
Kite at Suma Beach
Kobe

Considerations and applications for an effective high-flux IXS setup

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APS, ANL, USA, September 2016

Main Points For This Talk

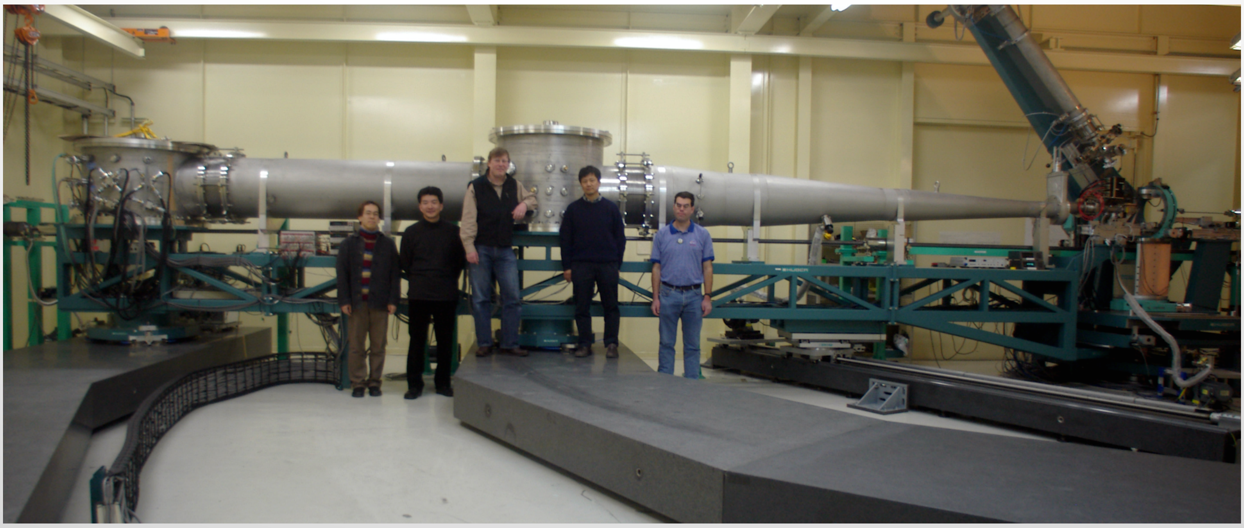
Introduce SPring-8 meV-IXS beamlines & some results.

There are significant – even great - opportunities with an "echo" spectrometer.

Some questions & issues worth mentioning.

The First Instrument at SPring-8

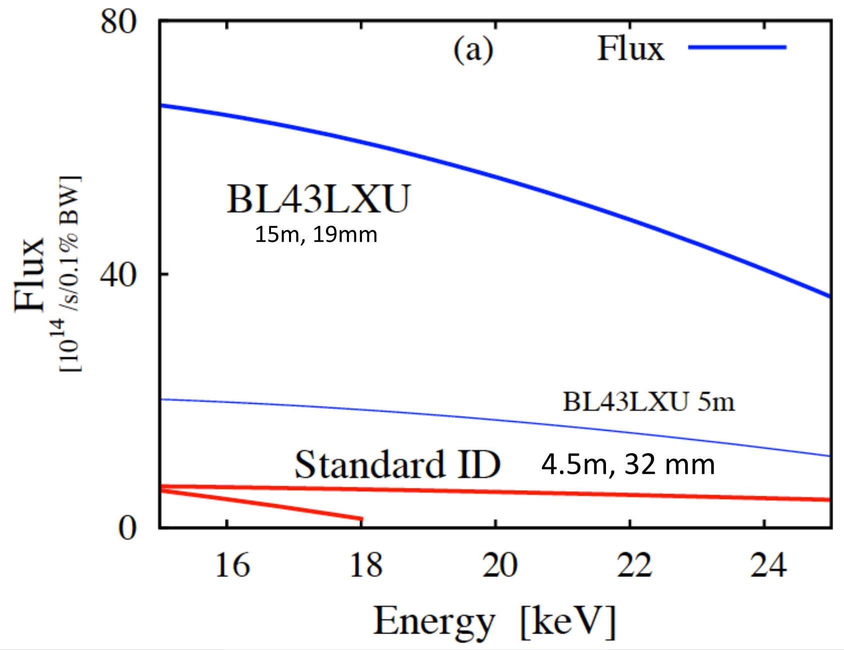
(BL35XU)



Operational from ~2002

Baron, *et al*, J. Phys. Chem. Solids (2000)

SPring-8 IDs for IXS



BL43LXU Collaborators

RIKEN-JASRI Collaboration

Initial Discussions & Design (Beginning in 2004):

Electron Optics: Kouchi SOUTOME, Hitoshi TANAKA
Insertion Devices: Takashi TANAKA, Hideo KITAMURA
Mono & Cooling: Tetsuro MOCHIZUKI
Front End: Sunao TAKAHASHI
Hutches and Shielding: Kunikazu TAKESHITA
Transport Channel & Optics: Haruhiko OHASHI, Shunji GOTO
Spectrometer (2008-): Daisuke ISHIKAWA

More Complete List of Contributors Includes:

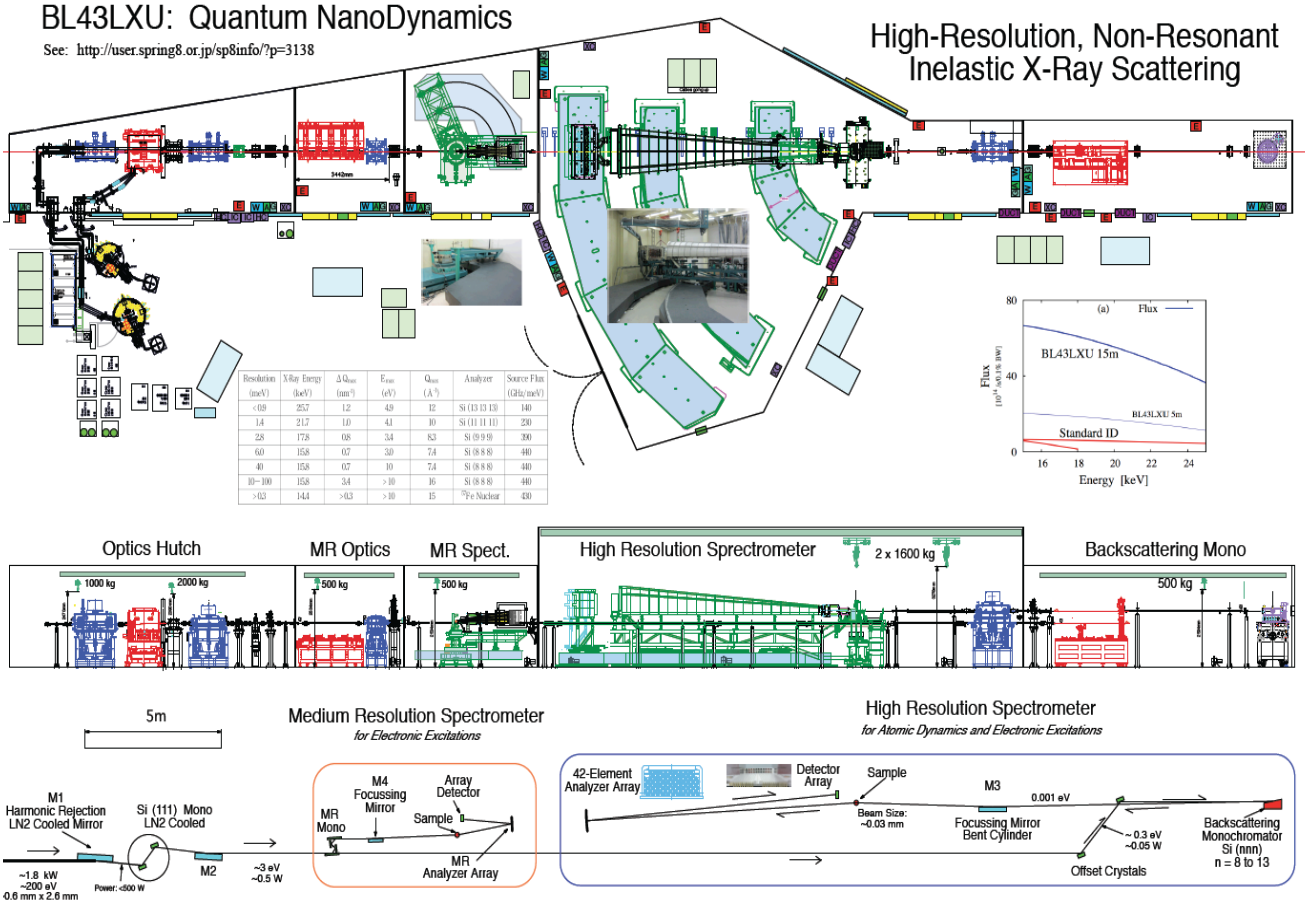
M. Abe, H. Aoyagi, H. Arita, N. Azumi, D. Ellis, K. Fukami, H. Fukui, Y. Furukawa, S. Goto, Y. Harada, D. Ishikawa, Y. Ishizawa, H. Kimura, H. Kitamura, H. Konishi, T. Matsushita, Y. Matsumoto, T. Mochizuki, N. Murai, H. Ohashi, T. Ohata, H. Ohkuma, M. Oishi, M. Oura, S. Sasaki, J. Schimizu, Y. Senba, M. Shoji, K. Sorimachi, K. Soutome, S. Takahashi, M. Takata, K. Takeshita, T. Takeuchi, H. Tanaka, T. Tanaka, S. Tsutsui, H. Uchiyama, T. Wagai, J. Yahiro, M. Yamamoto, H. Yamazaki

Director/Facilitator: T. ISHIKAWA

BL43LXU: Quantum NanoDynamics

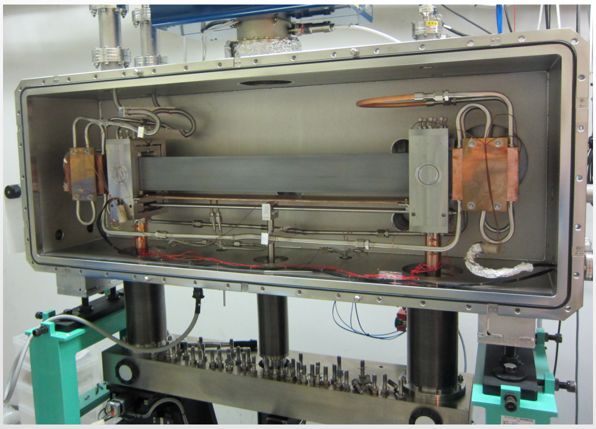
See: http://user.spring8.or.jp/sp8info/?p=3138

High-Resolution, Non-Resonant Inelastic X-Ray Scattering



Resolution (meV)	X-Ray Energy (keV)	ΔQ_{max} (nm^{-1})	E_{max} (eV)	Q_{max} ($Å^{-1}$)	Analyzer	Source Flux (GHz/meV)
<0.9	25.7	1.2	4.9	12	Si (13 13 13)	140
1.4	21.7	1.0	4.1	10	Si (11 11 11)	230
2.8	17.8	0.8	3.4	8.3	Si (9 9 9)	390
6.0	15.8	0.7	3.0	7.4	Si (8 8 8)	440
40	15.8	0.7	10	7.4	Si (8 8 8)	440
10−100	15.8	3.4	>10	16	Si (8 8 8)	440
>0.3	14.4	>0.3	>10	15	^{57}Fe Nuclear	430

High Heat-Load Mirror (M1)



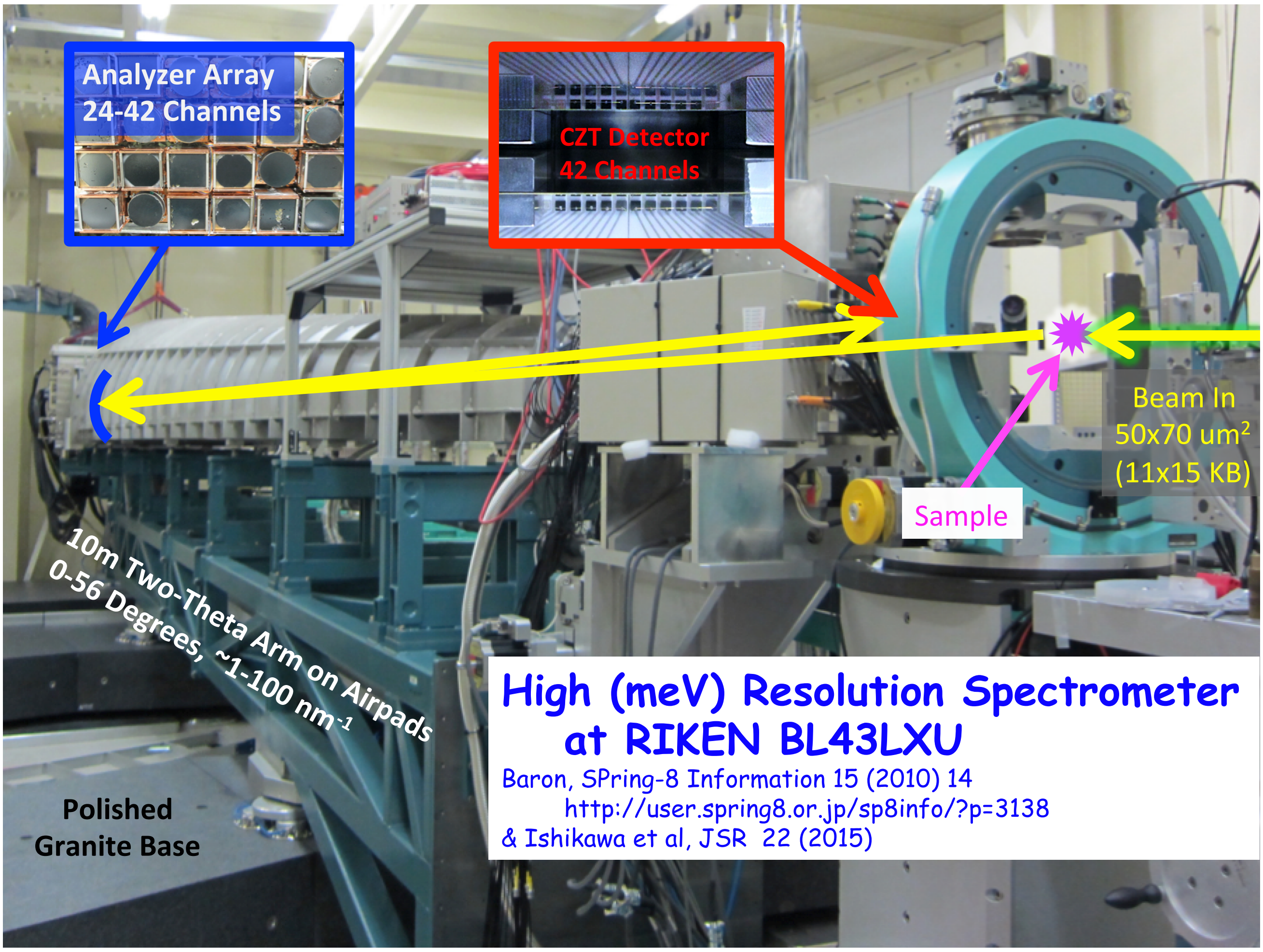
Reduces incident beam (<1800W) to
<500 W onto LN2 Si(111) Mono

Issues with
- Silicon Polishing
- Mirror Mask Design
- Vacuum Chamber Design
- Bender Shaft T-Control
- In-Vac Support T-Control

Note: Vibrations << urad level

Other Major Unexpected Issue

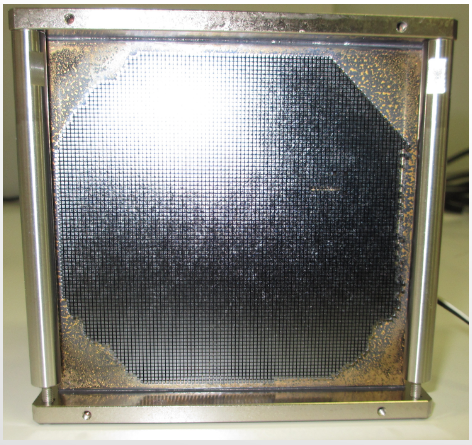
Analyzer Crystals (company quit)

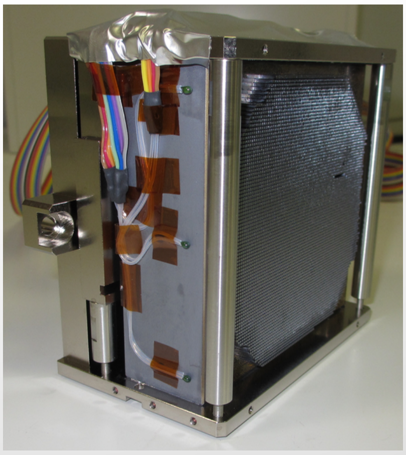


High (meV) Resolution Spectrometer at RIKEN BL43LXU

Baron, SPring-8 Information 15 (2010) 14
http://user.spring8.or.jp/sp8info/?p=3138
& Ishikawa et al, JSR 22 (2015)

BL43LXU Analyzer Crystals



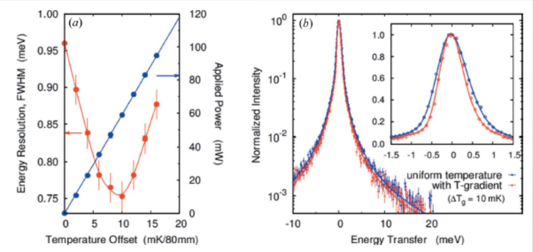


9.8 m Radius, 90x94 mm^2
50 or 60 μm blade, 3-5 mm depth, ~1 mm pitch
Channel width (after etch): ~ 0.15 mm

AQRB
Sep. 2016

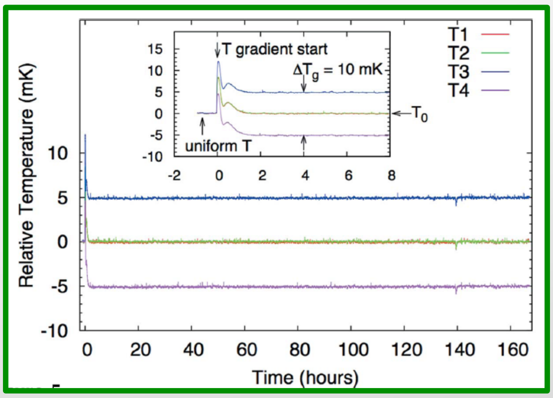
Temperature Gradient Analyzers

Can remove one of the geometric contributions to the analyzer resolution by making a temperature gradient across the analyzer in the scattering plane.



(13 13 13): 0.9 -> 0.75 meV

(11 11 11): 1.4 -> 1.25 meV



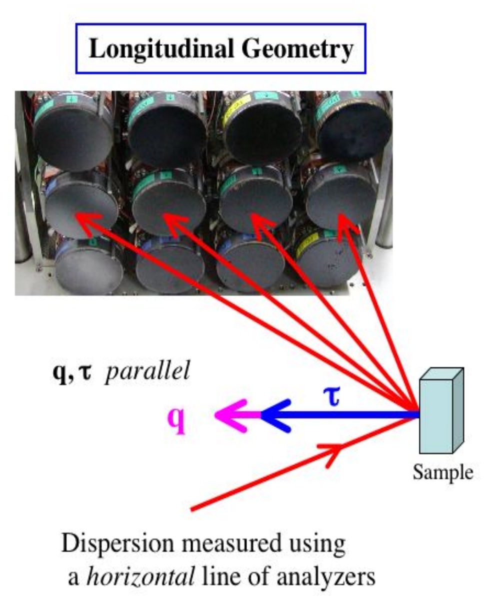
Analyzer T: Stable to ~0.3 mK
Gradient ~10 mK for optimal resolution

Ishikawa et al, JSR 2010, 2015

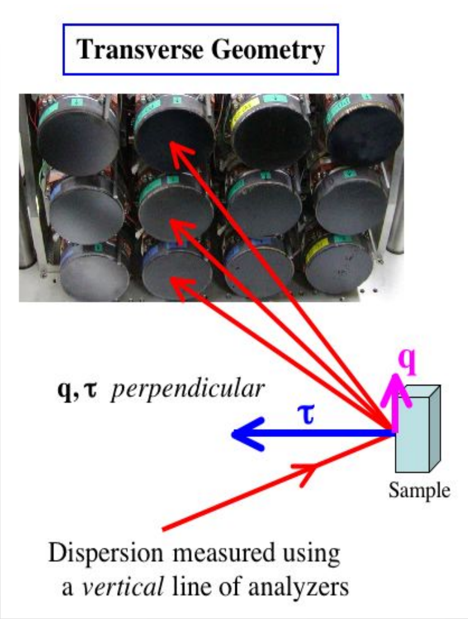
Analyzer Array

Q = q + τ

q = reduced momentum transfer in first zone
τ = nearest Bragg point



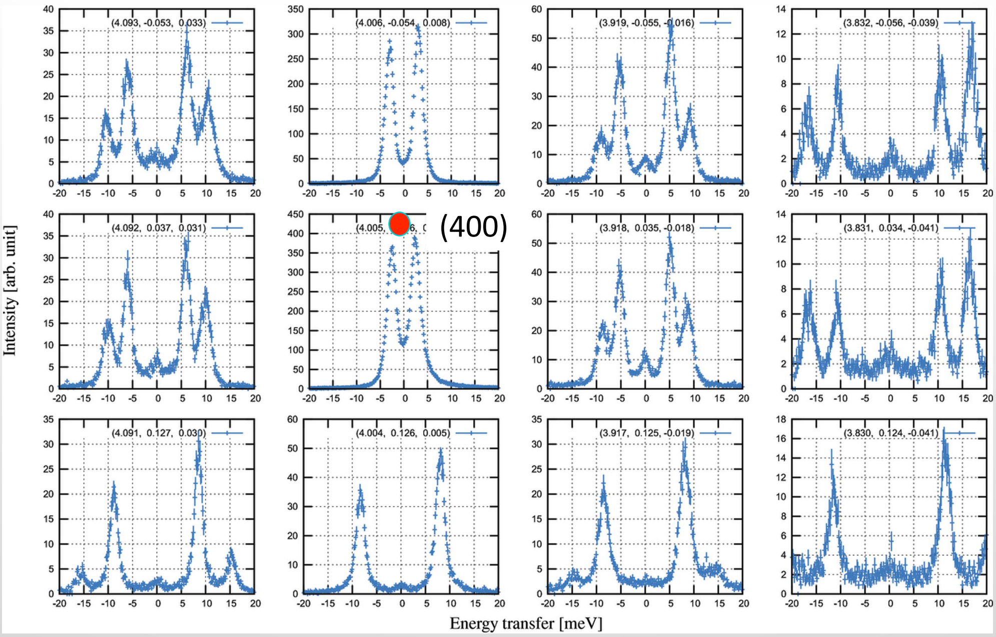
Dispersion measured using
a *horizontal* line of analyzers



Dispersion measured using
a *vertical* line of analyzers

Parallel Data Collection

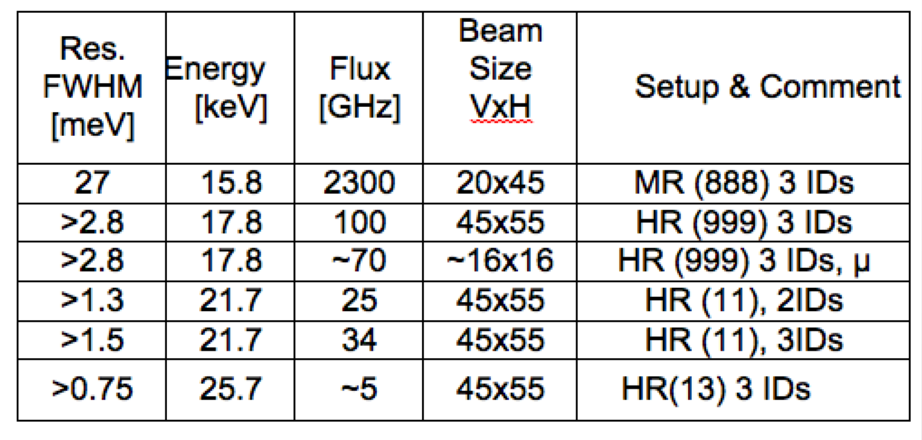
Measuring TA modes



MgO About (400) Bragg Point using 12-Analyzer Array

Fukui et al, JSR 2008

Present Performance



Res. FWHM [meV]	Energy [keV]	Flux [GHz]	Beam Size VxH	Setup & Comment
27	15.8	2300	20x45	MR (888) 3 IDs
>2.8	17.8	100	45x55	HR (999) 3 IDs
>2.8	17.8	~70	~16x16	HR (999) 3 IDs, μ
>1.3	21.7	25	45x55	HR (11), 2IDs
>1.5	21.7	34	45x55	HR (11), 3IDs
>0.75	25.7	~5	45x55	HR(13) 3 IDs

Experiments

~1/3 High Pressure (DAC) and usually high temperature
Small Samples: >~ 10 um diameter
Need space around the sample for laser heating (+- 100 mm)
Faster measurement is better for (unstable!) liquids

>~1/3 Complex Materials
Usually require a cryostat
Sometimes furnace (e.g. ferroelectrics)
Often desire to investigate weak modes -> flux limited

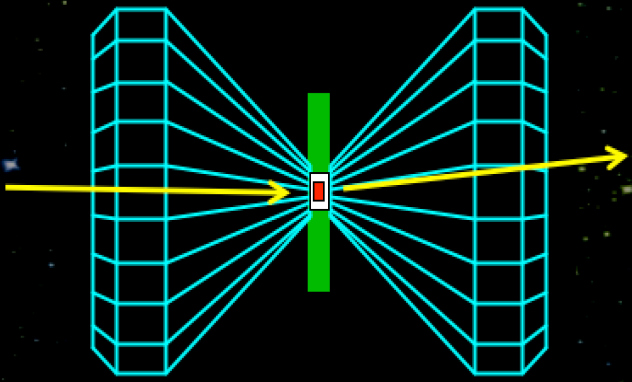
<~1/3 Disordered Materials
Resolution (FWHM & tails) generally an issue.

Conditions:
Beam Size: 50-100 um, Standard, ~15 um Possible
T: 2K – 800K (specific user groups: 1500K to 3000K)
P: 0~200 GPa DACs (User groups: He to 300 Bar)
H: up to 7T (BL43)
Online area detector for diffraction

Diamond Anvil Cells

P > 200 GPa
T > 3000 K

Large (60 deg., +)
Opening Angle



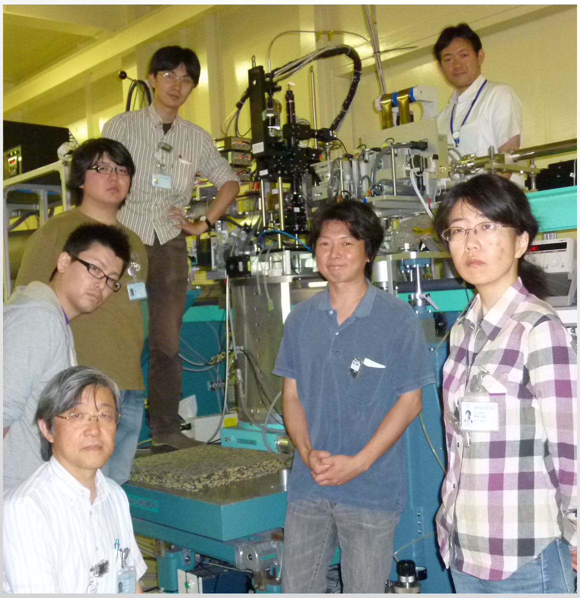
Diamonds: 2 x 1.5mm Thk
Sample: ~ Φ20 µm x 5µm Thk
Also Gasket & Pressure Medium
P increases -> Smaller Sample & Gasket Hole

Std Cell
Laser

Cell with Internal Heating

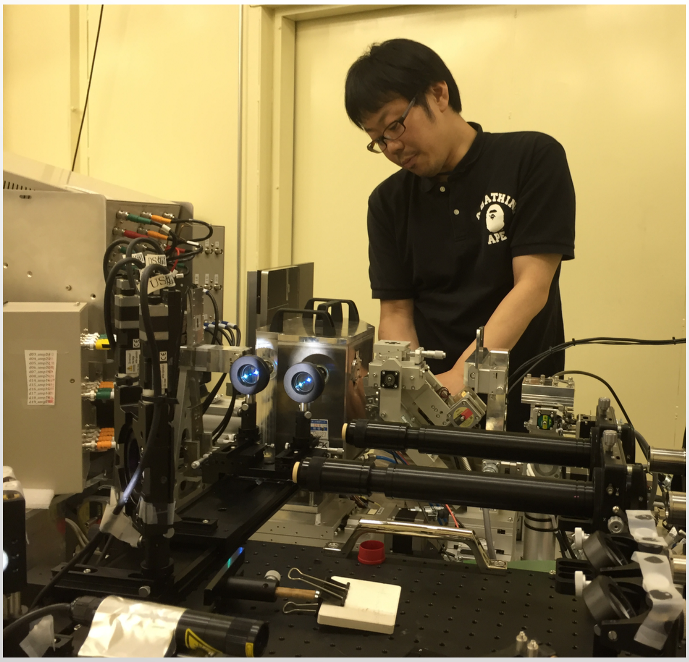
Small samples, Signal low, Poor signal to noise

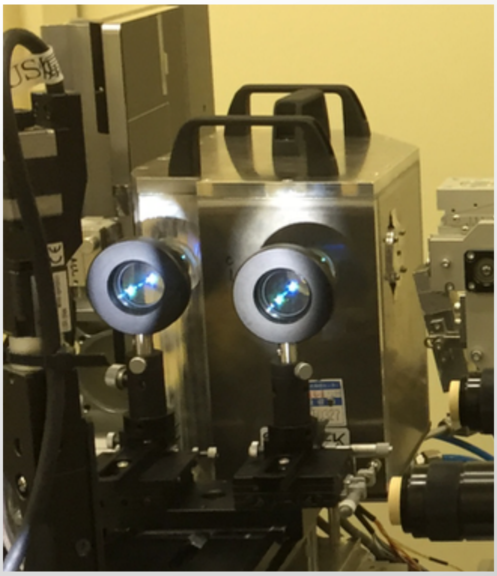
Tohoku/RIKEN system



Fukui, et al, JSR 2013

Tokyo Tech System



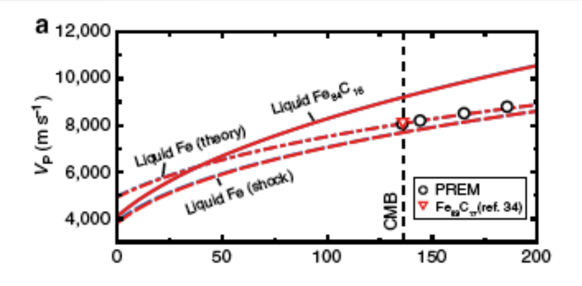


Nakajima, Tateno, Imada, Hirose et al

Its Not (only) Carbon In the Core

The earth's is, mostly, but not entirely iron. The density is too low (by ~10%) to be only iron -> some other lighter element must be present.

Based on first HP,HT LIQUID measurements that lighter element can not be simply carbon: the sound velocity would not agree with seismic measurements



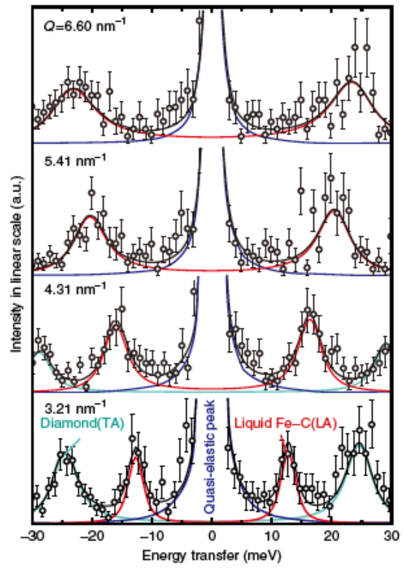
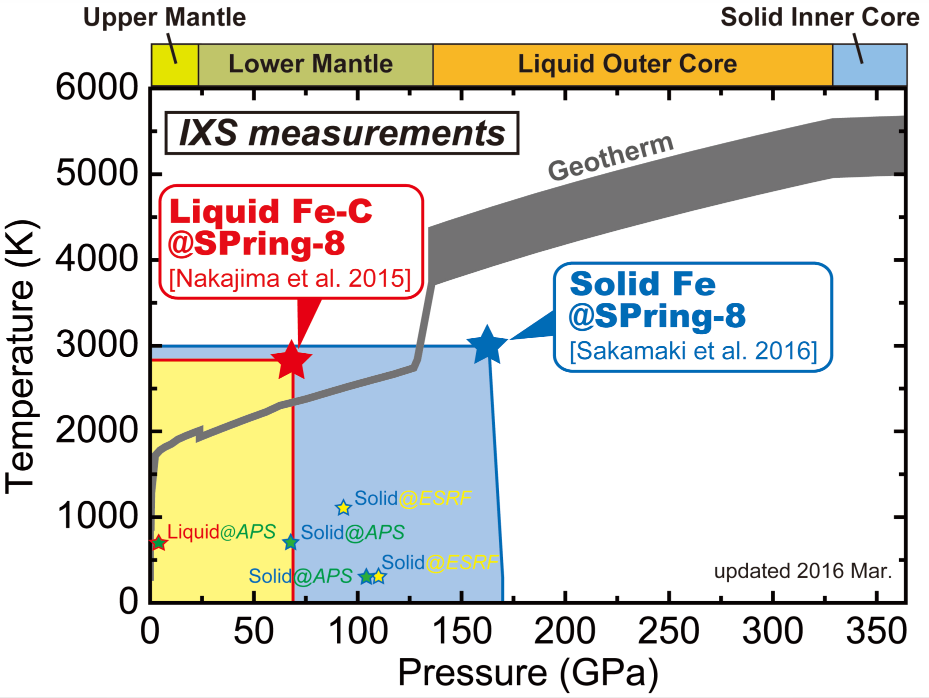


Figure 1 | Typical inelastic X-ray scattering spectra. These data were collected at 26 GPa and 2,530 K at momentum transfers Q, as indicated. The spectra include three components: a quasi-elastic peak near zero energy transfer (blue), longitudinal acoustic (LA) phonon mode of liquid $Fe_{84}C_{16}$ (red), and transverse acoustic (TA) phonon mode of diamond (turquoise).

Nakajima et al, Nat Comm 2015

Extreme Conditions



Faster Experiments help a lot when in marginally stable conditions

Sound Velocity. Viscosity.

Next Generation Options

Spherical Analyzers: Already discussed: robust instruments
Many parallel momentum transfers. Basically back to Doerner, *et al.* (80's)

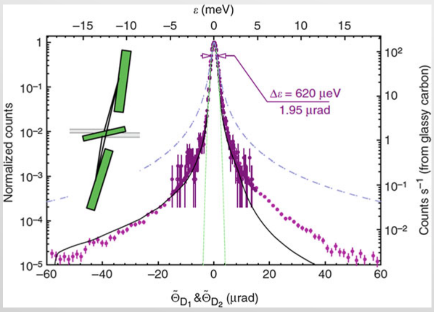
Replace the *figured analyzer* by a *collimating optic* after the sample
followed by flat crystal optics. (note also Bortel et al 2000, Sturhahn et al 2011)
"Post Sample Collimation"

Shvyd'ko's designs: Refractive Bragg Optics (CDW, CDDW, CDFDW… "echo")
Combine Bragg backscattering with refractive angular dispersion.
Operate at low (9.1 keV) energy
Can have extremely sharp tails on the resolution
Parallelization of energy transfers – enhanced efficiency (potentially huge)
(Shvyd'ko et al 2006…2016)

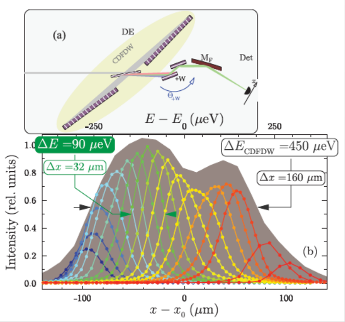
Shvyd'ko's Designs

CDW, CDDW	Spectrograph	"Echo"
Simplest No Parallelization	Dispersive Geometry Parallel Output	Parallel Dispersive Geometry Input & Output
1	~N	~N^2
Demonstrated (APS) Commissioning (NSLS-II)	Limited Test	Under Discussion

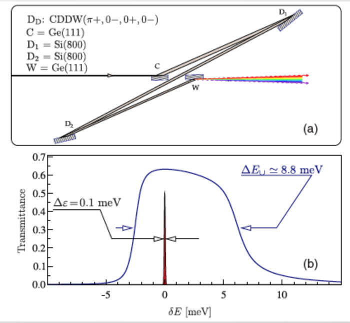
N: ~5 to 500



Shvyd'ko et al, Ncomm 2014



Shvyd'ko et al, PRA 2013



Shvyd'ko et al, PRL 2016

Also: 0.1 /45 meV & 1/85 meV
Shvyd'ko, PRA 2015

Spectrometer Applications & Issues

Total Energy Resolution FWHM	Energy Window (Larger is Better)	Q Resolution	Q Range (Larger is Better)	For	Setup
~0.02 meV	>0.2 meV (+) >1 meV (++) >2 meV (+++)	~0.01 nm^{-1}	> ~3 nm^{-1}	Glasses, Liquids, QXS Acoustic Phonons & Widths	"Echo"
		~0.10 nm^{-1}	> 25 nm^{-1} (>50)	Optical Phonon Line Widths	
~0.1 meV	>5 meV (+) >10 meV (++) >50 meV (+++)	0.05 - 0.25 nm^{-1}	> 25 nm^{-1} (>50)	Great Liquid Instrument	"Echo" (Spectrograph)
		0.1 - 0.5 nm^{-1}	> 50 nm^{-1} (>90)	Great Phonon Instrument	
~0.5 meV	>10 meV (+) > 50 meV (++) > 100 meV (+++)	0.1-0.5 nm^{-1}	> 50 nm^{-1} (>90)	Liquid Survey Instrument	"Echo" & Spectrograph
				Weak Mode Instrument	

Q$_{max}$ (9.1 keV, λ=1.36Å) = 92 nm^{-1}
Q(90 deg) = 65 nm^{-1}
Q(1 deg) = 0.8 nm^{-1}

Minimum **Q** ->
Focus Dependent

High Resolution Applications

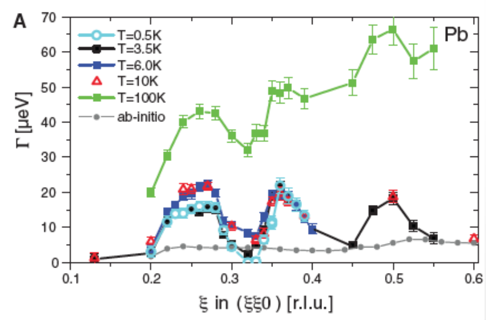
(<0.1 meV)

Obvious application to liquids and disordered materials
in a mostly new regime -> Other Talks

Coupling between systems:
Electron-Phonon Coupling
Spin-Phonon Coupling

Directly visible in linewidths (on top of anharmonic contribution…)
Pushes theory (but it needs pushing) but there.

Phonon Lineshapes in Superconductors



Aynajian…Keimer, *et al,*
Science 2008

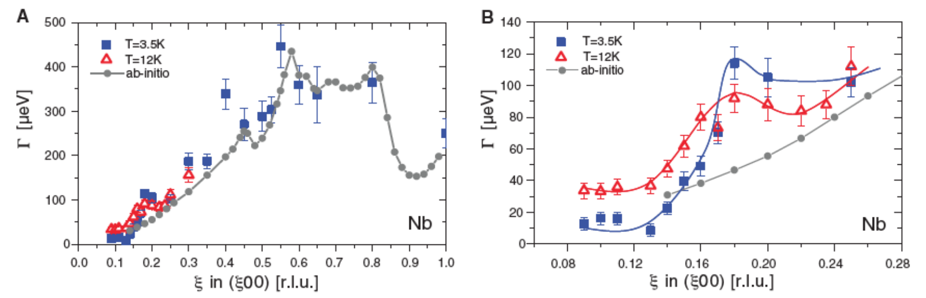


Fig. 4. (**A**) Linewidths of transverse acoustic phonons along $q = (\xi, 0, 0)$ in Nb at two different temperatures. The gray symbols are the results of lattice-dynamical calculations, as described in the text. (**B**) Blowup of the low-q segment of (A). The corresponding E is provided by the scale at the top. The lines are guides to the eye. Error bars indicate the statistical errors.

“Medium” Resolution Applications

(say: 0.2-0.5 meV)

Many experiments done at present facilities.

Liquid Experiments over larger Q/E ranges.

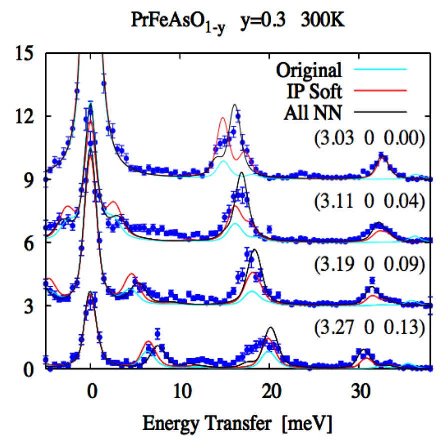
Phonons in complex materials.

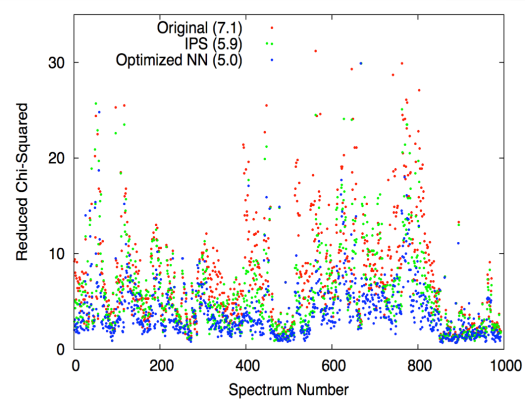
A More Complicated Sample

Slides with unpublished data removed.

Water and $BaBiO_3$:

Dynamical model from *Fitting Spectra*





Improvement by allowing parts of nearly all NN bonds to change (Baron, SR&FEL Handbook 2016).

Issues: More info on oxygen modes needed.
Also really need to include 2-phonon contribution (slow)
Start with symmetrized magnetic model (*Murai et al*, PRB2016)

General way to approach IXS – Reverse the Exodus

Caution

Nominal rate increases are **HUGE**: N or N^2
where N is 5-500, compared to a conventional spectrometer

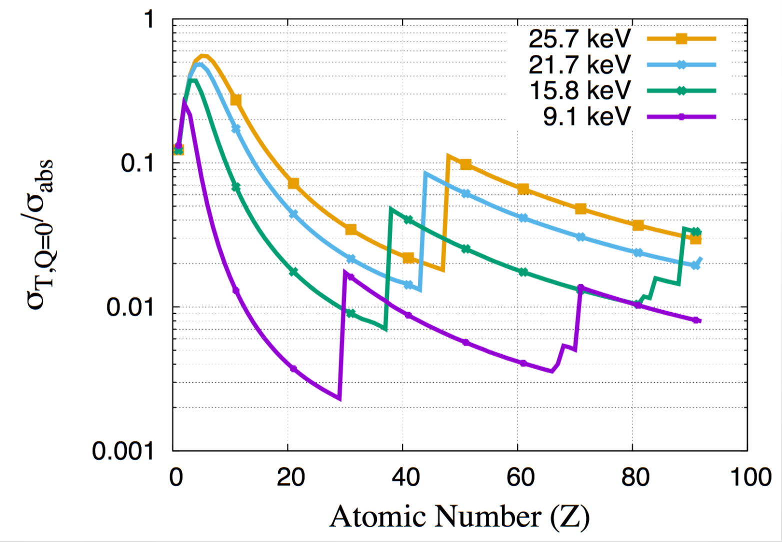
But: Energy resolution is much smaller: 1/10 or 1/100
Q resolution may need to be much better: 1/10 or 1/100
Energy is much lower: Losses on thick samples (1/5??)
Losses into sample environment (1/5??)

Very large improvement is possible – but still finite.
Care is needed.

(Radiation damage also an issue but dispersive setup helps).

Absolute Energy Matters

(generally higher is better)



Plot shows relative signal for a thicker (10, 100 um) sample.

Radiation damage scales similarly (x factor of energy – so slower)

Higher energy worse for Q Resolution

Questions

What are the resolution function tails like?

What are the limits on sample thickness/projection?
Is a grazing incidence geometry on the sample (e.g. thin film) possible?

What to do when you must have a small (1 or 5 or 10 um) spot size?
High Pressure, ***New Material***

Can one reasonably switch from "echo" to spectrograph operation?
For same scan range: just add slit/chan-cut? Or replace mono?
Larger scan range possible for spectrograph? Relationship?

Can one gain scan range by increasing the arm length?
for both the spectrograph and/or "echo"

Is it possible to (usefully) do this at 20 keV ?

Optics Issues

At what level are the designs for different spectrometers
(dE, Window, Q, dQ) mutually compatible/exclusive?

Parameter lists including crystal sizes, arm lengths, etc.

Tolerance numbers: Angle/Polishing/Temperature etc.

Two Comments

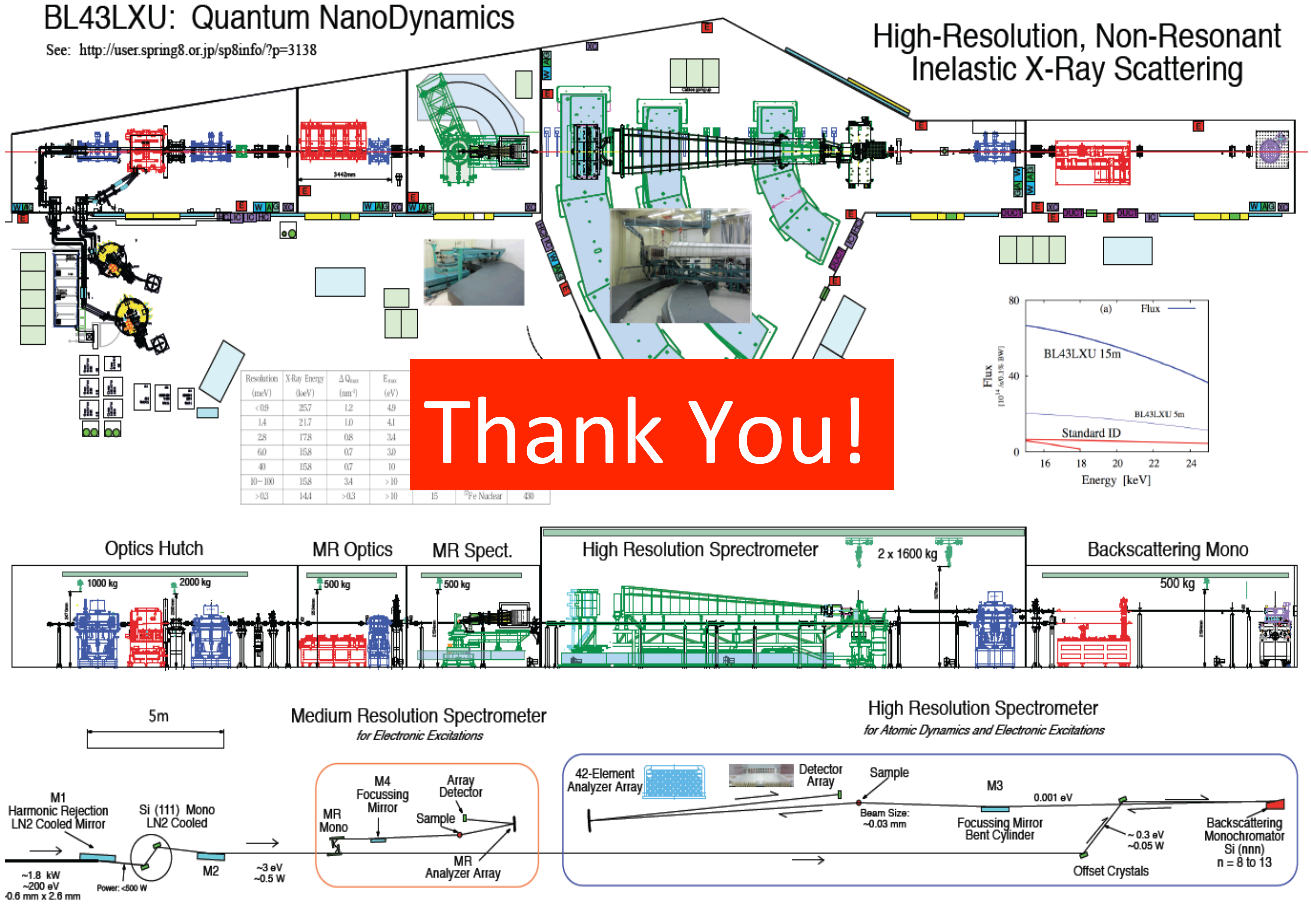
The potential of echo/spectrograph operation makes refractive Bragg optics (Shvyd'ko's designs) extremely attractive for both new investigations and significantly improved older style investigations, with the potential to push the state of the art greatly beyond what is possible today.

The spectrometers appear to be difficult practical optics problems, requiring significant funding, time, manpower and experience to make **reliable**.

BL43LXU: Quantum NanoDynamics

See: http://user.spring8.or.jp/sp8info/?p=3138

High-Resolution, Non-Resonant Inelastic X-Ray Scattering



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40	15.8	0.7	10			
10–100	15.8	3.4	>10			
>0.3	14.4	>0.3	>10	15	^{57}Fe Nuclear	430

Thank You!