Complex environment engineering diffractometer (CEED)

Conceptual design update
Update of performace characteristics by MC simulations

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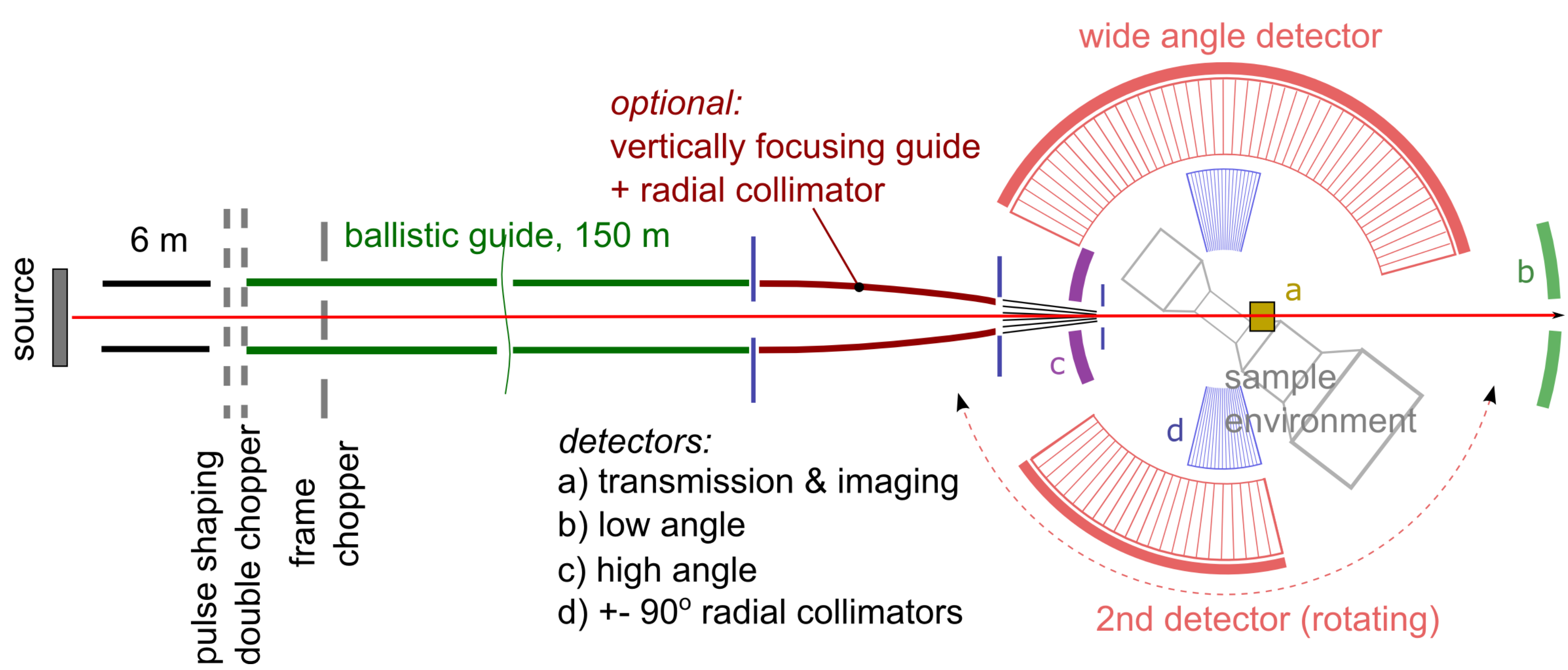
New features tested by MC simulations

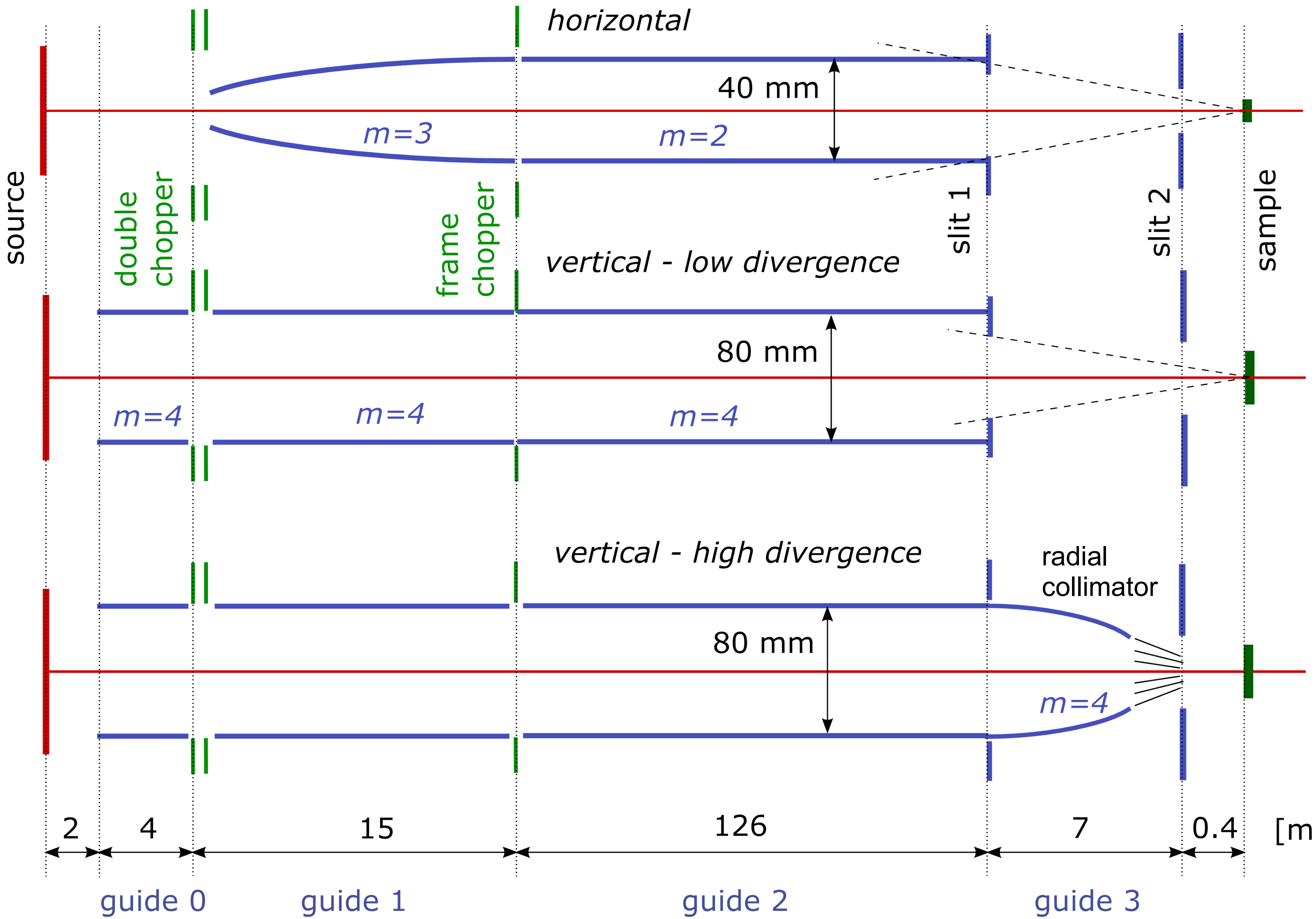
- Updated neutron guides geometry
- Radial collimators for small gauge volumes
- Double chopper for constant $\Delta\lambda/\lambda$ resolution
- Double frame option
- New virtual samples for "engineering" materials: duplex steel, TiAl alloy

CEED design

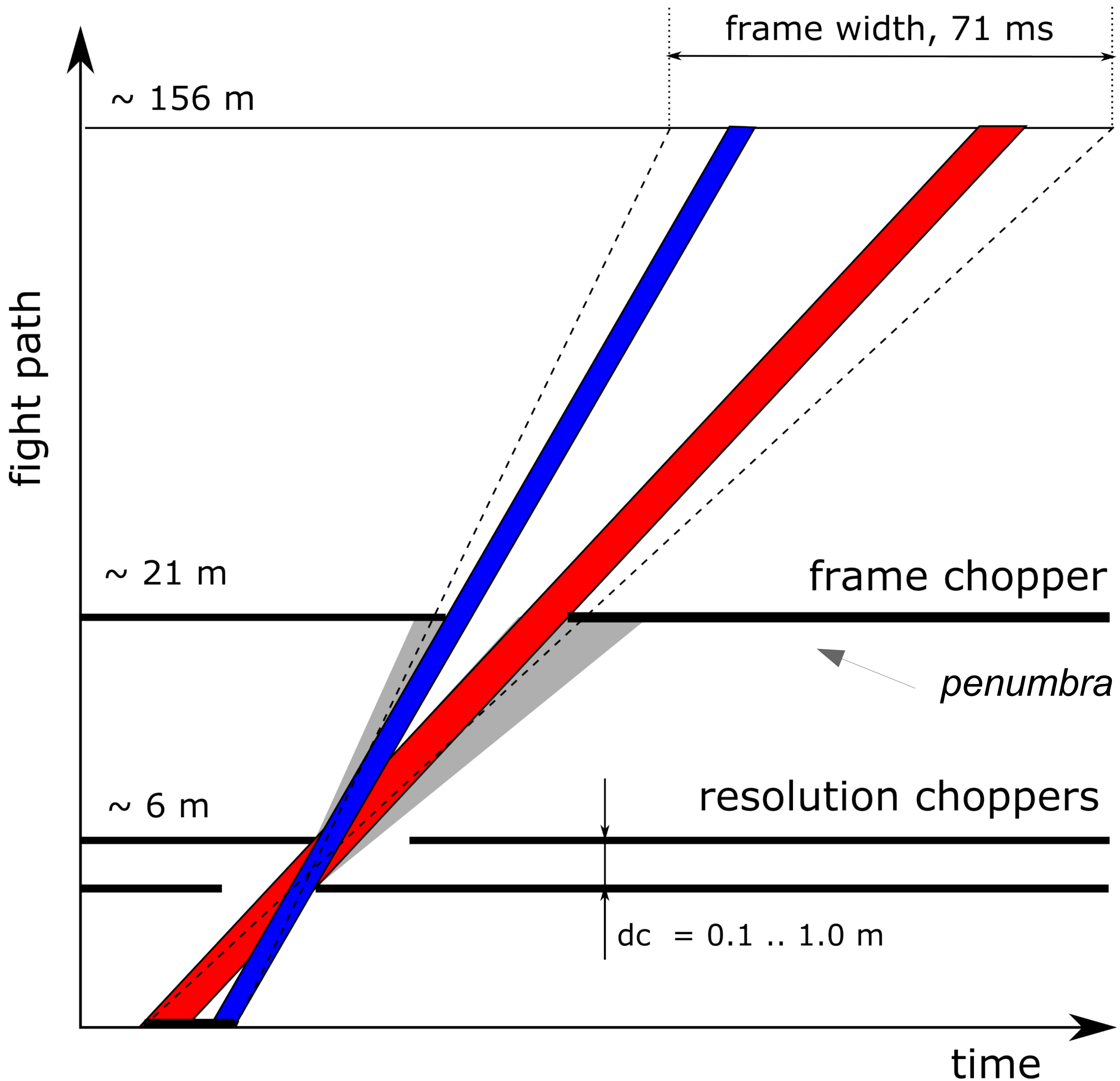
a very schematic view ...



CEED design - primary beam



Double chopper for pulse shaping



Test setup:

2-frames

λ_1=1.8 Å

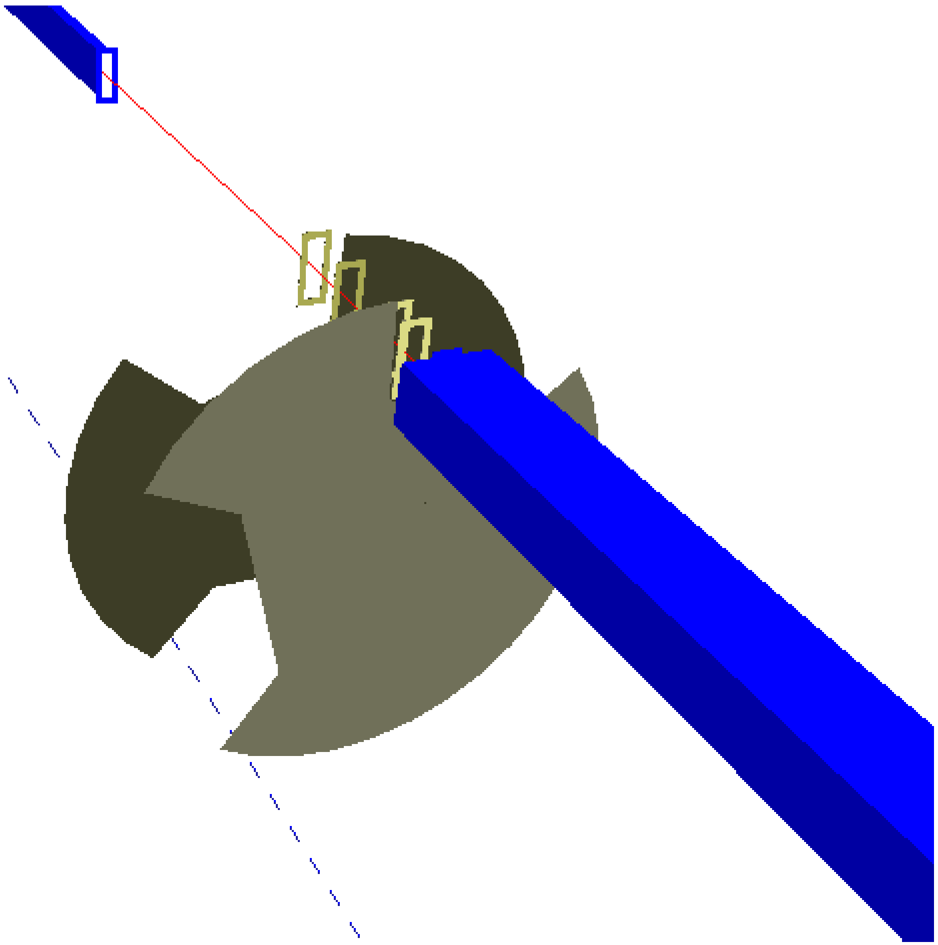
λ_2=3.6 Å

total range:

$\Delta\lambda$ = 0.9 .. 4.5 Å

similar e.g. to D33/ILL but limited source pulse duration = limited band width

Double chopper



RESTRAX view of the simulation model

Chopper characteristics

outer radius: 350 mm
frequency: 140 Hz
window angles: ~ 54 and 72 deg

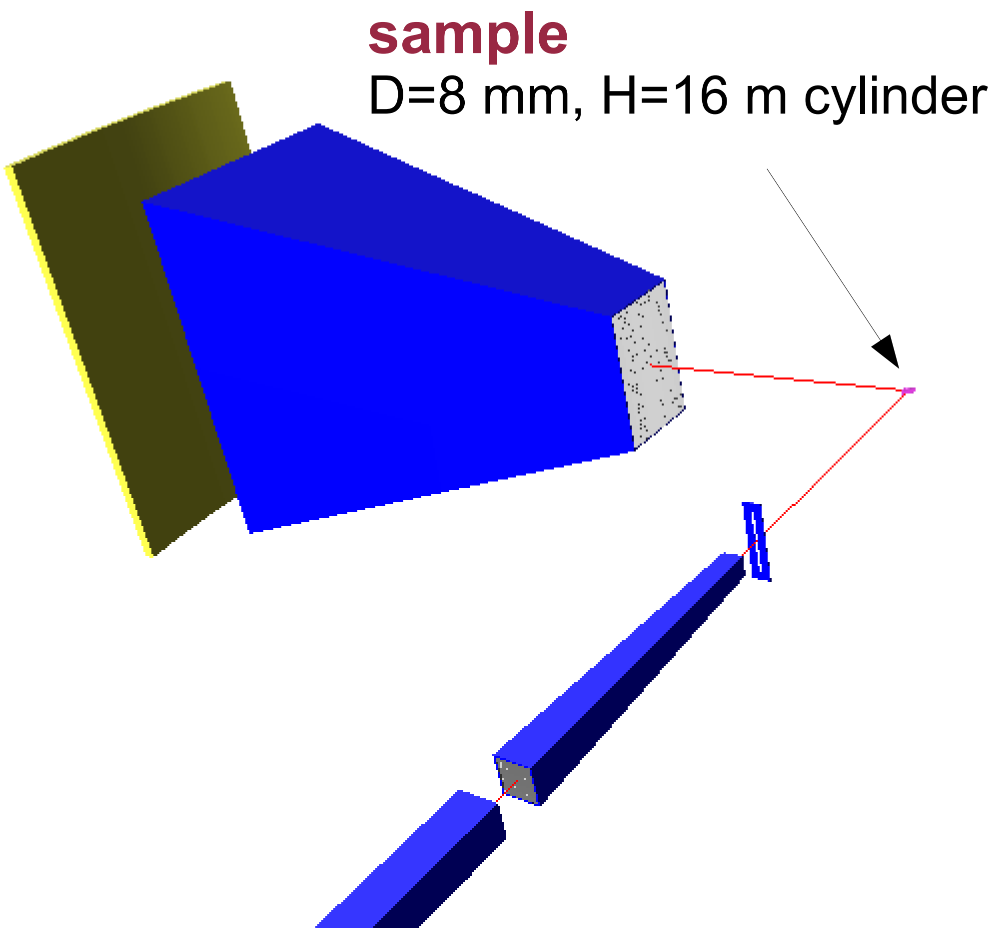
distances:

high resolution (HR)
0.2 m ... τ = 50 μs at λ=1 Å

low resolution (LR)
1.0 m ... τ = 250 μs at λ=1 Å

Two choppers operating in "blind" mode:
chopper 1 closes when chopper 2 opens - provides flat $\Delta\lambda/\lambda$– resolution curve

Sample area at 90° configuration



RESTRAX view of the simulation model

Incident beam

free path to the sample: 400 mm

vertical: radial collimator

acceptance angle	3 deg
number of slits	17
length:	400 mm

horizontal: slit, variable width

Scattered beam

free path to the sample: 400 mm

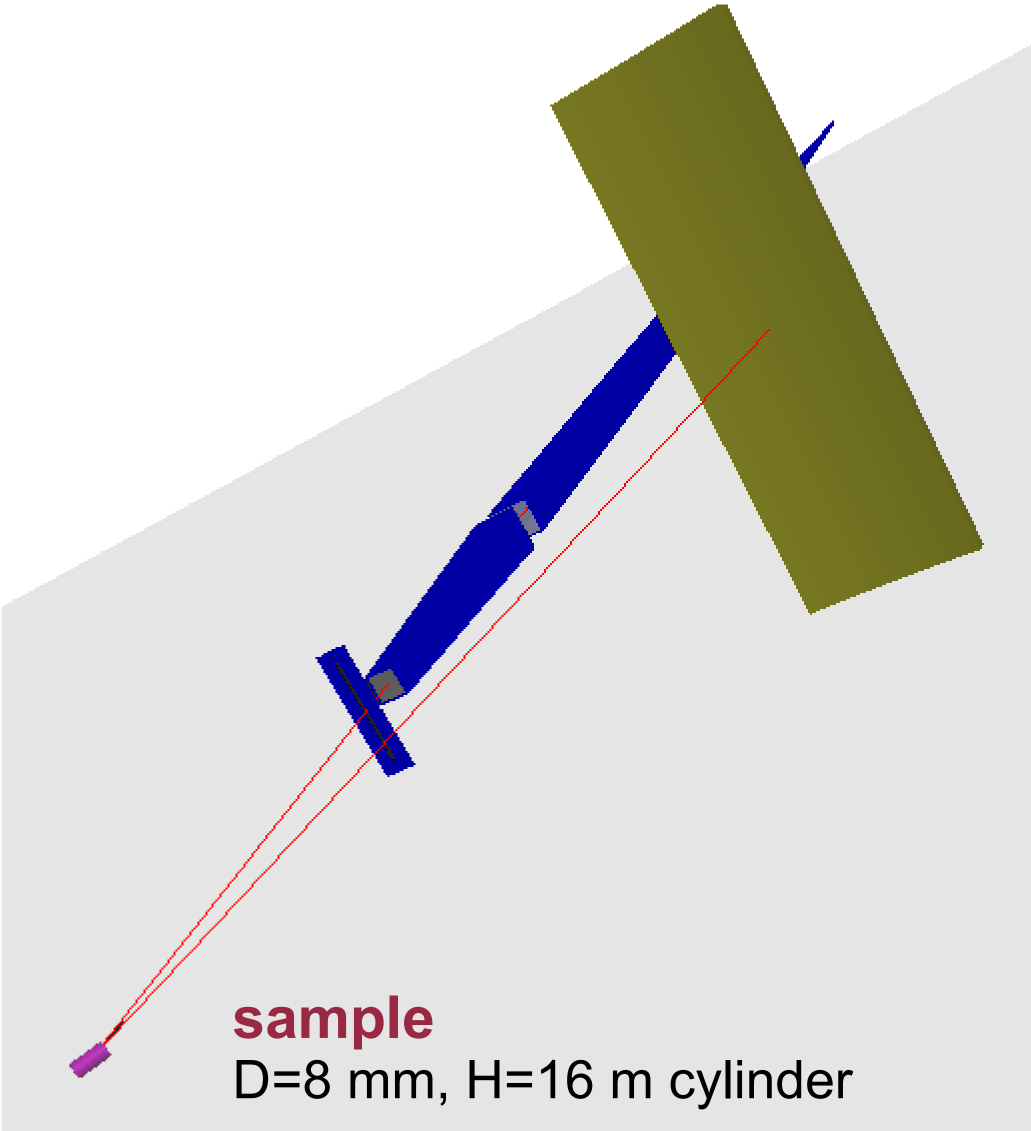
vertical: no collimator

acceptance angle	30 deg

horizontal: radial collimator

acceptance angle	20 deg
number of slits	81
length:	800 mm

Sample area at 170° configuration



RESTRAX view of the simulation model

Incident beam

the same as at 90°

Scattered beam

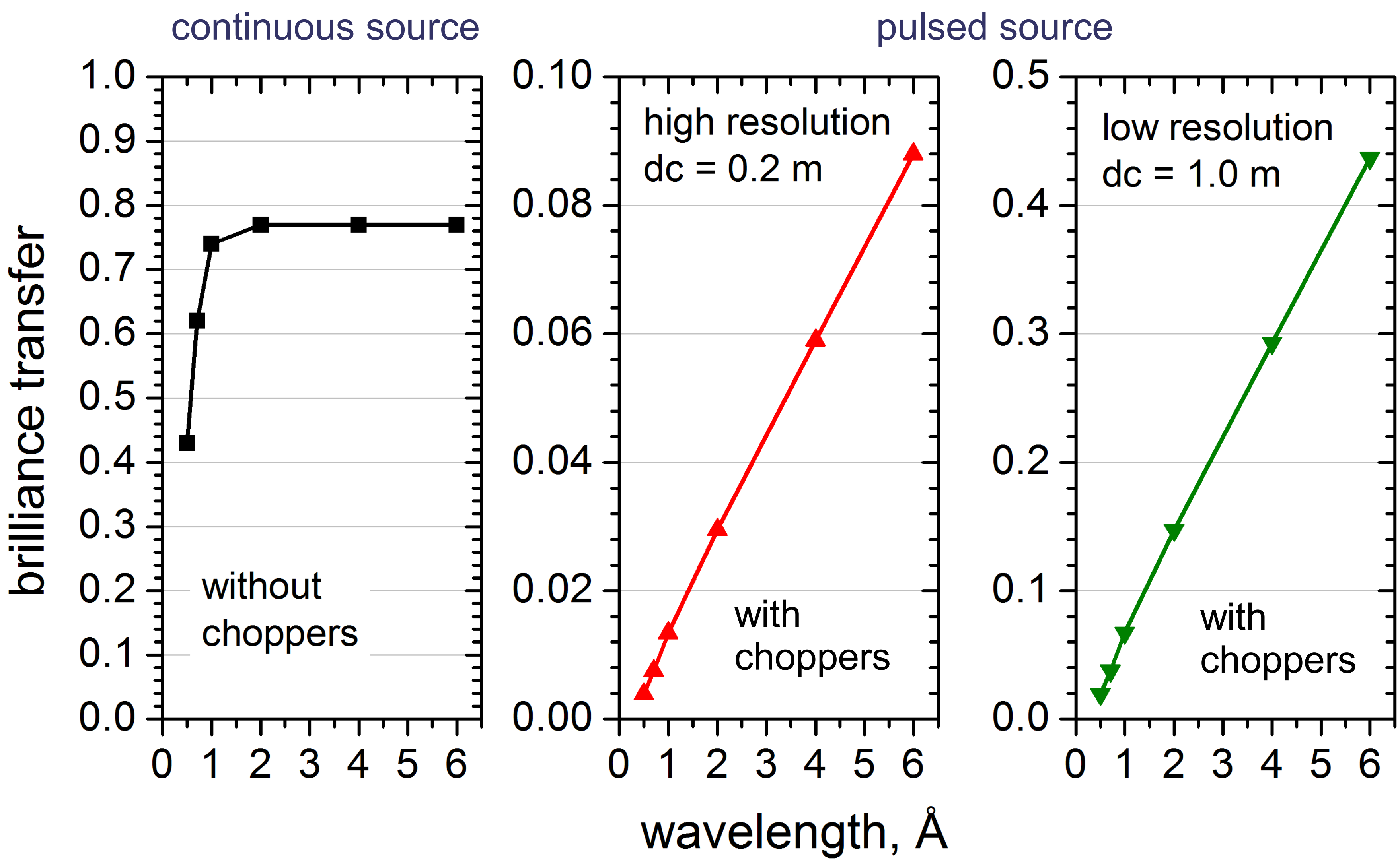
vertical: no collimator

acceptance angle 30 deg

horizontal: no collimator

acceptance angle 10 deg

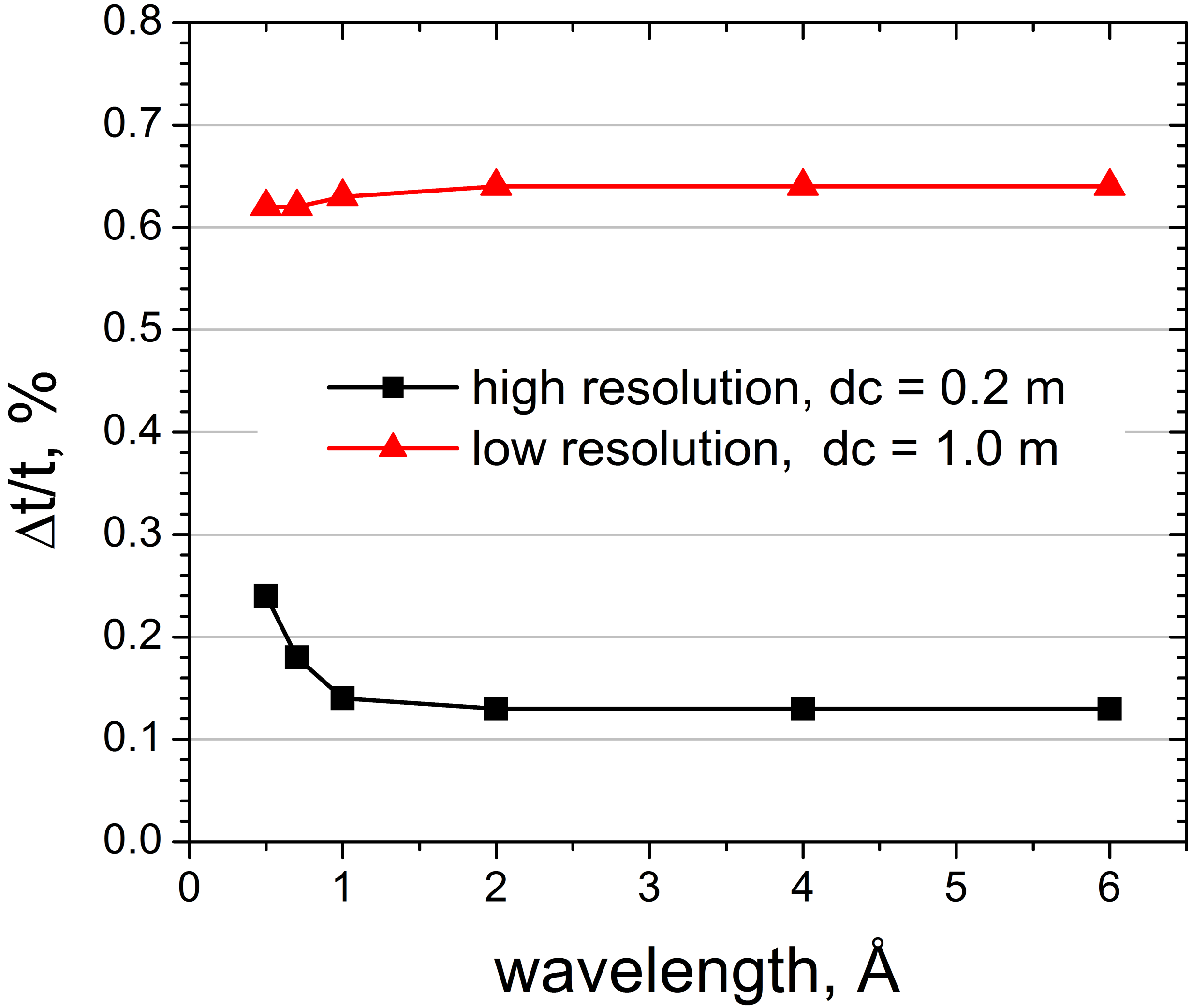
Brilliance transfer to the sample   no radial collimators



Brilliance transfer as a function of wavelength

integration volume: dS = 5 x 10 mm^2, dΩ = 0.3 x 0.3 deg^2

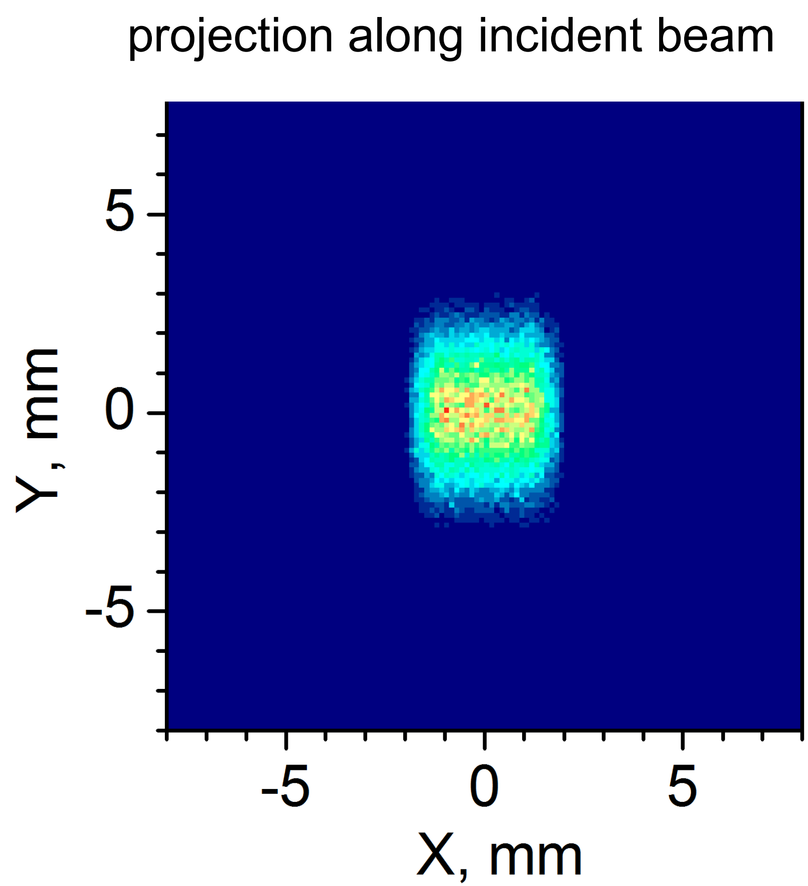
Time resolution

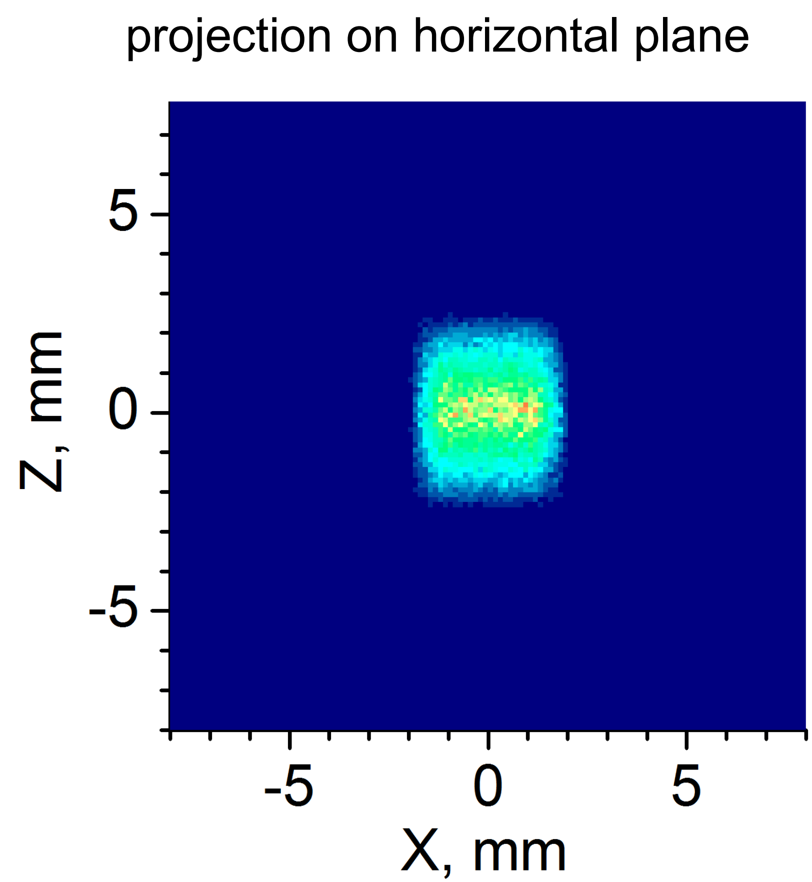


Nearly constant Δλ/λ resolution as produced by the double chopper for different distances, *dc*=0.2 and *dc*=1.0 m.

Beam width 2 cm => worse resolution at short wavelengths

Gauge volume, 2θ = 90°





Gauge volume is defined by the **two radial collimators**
- vertical (before the sample)
- horizontal (after the sample)

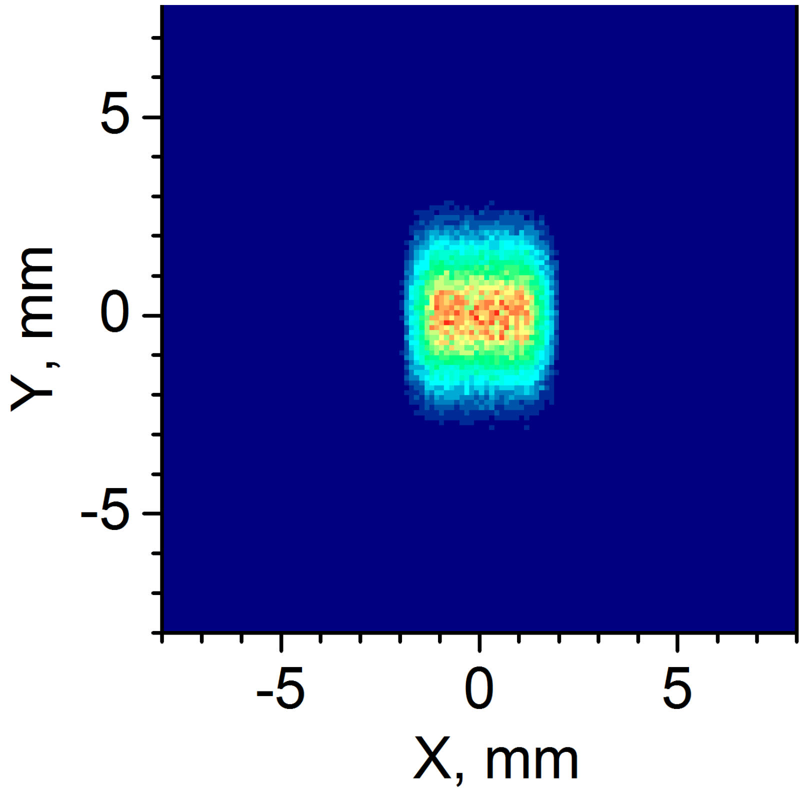
and input slit

free space around the sample: *R*=400 mm

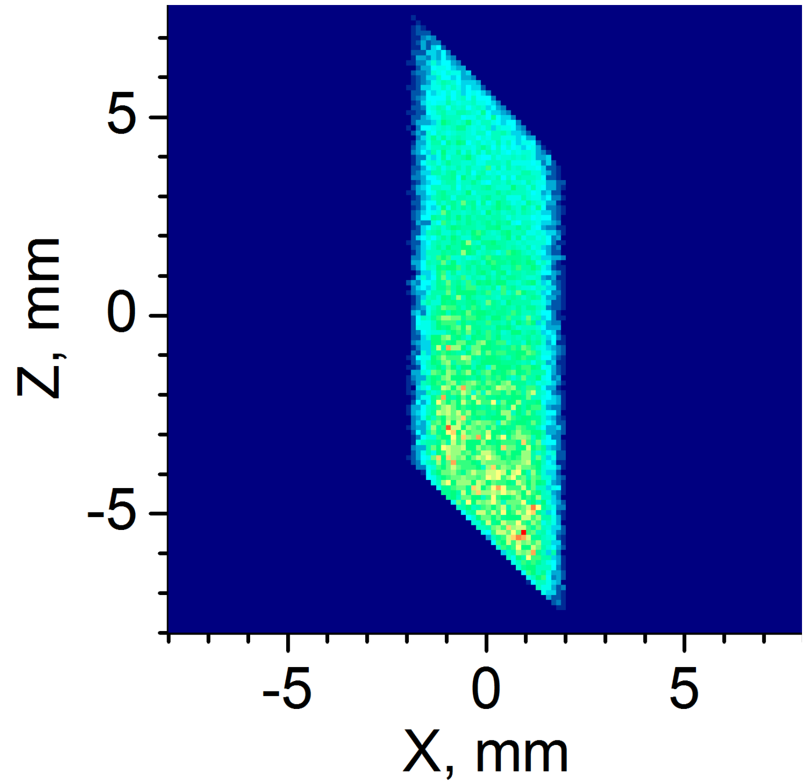
Integrated volume:
~ 25 mm^3

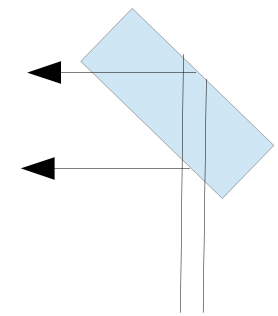
Gauge volume, 2θ = 170°

projection along incident beam

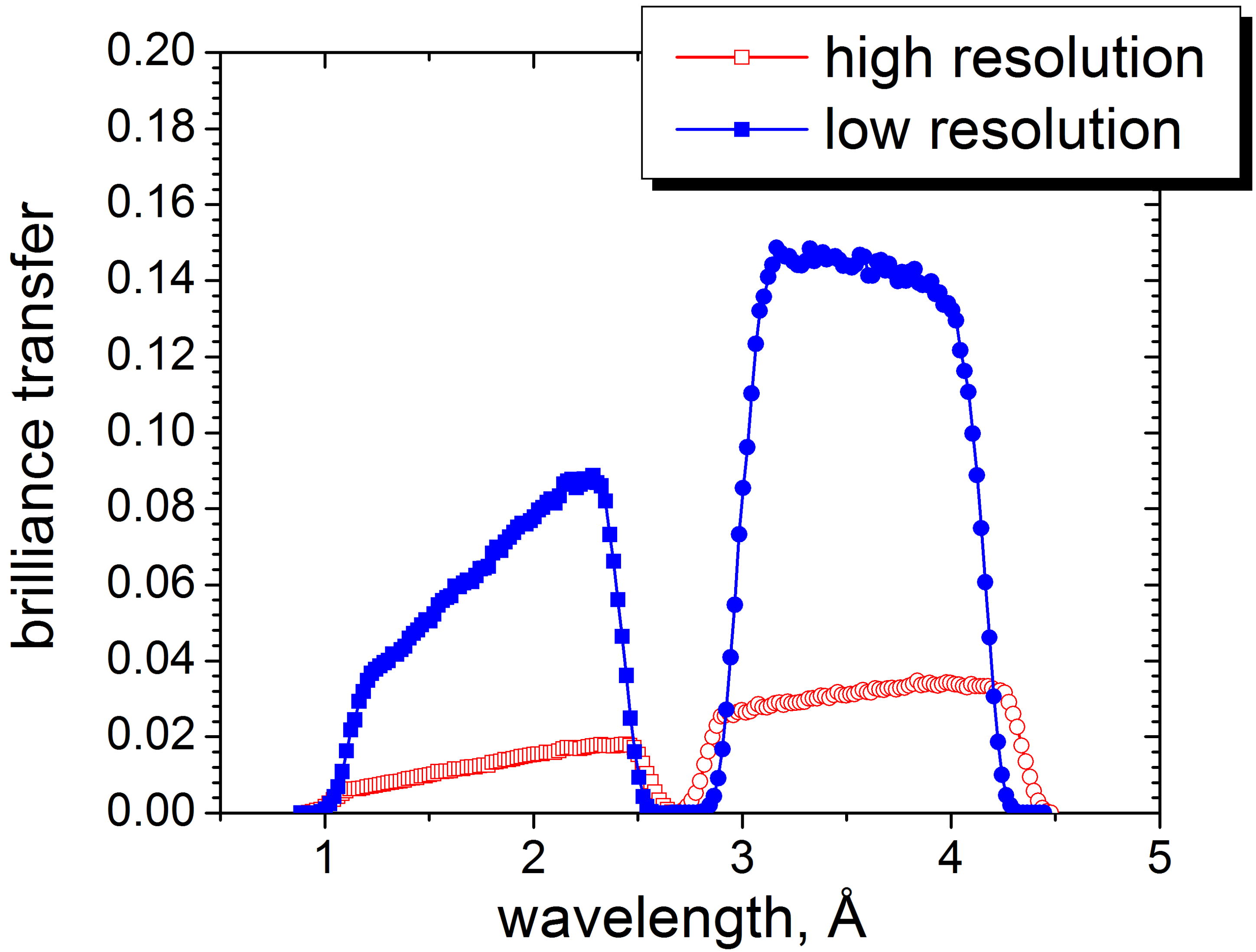


projection on horizontal plane



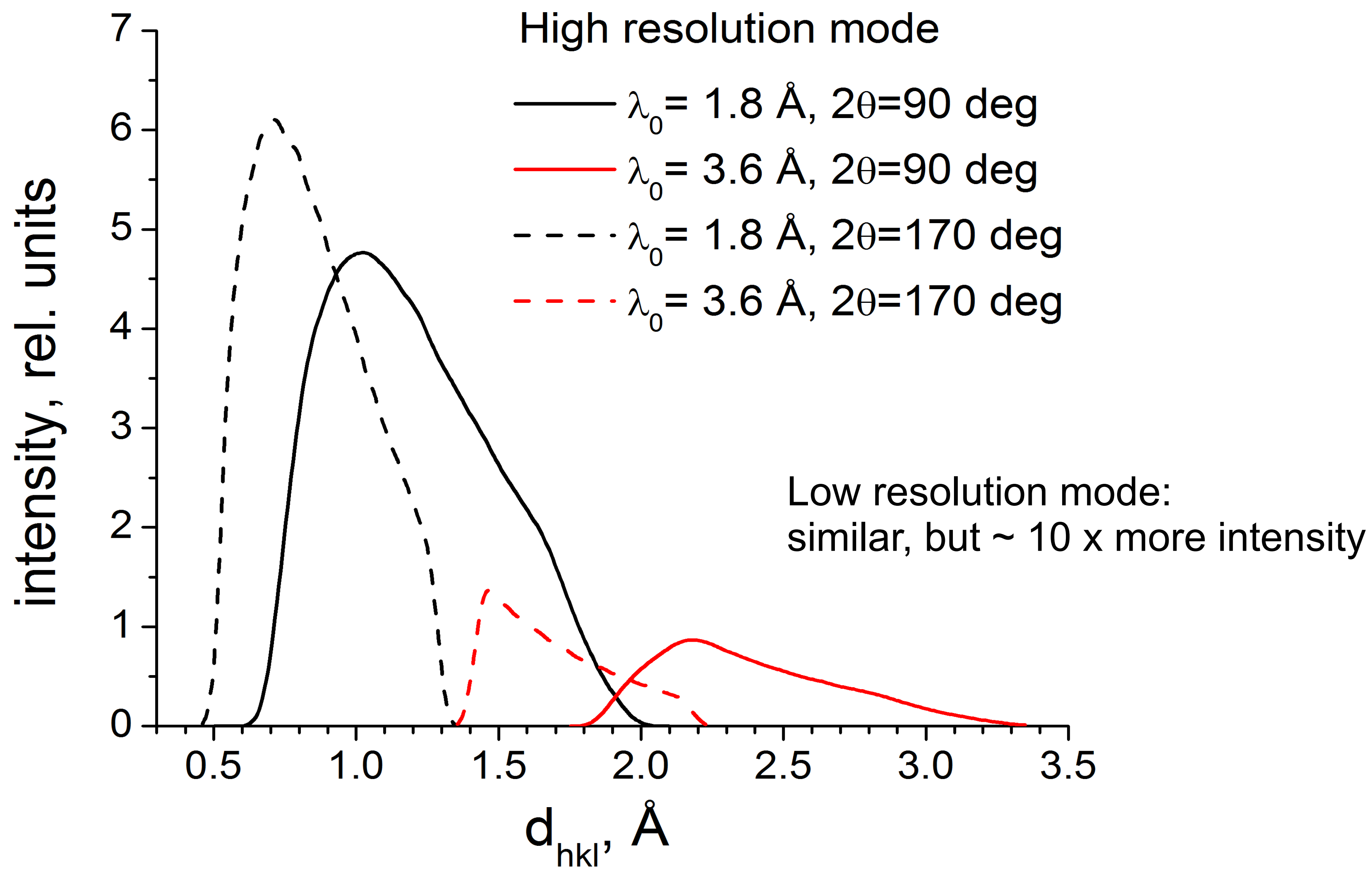


Brilliance transfer
including choppers and radial collimators



integration volume: dS = 3 x 3 mm^2, dΩ = 0.002 x 0.02 sr

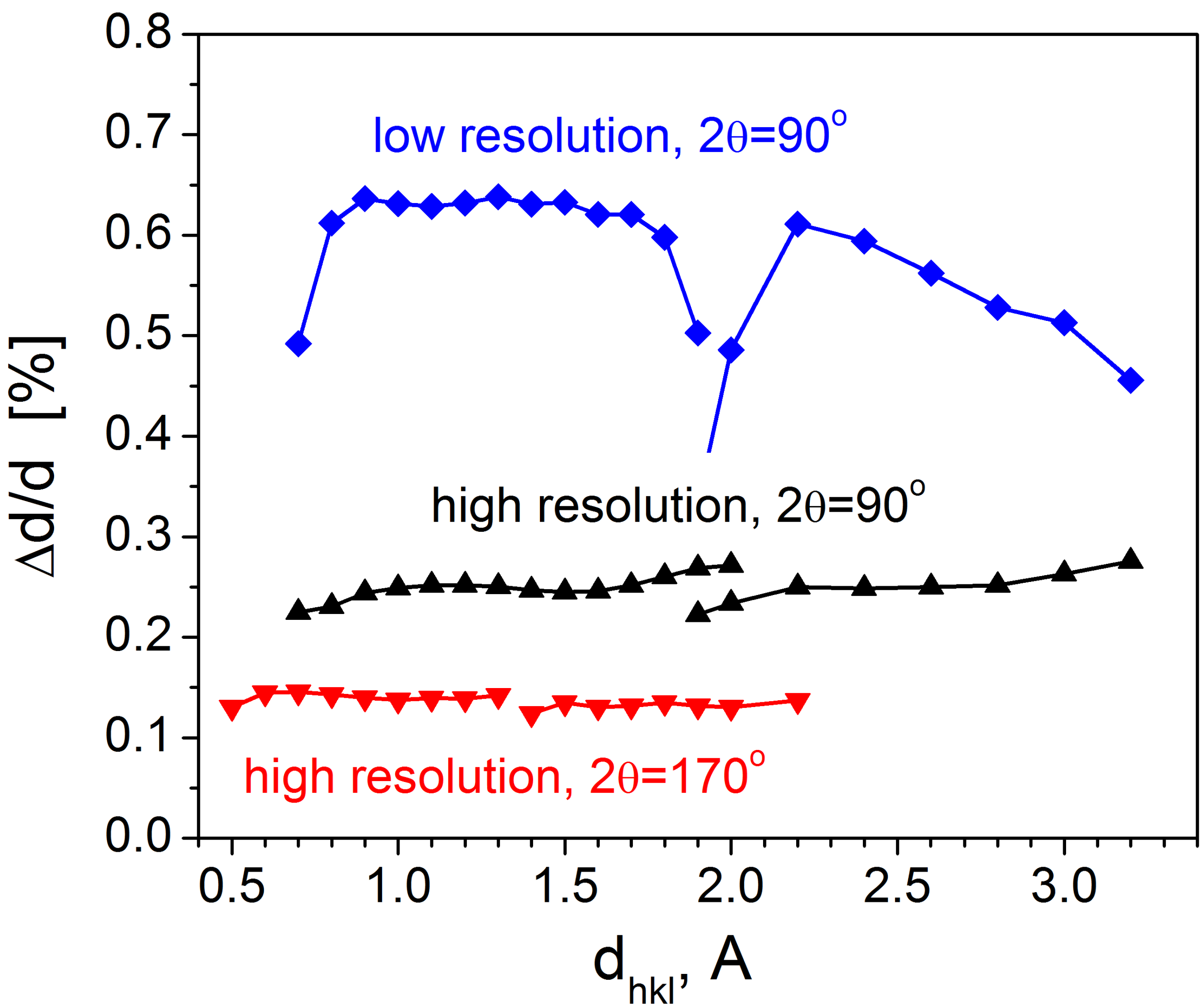
Isotropic scattering



Conversion to d_{hkl} scale is the same as for a powder sample (event based analysis)

Resolution Δd/d

Simulation with callibration sample (equal F^2 and equidistant *d* values)



Resolution curves for high and low resolution modes

NOTES:

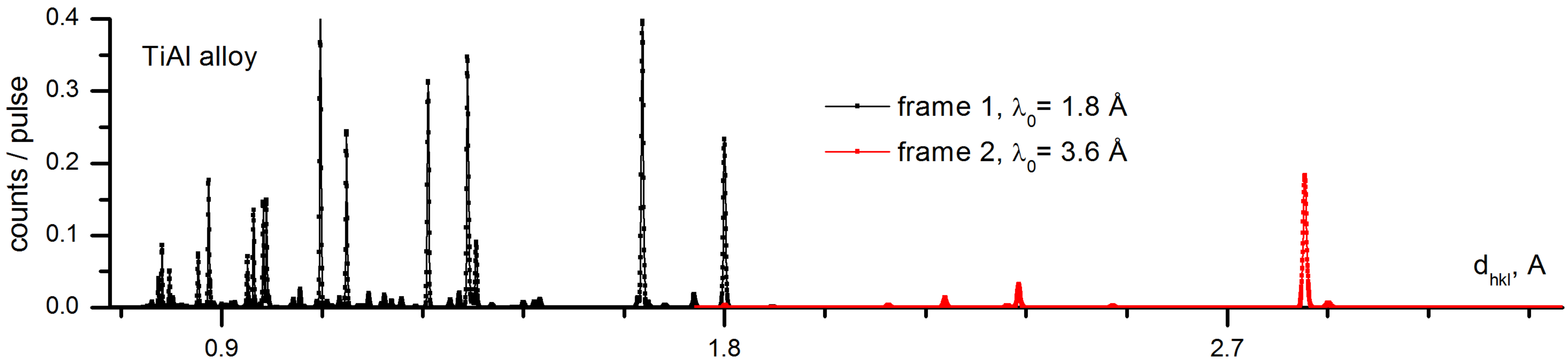
Resolution includes the contribution of beam divergence, sample size etc. (dominant at high resoluton)

d-range is reduced for the *low resolution* mode due to the penumbra effect

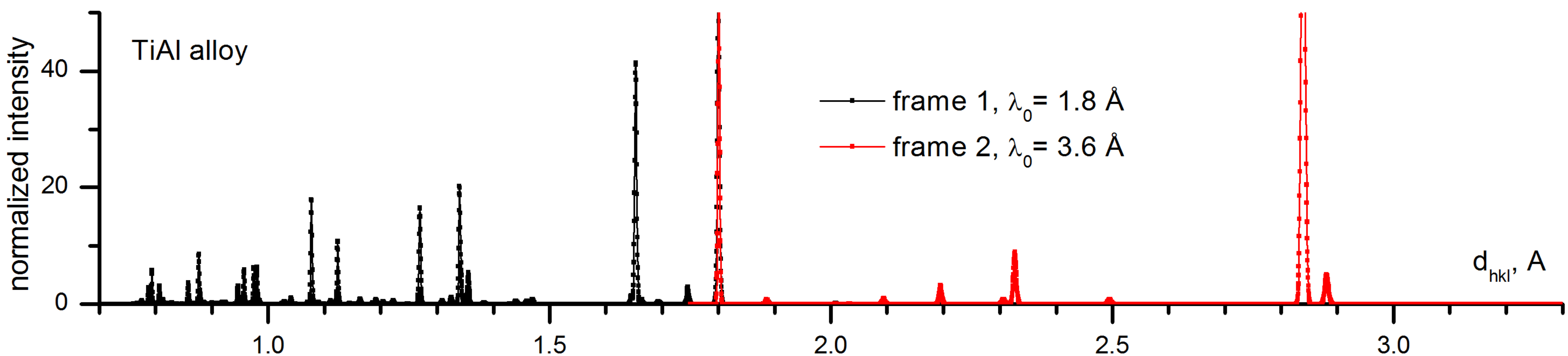
Simulated experiment 1: **TiAl**

high resolution mode (as described before)
two wavelength frames
detector range 80 - 100 deg

simulated count rate



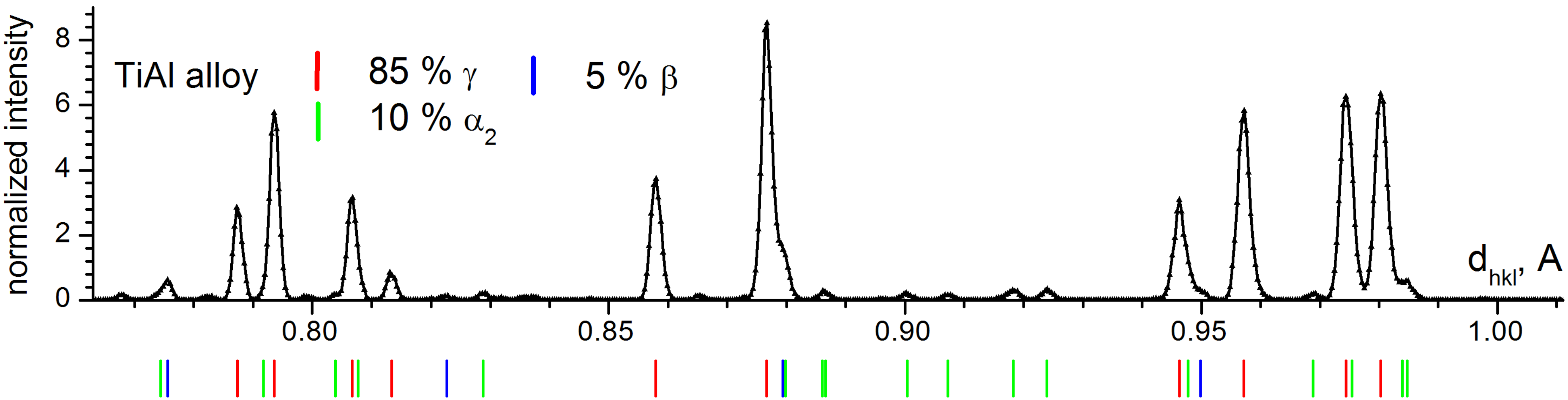
normalized with Vanadium



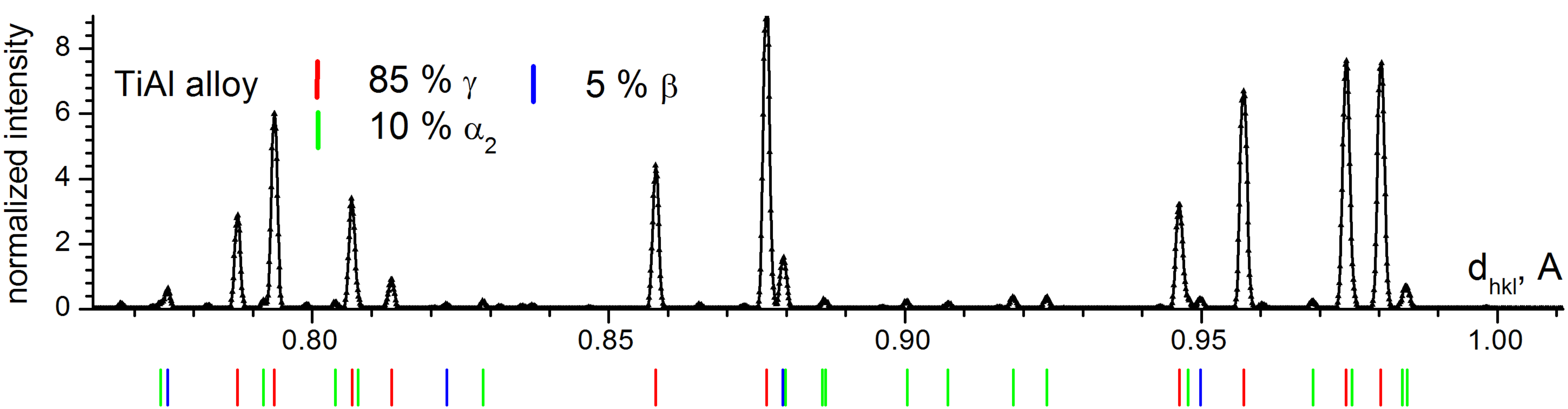
Simulated experiment 1: **TiAl**

comparison of detector angles *zoom at low d*

detector range 80 - 100 deg

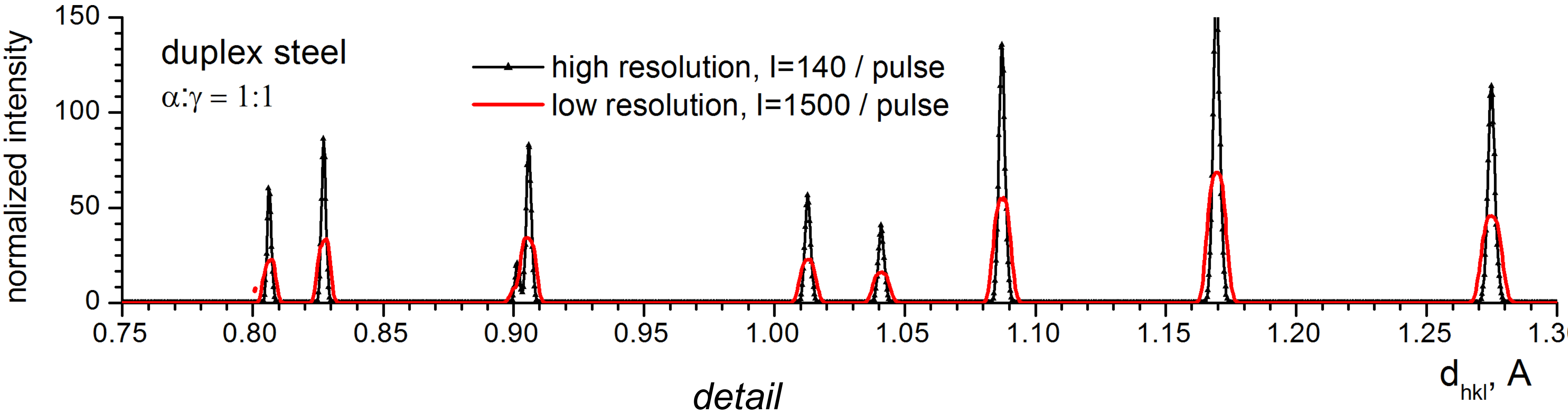


detector range 165 - 170 deg



Simulated experiment 2: **duplex steel**

comparison of low and high resolution modes *zoom at low d*



detail

wavelength band 0.9 - 2.7 Å
detector range 80 - 100 deg

Summary

- Detailed model of CEED instrument concept is available
- Small gauge volume feasible with radial collimators at ~ 40 cm from the sample (minor loss of intensity)
- Flat $\Delta\lambda/\lambda$ resolution curve, tunable with the double chopper
- Penumbra effect - significant reduction of usable bandwidth (mainly at low resolution and high λ) => *should the instrument be longer?*
- double frame mode: possible, but not easy to configure, avoid cross-talk effects etc.
- tests with virtual samples - basis for intercomparisons and testing data analysis in future