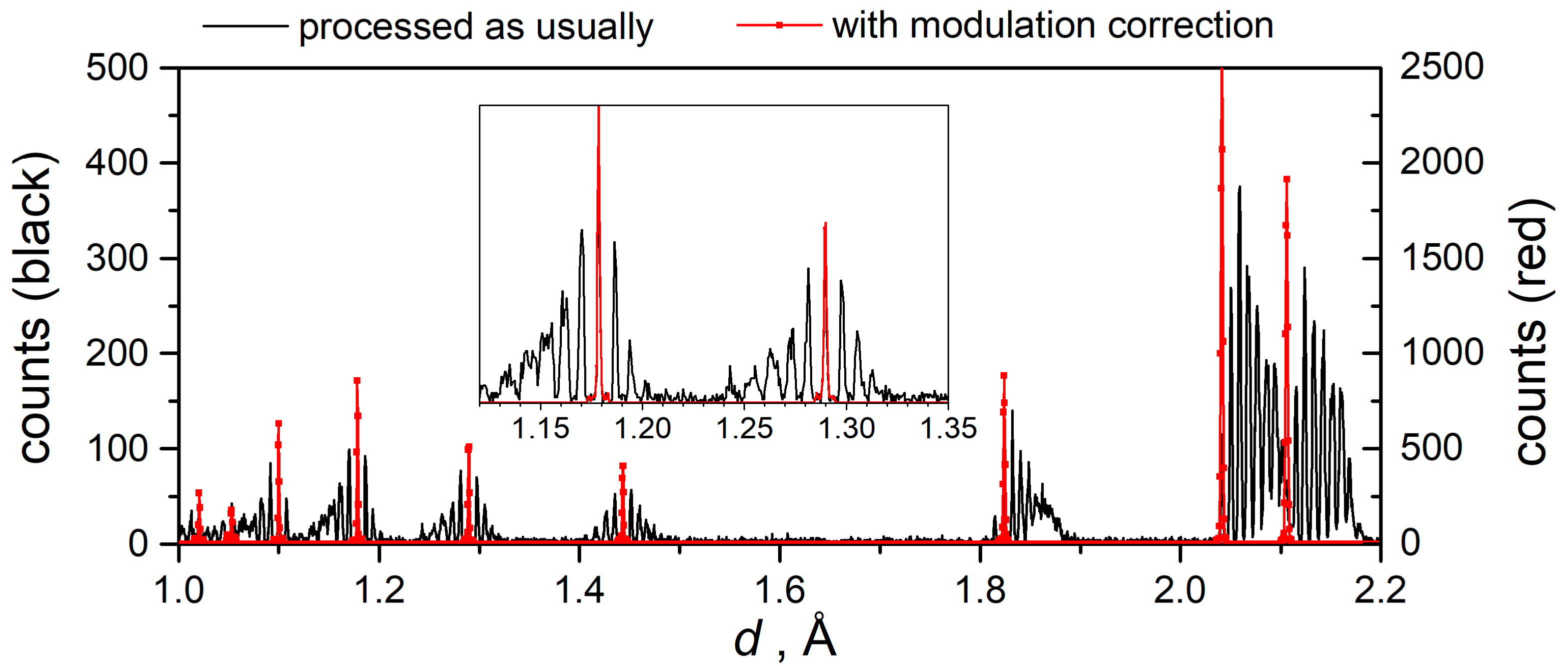
Accumulated diffractograms assuming a single chopper window (black) and with account for the modulation (red).



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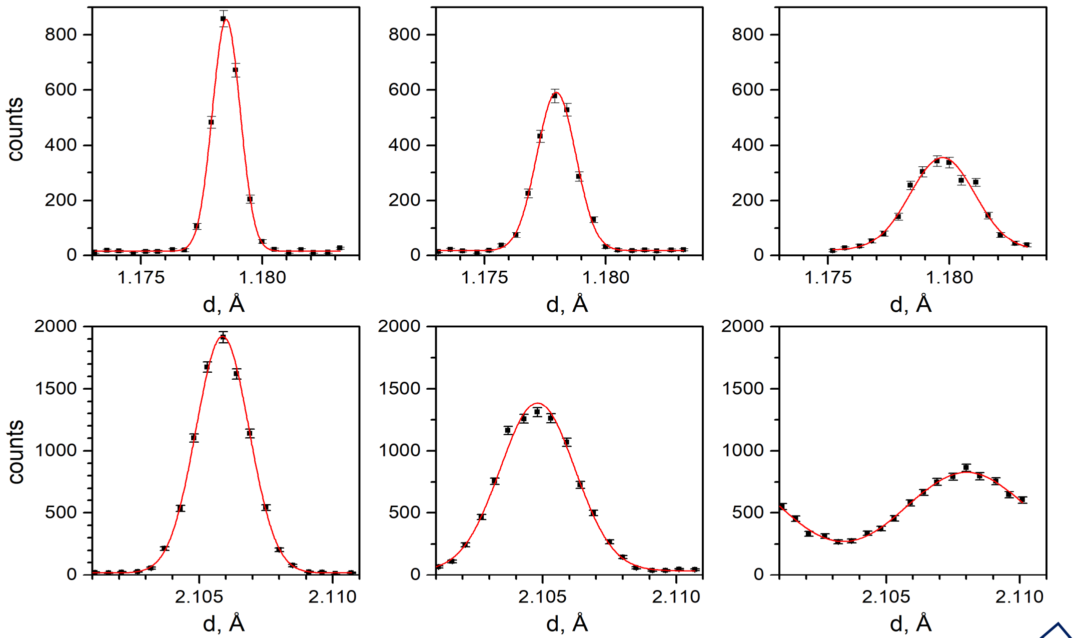
Diffraction peaks after data reduction + Gaussian fit.

stress free	ε=-500 $\mu\varepsilon$ σ=500 $\mu\varepsilon$	ε=1000 $\mu\varepsilon$ σ=1000 $\mu\varepsilon$



α-Fe(211)

γ-Fe(111)

Simulated counts were scaled to 60 s exposure time at 5 MW power + Poisson noise added.

	original	fit Fe(211)	fit Fe(111)
peak shift	-500	-471 *(21)*	-506 *(14)*
broadening	500	479 *(60)*	469 *(90)*
peak shift	1000	1020 *(42)*	1016 *(170)*
broadening	1000	1031 *(140)*	1053 *(70)*

For strong peak broadening, sum of 3 equal peaks separated by the modulation period have to be taken as the fitting function.

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Requirements

- We prefer raw data as a list of events rather than a 2D matrix (t, θ)
  NOTE: ~ 10^5 counts in the diffraction signal is enough, but a high pixel resolution is required (δt < us, δθ < 0.05 deg) => ~ 10^7 pixels in a matrix.
- Recording of the modulation chopper phase is necessary.
  A drift by > 1μs causes observable pseudo strains.
- Interactive UI allowing control of the data reduction steps explained above:
  - 2D plots: I(θ, t), I(sin θ, t/sin θ)
  - 1D plots: I(t/sin θ), I(d_{hkl})
  - assignment of the diffraction sub-lines to the chopper slit index
  - selection of valid areas on the I(θ, t) map

Conclusions

- Data reduction to the standard 1D diffractograms is feasible (validated on synthetic data) => using of standard data analysis SW (FullProf, MAUD, Jana, ...) should be possible.
- Suitable for lattice strain measurements (peak shifts and broadening).
- Limited use for low-symmetry and multiphase materials (too many overlaps)
- Rietveld analysis to be tested. Normalization of intensities: using of an isotropically scattering sample (PE, plexi glass, V) should work, but ...
- Possible additional problems with d_0 determination: uncertainty of $\pm\frac{\Delta T}{t}d_0$.
- Peak broadening limited to $<\frac{\Delta T}{t}$ (should be OK for usual bulk materials, but not for fine grained phases)
- Options for 2D pattern fitting to be investigated ...