Twin Peaks

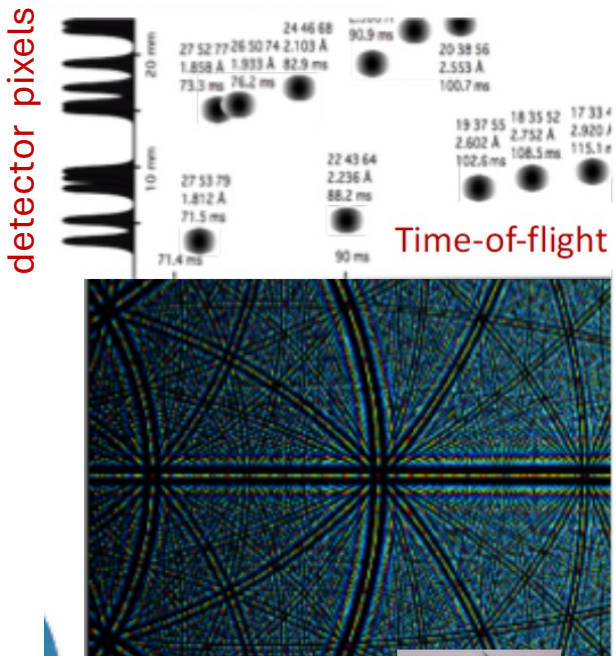
Single-crystal diffractometer

Werner Schweika – Diffraction STAP meeting 22.10.2025

NMX

macromolecular crystallography

full pulse TOF Laue, L~ 150m
cold moderator $\lambda > 1.8$Å
small divergence, small beam
large unit cells



Single crystal diffraction

TWIN PEAKS

hope for support from **You, ESS, FZJ, PSI, ISIS, Bilbao, Edinburg, ….**

keep it simple – high benefit/cost

similar, cold spectrum ~1.8 - 6Å

bi-spectral ~0.8-5Å

not so very large unit cells
full pulse TOF Laue, L~ 60m
very intense beam > ~ 10 x SNS, 100 x ISIS TS2
large solid angle of detection - like WISH-2
small instrument

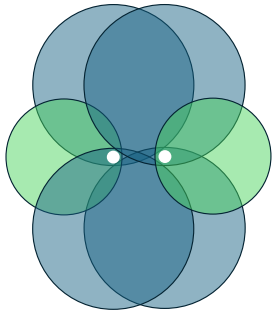
we can have both instruments at one beam port S4

probably both in total cheaper than any other previous ESS instrument

prime application **high pressure DAC** from synchrotron community

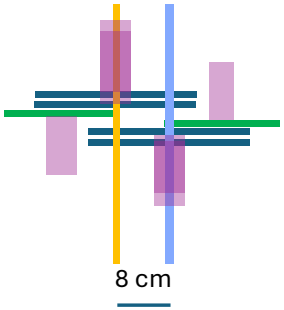
courtesy of
Bianca Haberl, Univ. Canberra
Damian Paliwoda, ESS
Andrzej Grzechnik, RWTH Aachen Univ.

<u>Options</u>
Pulse shaping small choppers
d ~ 25 cm resolution > ~20 µs, 150µs for 0.5% at 2Å
guide kink (MAGIC)
simply no T0 chopper
polarised n for dynamical nuclear polarisation – IMAGINE-X ORNL
polarised protons: converting inc background => 106 b coherent signal



TWINS for single crystal diffraction
cold and bi-spectral at a single beam port S4

neutron time-of flight Laue diffraction
full pulse (like NMX) or with pulse shaping
=> world leading highest flux
=> high pressure DAC



small double disk chopper - simple, cheap (MAGIC)
~400 – 450 Hz fix d ~ 25 cm 3 or more sub-pulses
possible resolution > ~15µs, 3 choices
optimal resolution ~ 100µs – 200µs, or **full pulse**

Overlap / band selecton chopper **14 Hz**, d=18 cm
opening / closing time 1.26 ms/cm
(conceptually similar to DREAM)

~~T0 chopper~~ not needed with kinked guide
guide – semi elliptic - small < ~4cm
kink - could be polarising for DNP
... monitor, heavy shutter

in bunker

length 60m – 70m
bandwidth 1.8Å – 5.8Å cold spectrum
0.8 Å ~ 5 Å bispectral
collimation **fix** focusing 0.2°-0.5°
or change absorbing to focusing end
sample size < 8 mm (diffuse scattering) to ~ 1 mm
detector resolution < ~2mm x 2mm
~ 50 – 100 cm from sample
large solid angle
scintillation detector in vacuum
type **SONDE**(FZJ,SKADI) or WSF(ISIS,CDT)