

Inelastic X-ray Scattering Spectroscopy

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Inelastic X-ray Scattering

"Normal" scattering experiment: static structure factor $S(q)$

Spectroscopy offers dynamic structure factor with $E =$ energy transfer

$S(q, E)$ – includes time dependence

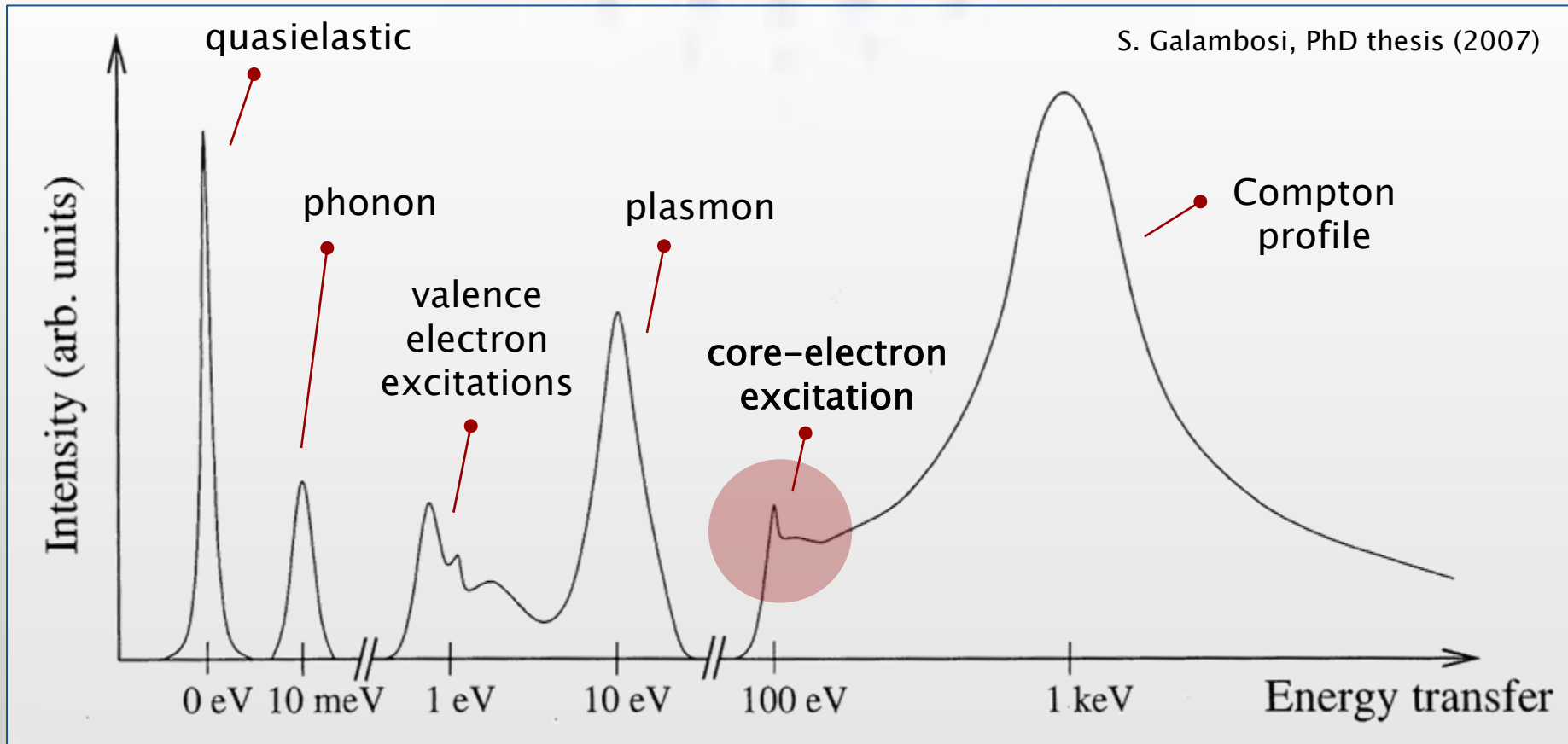
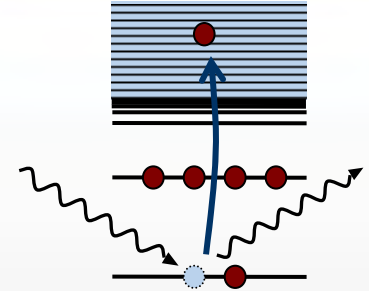
Typical q -range several $1/\text{\AA}$

Typical E -range tens to hundreds of eV

$S(q, E)$
{
 valence electrons: plasmons; electron-hole creation
 core electrons: absorption thresholds

Inelastic x-ray scattering

Access to a rich excitation spectra:



X-ray Raman scattering

IXS from core electrons

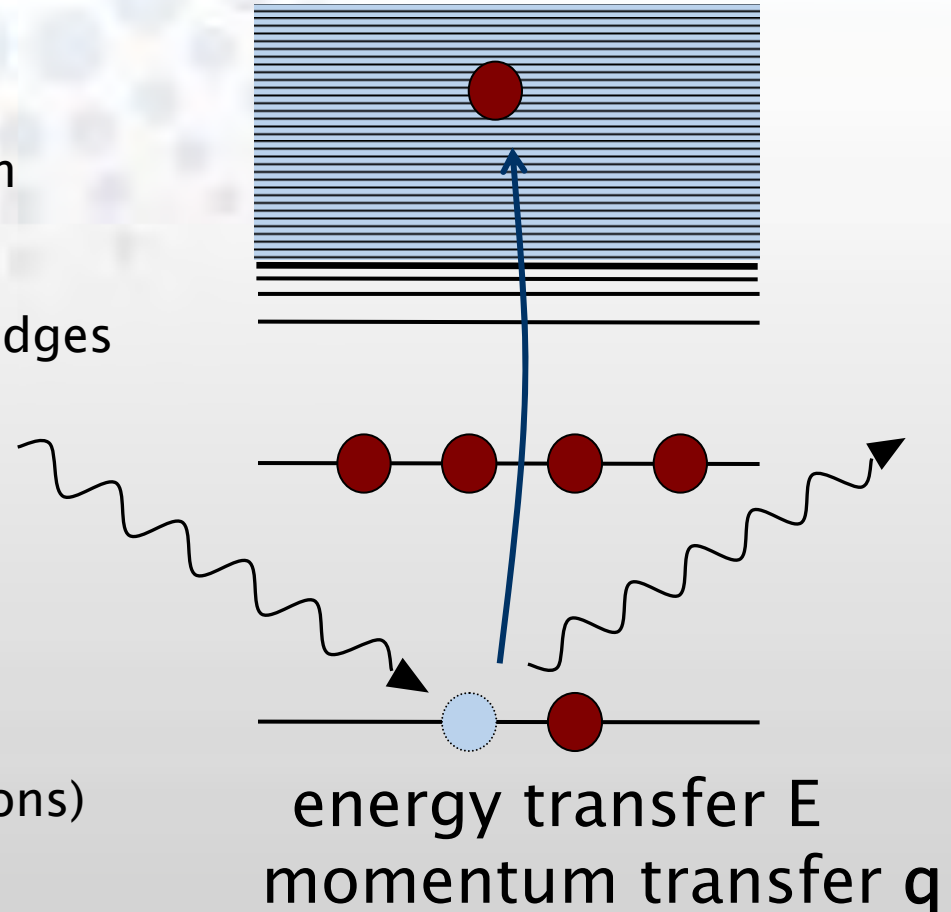
Powerful technique rapidly growing in popularity

Use hard x-rays to study soft x-ray edges

bulk-sensitive measurements
high pressure studies possible

Additionally momentum-transfer dependence (non-dipole contributions)

Photon energies can be chosen freely – only energy shift between incident and exit ray matters



Requirements

- Monochromator (1 eV bandwidth or better)
- Every photon counts
- 1D or 2D detector for the proposed design

Is more relaxed with:

- No small spot required
- No coherence required
- Can have large divergence
- Energy range can be chosen (often 8–12 keV)
- Both vacuum and high pressure are OK
- Sample can be gas, liquid, solid...

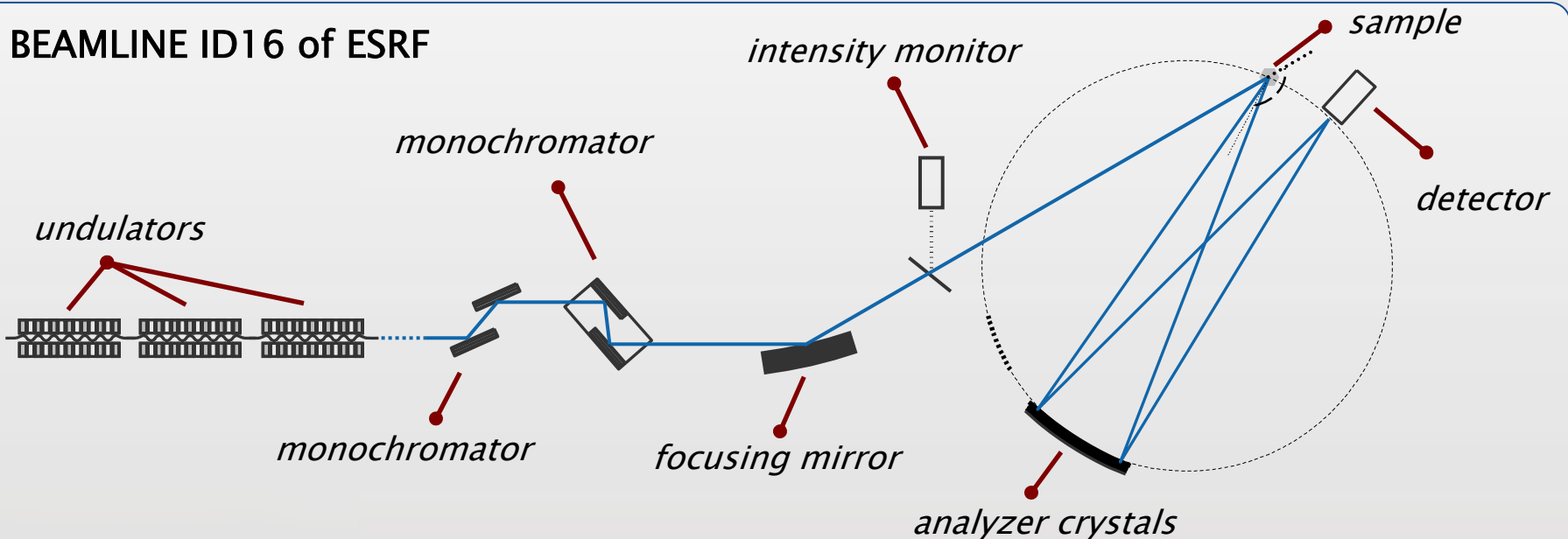
Instrumentation

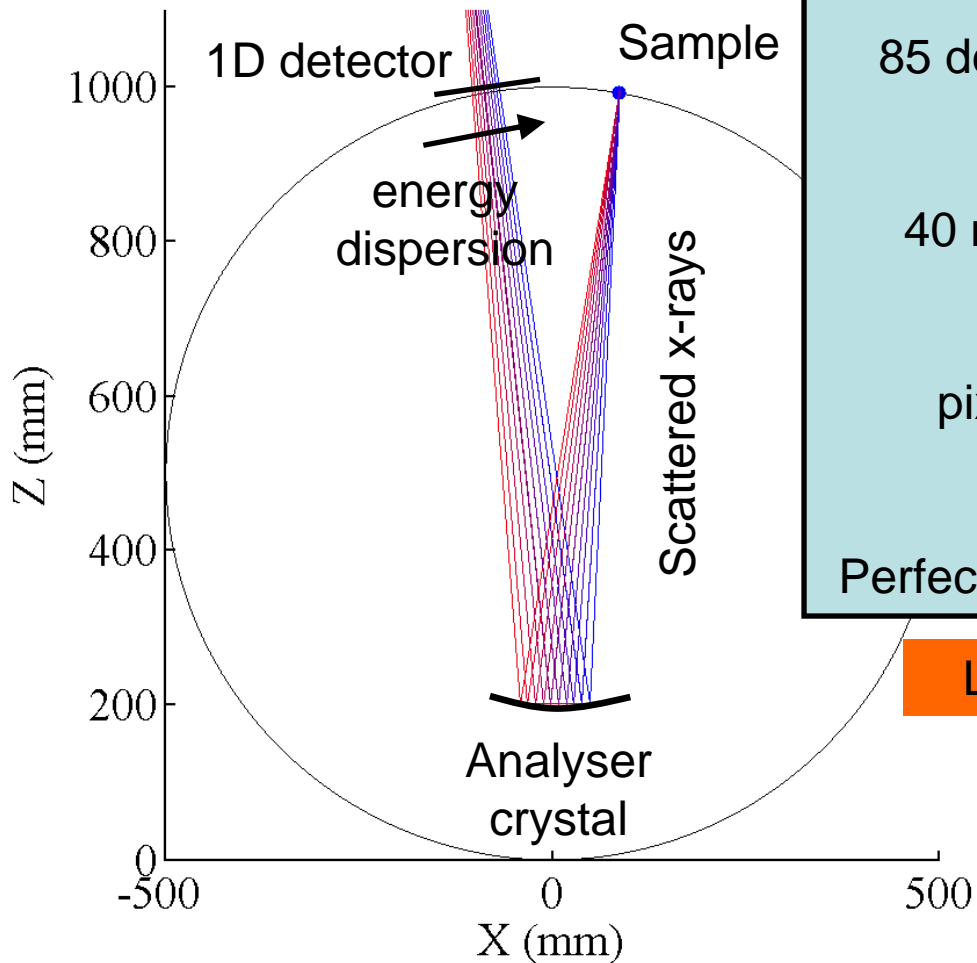
Crystal analyser spectrometers to reach 1 eV bandwidth or better

Often in synchrotrons operation in point-to-point scanning mode

BUT single-shot-image spectrum recording very well possible (suggested here)

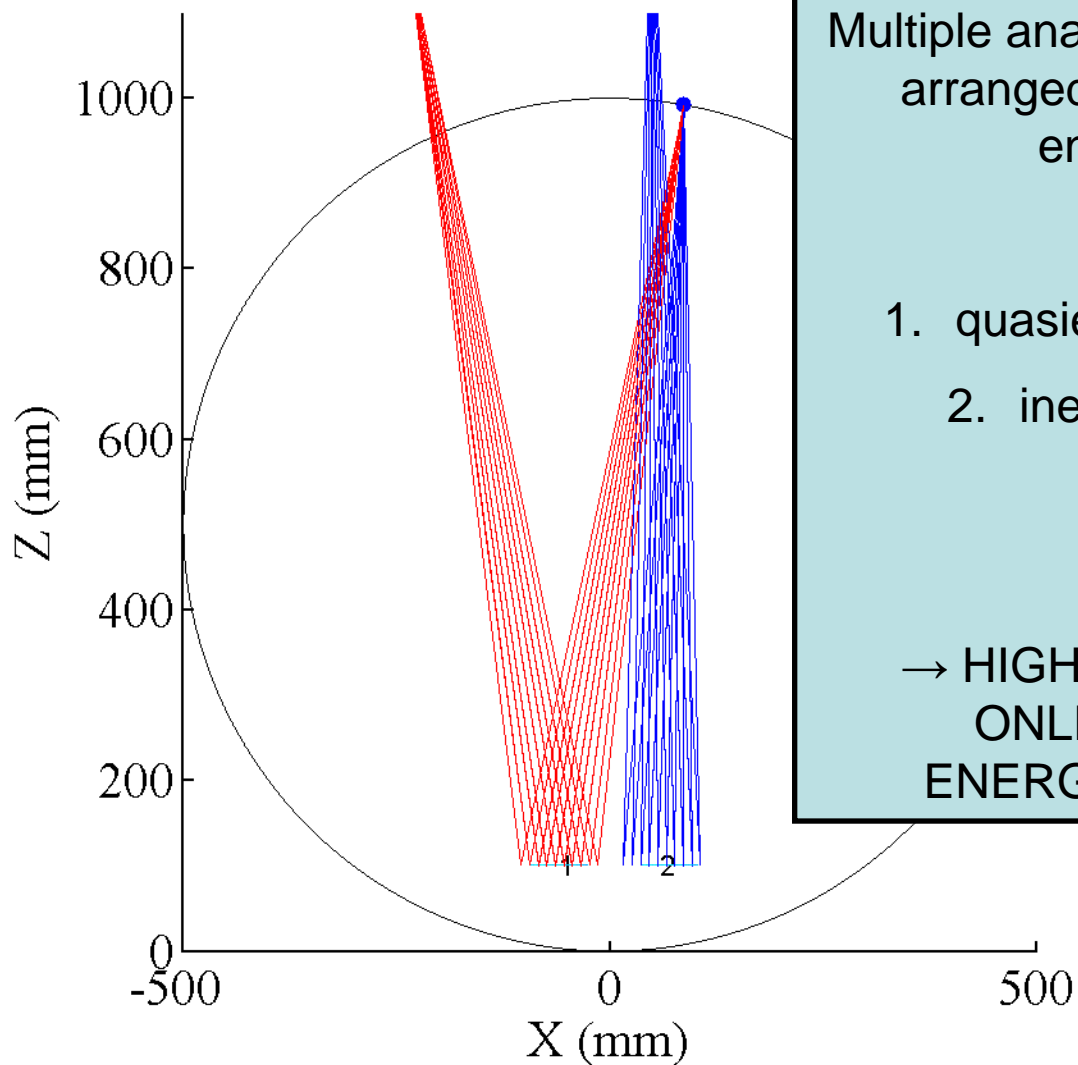
BEAMLINE ID16 of ESRF





Detection scheme:
 85 degree Bragg angle
 25 eV range
 40 mm long detector
 0.6 eV/mm
 pixel size 0.5 mm
 0.3 eV/pixel
 Perfect for 1 eV resolution!

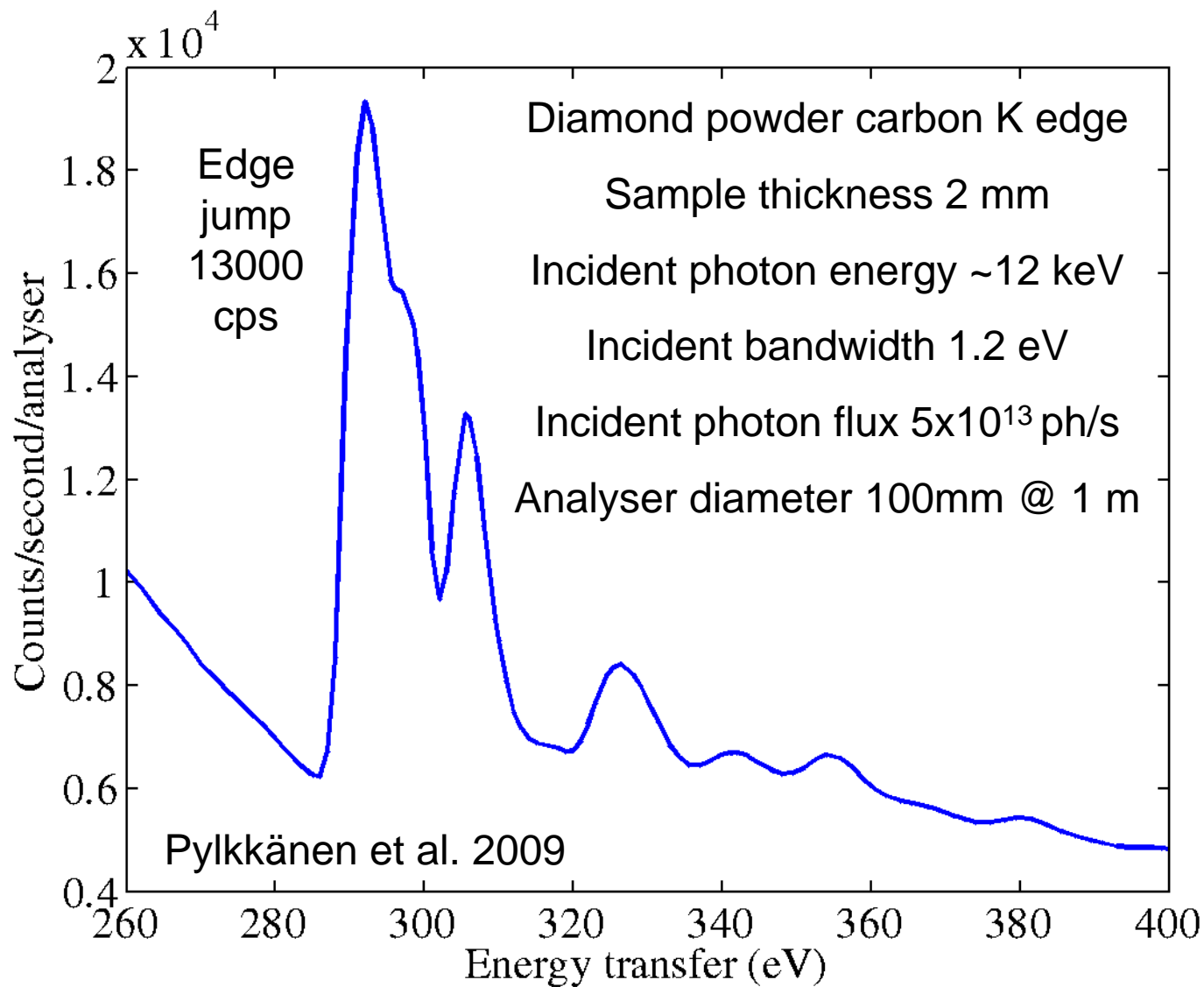
LPD detector OK



Multiple analyser crystals can be arranged to record different energy ranges

1. quasielastic scattering
2. inelastic spectra

→ HIGH-RESOLUTION
ONLINE INCIDENT-
ENERGY CALIBRATION



Incident photon flux at sample at 3rd generation synchrotron at 12 keV

$$\Delta E = 1.2 \text{ eV} \quad 5 \times 10^{13} \text{ ph/s}$$

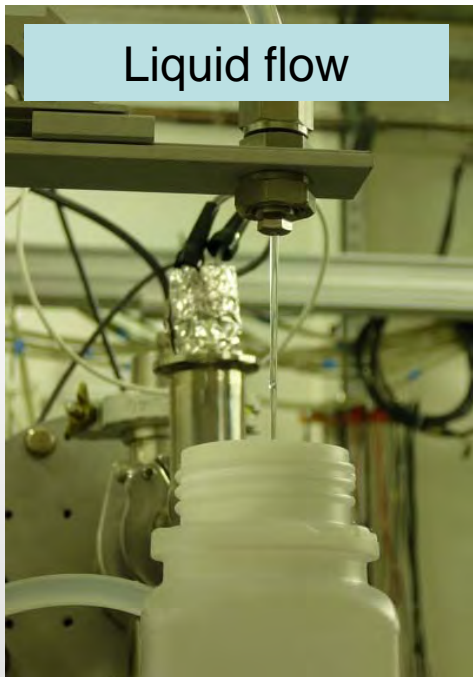
In 100 fs 5 photons (forget about it..)

Expected flux at XFEL at 12 keV

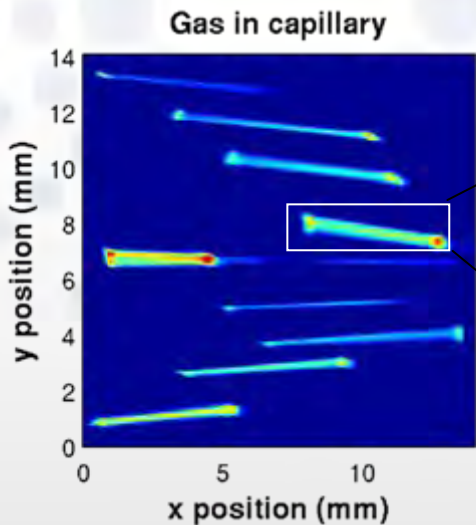
$$\Delta E = 0.1\% \text{ BW} = 12 \text{ eV} \quad 10^{12} \text{ ph/pulse}$$

$$\Delta E = 1.2 \text{ eV (w/10\% reflectivity)} \quad 10^{10} \text{ ph/pulse (ok!)}$$

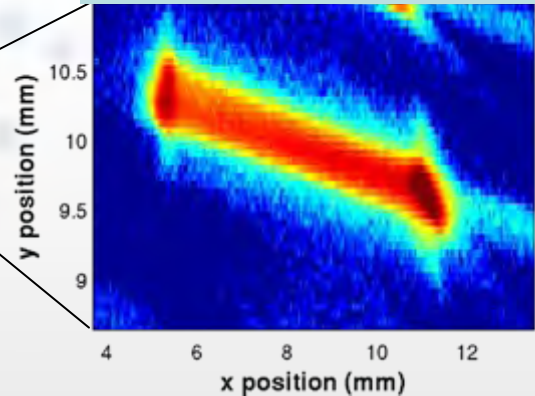
Sample (thickness)	Edge and its energy in eV	signal / pulse expected	# of integrations in order to reach 2-3% statistics	integration time for one delay time signal
diamond (2mm)	C K (290)	2 counts	1500 x 75	4 s
water (2mm)	O K (535)	0.5 counts	6,000 x 75	30 s
He 30 bar (6 mm)	He K (20)	0.02 counts	150,000 x 75	7 min



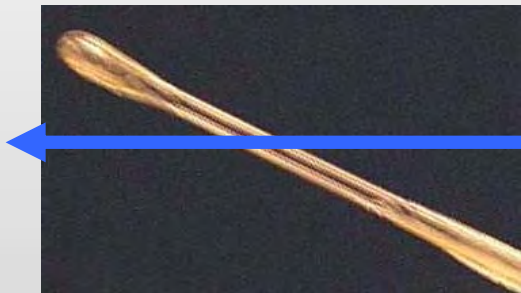
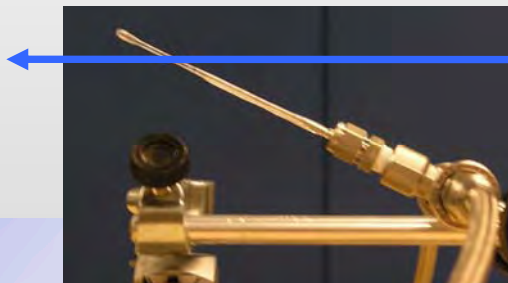
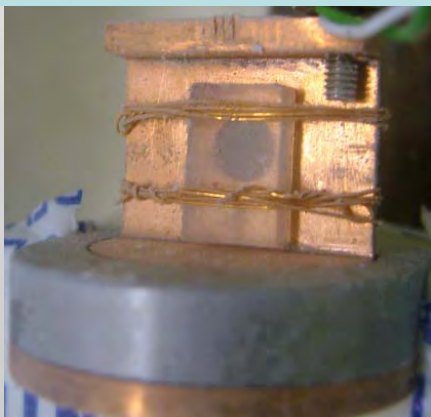
Liquid flow



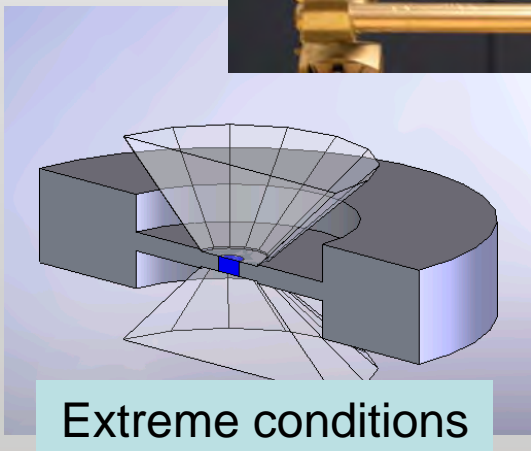
Pressurised gas



Extreme conditions



Sz. Galambosi et al. 2009



Extreme conditions

All samples are OK!

Checklist

Experiment	x-ray Raman spectroscopy
Spot size	Is not important (uncofused OK if sample large enough, line focus for better resolution)
Divergence	Not important
Beam quality	Energy ~constant
Energy	8–12 keV
Bandwidth	1 eV
Scanning	not necessary
How many photons destroy the experiment	Depends on sample
Burst mode	possible, depends on sample and detector
Diagnostics	not crucial
Complete vacuum setup	possible
Detector	at least 1D with at least 0.5 mm pixel size
Harmonics	$1e-6$ rejection OK

Thank you!!

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