Inelastic scattering spectroscopy with neutrons and X-rays to study superconducting materials:

Part I (some) general idea and (non-resonant) phonon studies

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Summary

- *Electron - phonons interactions and superconductivity in a nutshell*
- *Spectroscopies with X-rays and neutrons*
- *Inelastic X-ray Scattering spectroscopy*
- *Phonon anomalies in "conventional" superconductors*

Further readings

Basic textbooks in neutron and x-ray physics

- “Introduction to the Theory of Thermal Neutron Scattering”, G.L. Squires (Dover Publications,1996)
- “Theory of Neutron Scattering from Condensed Matter”, Stephen W. Lovesey (Clarendon Press, 1986)
- “Elements of Modern X- ray Physics”, Jens Als- Nielsen Des McMorrow (John Wiley & Sons, 2011)
- “JDN 10 – Diffusion Inélastique des Neutrons pour l'Étude des Excitations dans la Matière Condensée”, S. Rols, S. Petit, J. Combet et F. Leclercq-Hugeux (Eds.) (EDP Sciences, 2010)

Further readings

Advanced readings in x-ray physics

- "Core Level Spectroscopy of Solids", Frank de Groot, Akio Kotani (2008, CRC Press)
- "Introduction to High-Resolution Inelastic X-Ray Scattering", A.Q.R. Baron *arXiv:1504.01098*
- "Resonant inelastic x-ray scattering studies of elementary excitations", L. J. P. Ament, M. van Veenendaal, T. P. Devereaux, J. P. Hill, J. van den Brink, *Reviews of Modern Physics* **83** (2011)

Further readings

Basic textbooks in superconductivity

...there are many, my preferred one is:

- “Theory Of Superconductivity” (Advanced Books Classics), J. Robert Schrieffer (Perseus Books, 1999)

Further readings

Advanced readings in superconductivity

(non exhaustive list by far...)

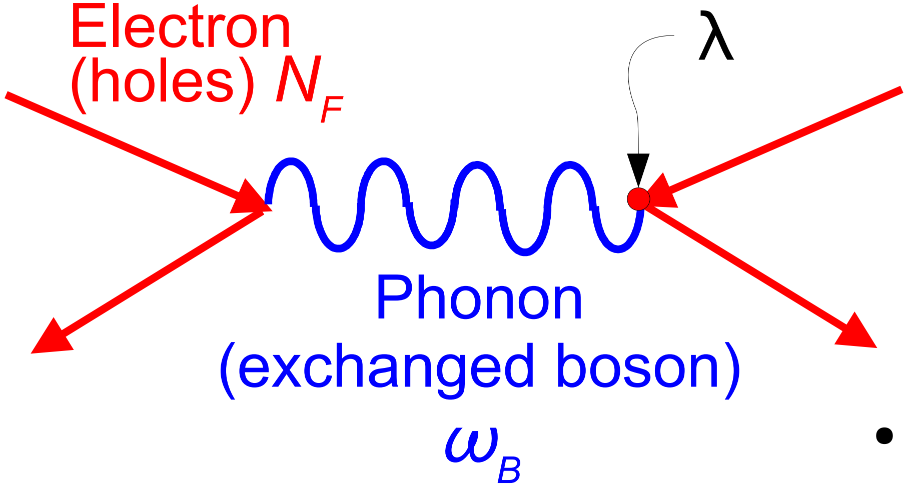
- J. P. Carbotte, *Rev. Mod. Phys*. **62** (1990) 1027.
- D. A. Bonn, *Nature Physics* **2** (2006) 159.
- D. J. Scalapino, *Rev. Mod. Phys*. **84** (2012) 1383.

Electron - phonons interactions and superconductivity in a nutshell

Superconductivity basic idea:

creation of “Cooper pairs” ⇨ “bosonic” charge carriers

Reciprocal space

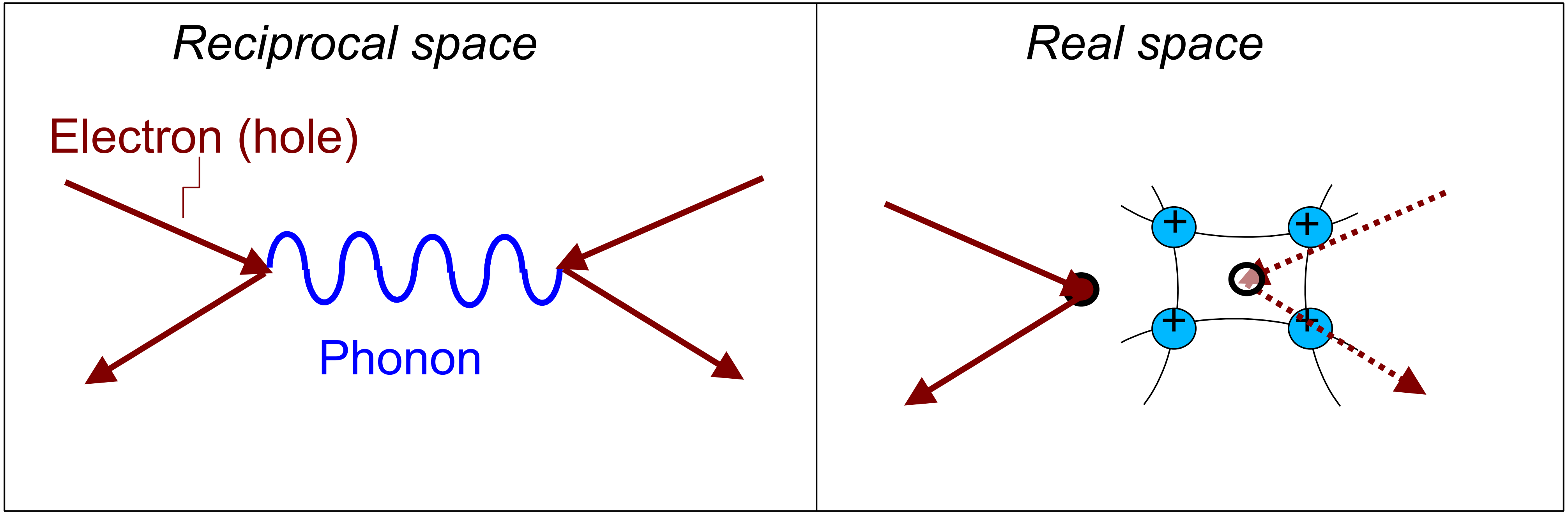


The transition temperature (Tc) is function of:

- the boson frequency (ω_B);
- the interaction strength (λ);
- the electron density @ Fermi surface (N_F).

Electron - phonons interactions and superconductivity in a nutshell

BCS model : - Boson formation by electron (hole) pairing
- Phonon mediated coupling



At Tc pair formation AND Bose condensation
Correlated state over a large x ~ 1000 Å
Isotopic effect - Isotropic (s-wave) pairing

Electron - phonons interactions and superconductivity in a nutshell

Superconductivity basic idea:

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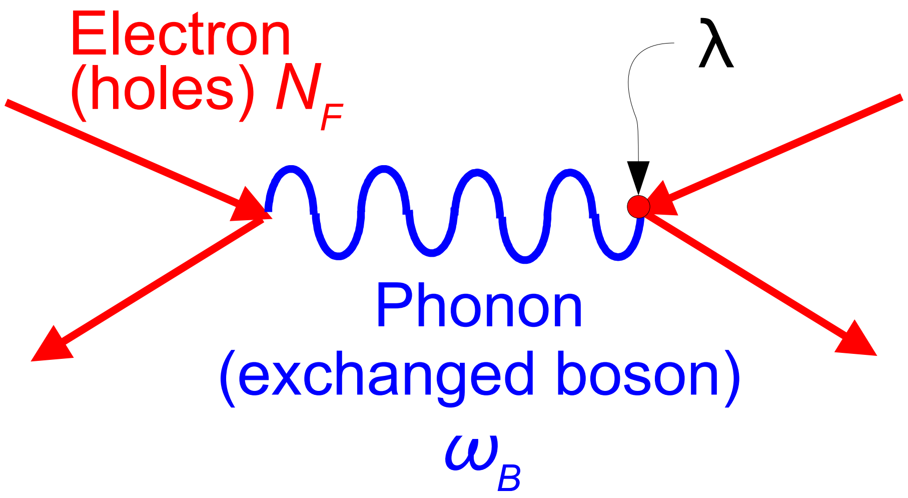

In weak coupling limit we have:

$$T_c^{weak} \sim \omega_B \exp\left(\frac{-1}{N_F V(\lambda)}\right)$$

(V pairing potential)

Electron - phonons interactions and superconductivity in a nutshell

Superconductivity basic idea:

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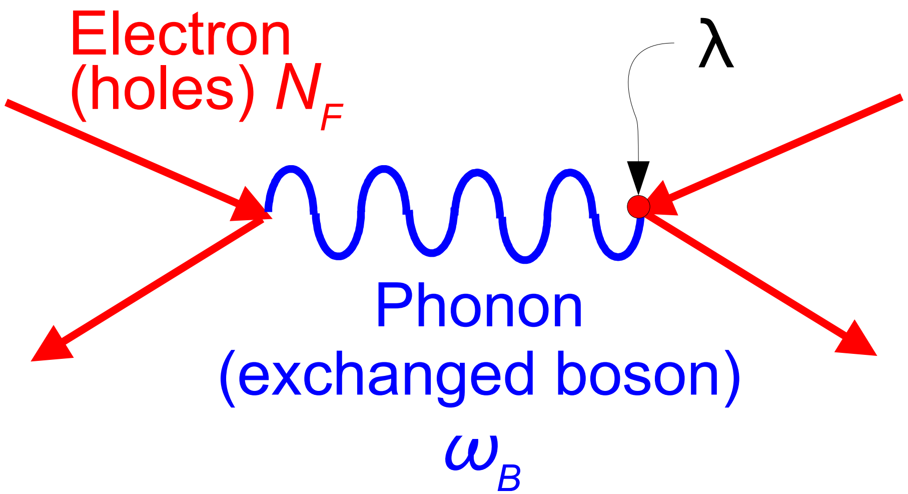


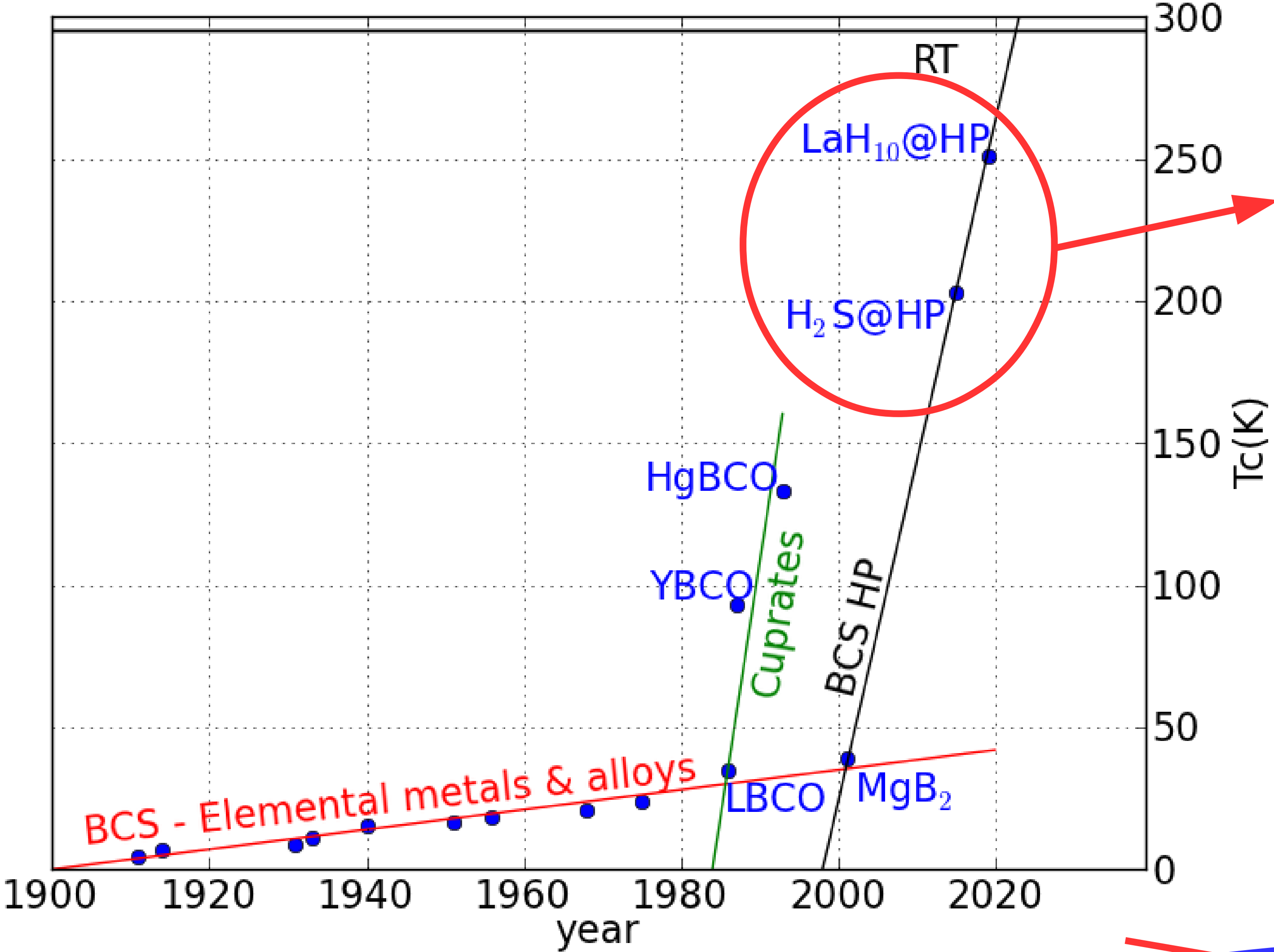
Looking to **strong coupling limit** :

$$T_c^{strong} \sim \omega_D \exp\left(\frac{-(1+\lambda)}{\lambda-\mu^*-(\langle\omega\rangle/\omega_D)\lambda\mu^*}\right)$$

in **elemental metal and alloys** (*i.e.* small phonon ω_D) $T_c < 30$ K

This also motivate the search for superconductors with **soft modes**

High temperature superconductivity quest



Today hydrides at high pressure reach 250-252 K

An order of magnitude higher than the supposed BCS limit!

How it is possible?

~~30 K Tc limit for BCS(?)~~

Spectroscopies with synchrotron and neutrons

synchrotron light sources

- ***Photon in - photon out***
  - *absorption*
  - *fluorescence*
  - *inelastic scattering*
  - *resonant inelastic scattering*
- ***Photoemission***

neutrons

Neutron in - neutron out

- *inelastic scattering*

List (approximately) exhaustive

*for **condensed matter only**!*

We can explore many excitations in solids,

but here we will focus on....

Spectroscopies with synchrotron and neutrons

synchrotron light sources

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Neutron in - neutron out

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We can explore many excitations in solids,

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neutrons

Neutron in - neutron out

- *inelastic scattering*

We can explore many excitations in solids,

but here we will focus on.... and (para)magnons (afternoon lecture).

Spectroscopies with synchrotron and neutrons

synchrotron light sources

- ***Photon in - photon out***
  - *absorption*
  - *fluorescence*
  - *inelastic scattering*
  - *resonant inelastic scattering*
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neutrons

Neutron in - neutron out

- *inelastic scattering*

We can explore many excitations in solids,

if you'd like to know whats happens to electrons, then....

Spectroscopies with synchrotron and neutrons

synchrotron light sources

- **Photon in - photon out**
  - *absorption*
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- **Photoemission**

neutrons

Neutron in - neutron out

- *inelastic scattering*

We can explore many excitations in solids,

if you'd like to know whats happens to electrons, then....

Spectroscopies with synchrotron and neutrons

synchrotron light sources

Photoemission

See tomorrow lecture :

“ Photoemission and angle-resolved photoemission :

A tool to probe the electronic structure of materials”

by Patrick Le Fèvre (SOLEIL synchrotron)

For correlated materials and superconductors see lecture (video, slides, text) and practicals (text, slides and solutions) by Andrés Santander Syro on: http://gdr-meeticc.cnrs.fr/ecole-du-gdr-meeticc-school_v3/

Spectroscopies with synchrotron and neutrons

synchrotron light sources

- ***Photon in - photon out***
  - *absorption*
  - *fluorescence*
  - *inelastic scattering*
  - *resonant inelastic scattering*
- ***Photoemission***

} *interaction with electrons*

- ***Photon-in photon-out***
  - *Mößbauer (& related)*

} *interaction with nuclei*

Spectroscopies with synchrotron and neutrons

neutrons

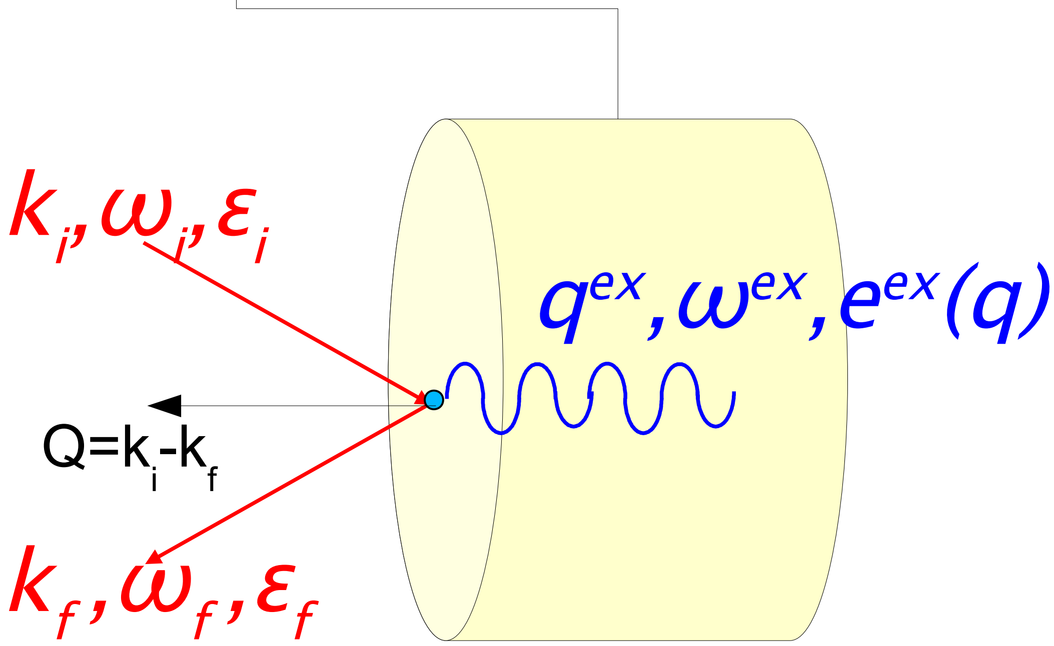
Neutron in - neutron out

- *inelastic scattering*

interaction with nuclei
(this lecture)
&
electron's spin
(lecture II)

Inelastic X-ray Scattering spectroscopy

A particle (photon, neutron, electron He atom...) probe a sample (in this lecture a crystal)

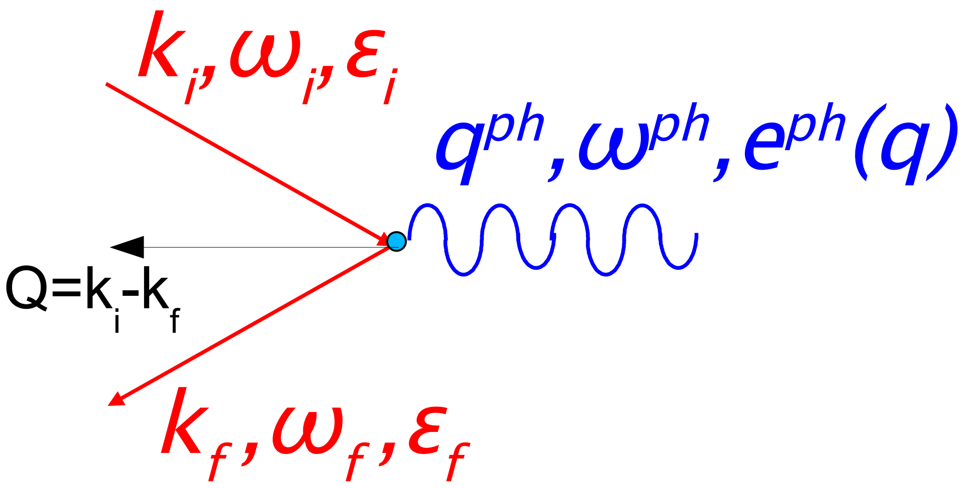


and exchange energy and momentum with an internal excitation (*e.g.* a phonon..)

With visible light is known since the works of Raman and Brillouin

Inelastic Scattering: kinematic

Phonon quasi-particle can scatter probe particle as photons, neutrons, electrons and even and He atoms

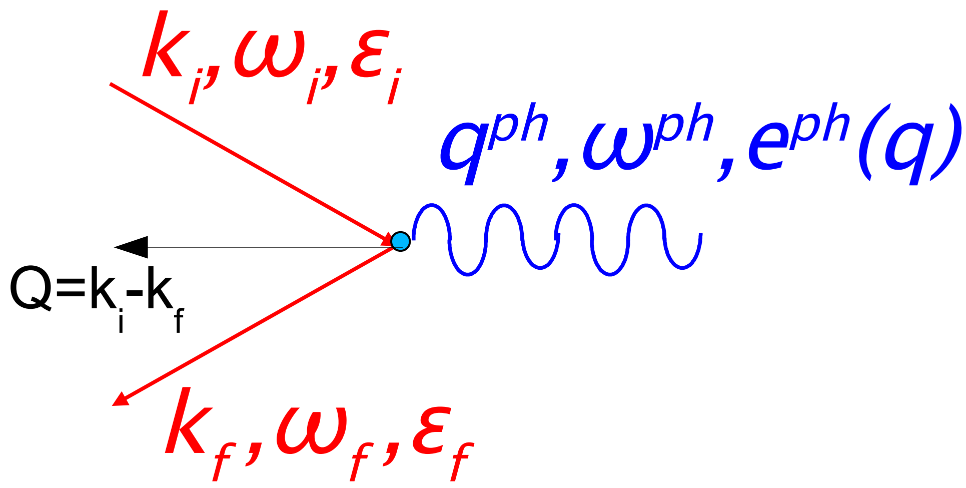


$$\hbar\omega_i - \hbar\omega_f = \hbar\omega_{ph}$$

$$\hbar k_i - \hbar k_f = \hbar Q$$

Inelastic Scattering: kinematic

Knowing energy (frequency), momentum (wave-vector) of both incident and scattered probes, one get energy and momentum of the phonon



$$\hbar\omega_i - \hbar\omega_f = \hbar\omega_{ph}$$

$$\hbar k_i - \hbar k_f = \hbar Q$$

Inelastic Scattering: kinematic

Like playing pool with phonons

Courtesy Wikiedia, Childzy

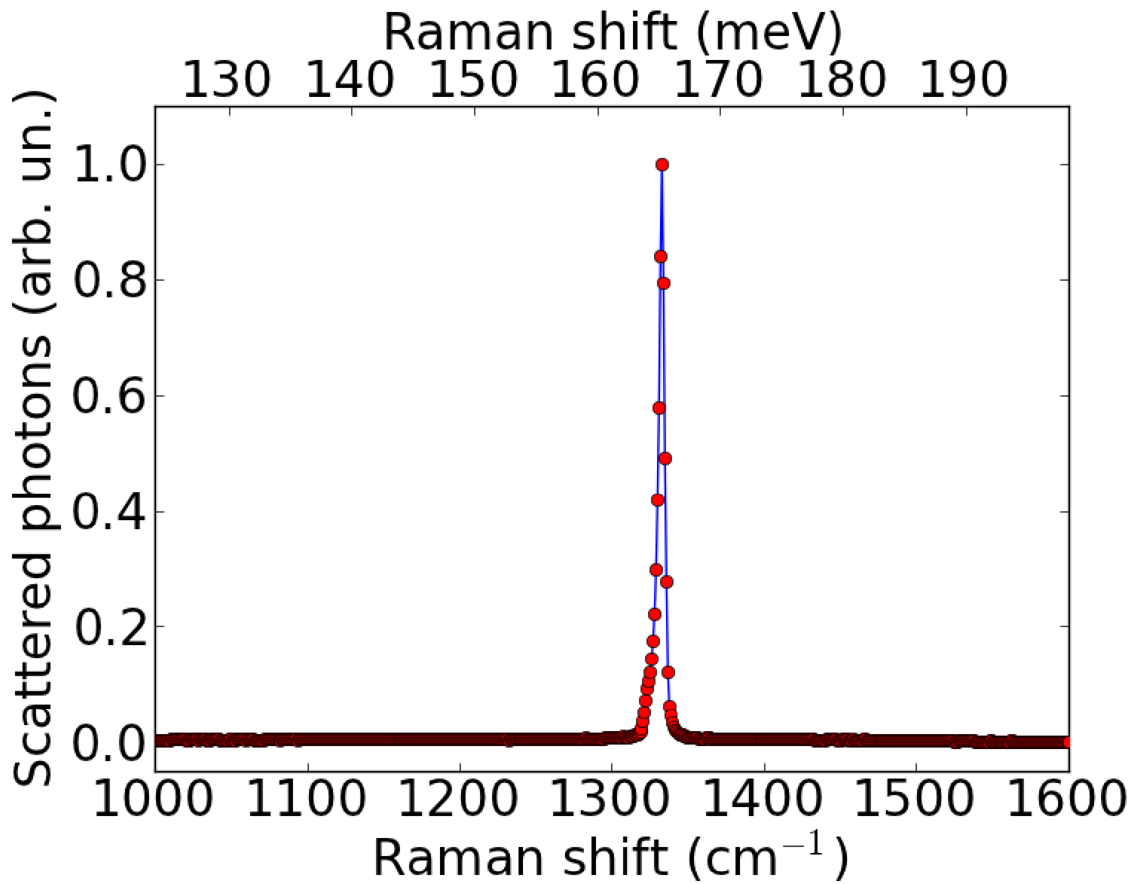
$$\hbar\omega_i - \hbar\omega_f = \hbar\omega_{ph}$$

$$\hbar k_i - \hbar k_f = \hbar Q$$

Phonon parameters from inelastic scattering

Energy of the phonon line :

→ Phonon frequency



Just like Raman with neutrons or X-ray.
(Data from diamond standard)

Two big difference with visible light Raman:

1) the reciprocal space access (see next slides)

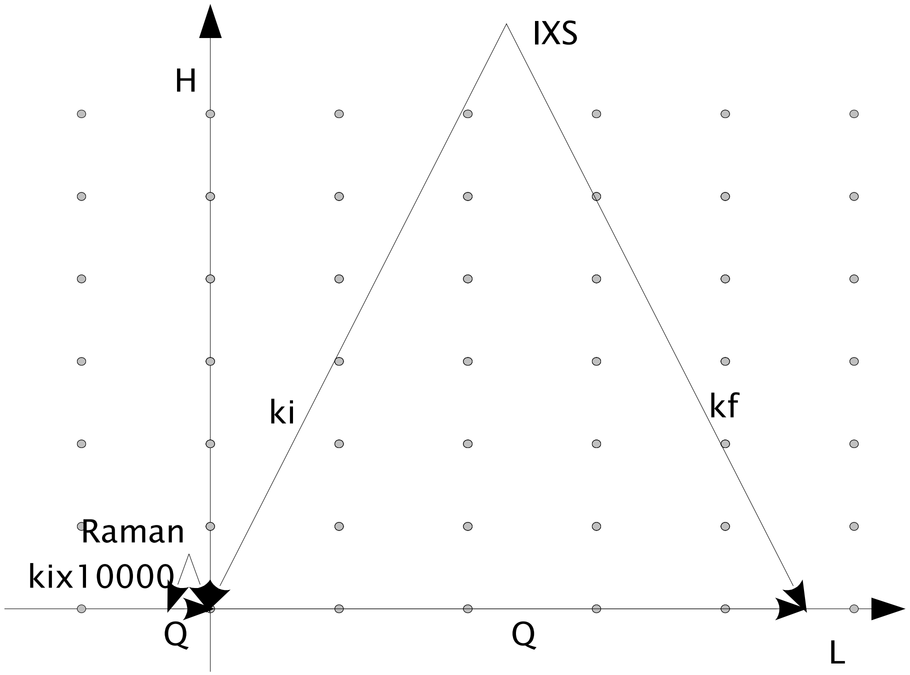
2) the photon-matter interaction (cross-section)

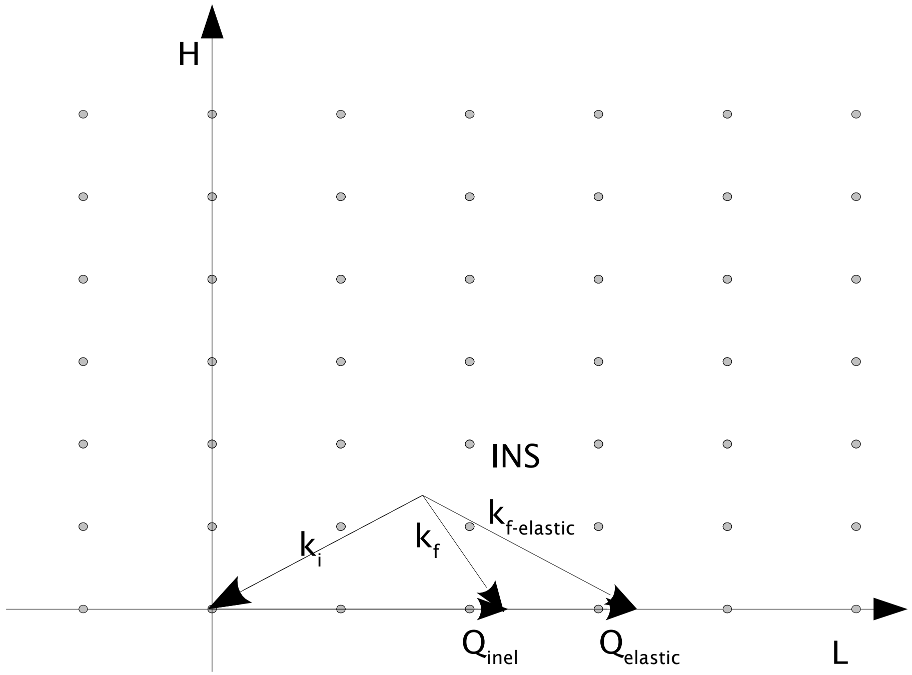
Scattering vectors for typical incident energies:

2.5 eV visible light (496 nm wavelength ⟺ green);

17793 eV X-ray from Si(999);

14 meV neutrons (tuned to best graphite filter windows).





M. d’Astuto and M. Krisch JDN **10** (2010)

Phonon parameters from inelastic scattering

Energy of the phonon line :

→ Phonon frequency

Here an example using X-rays in diamond (neutrons would be the same)

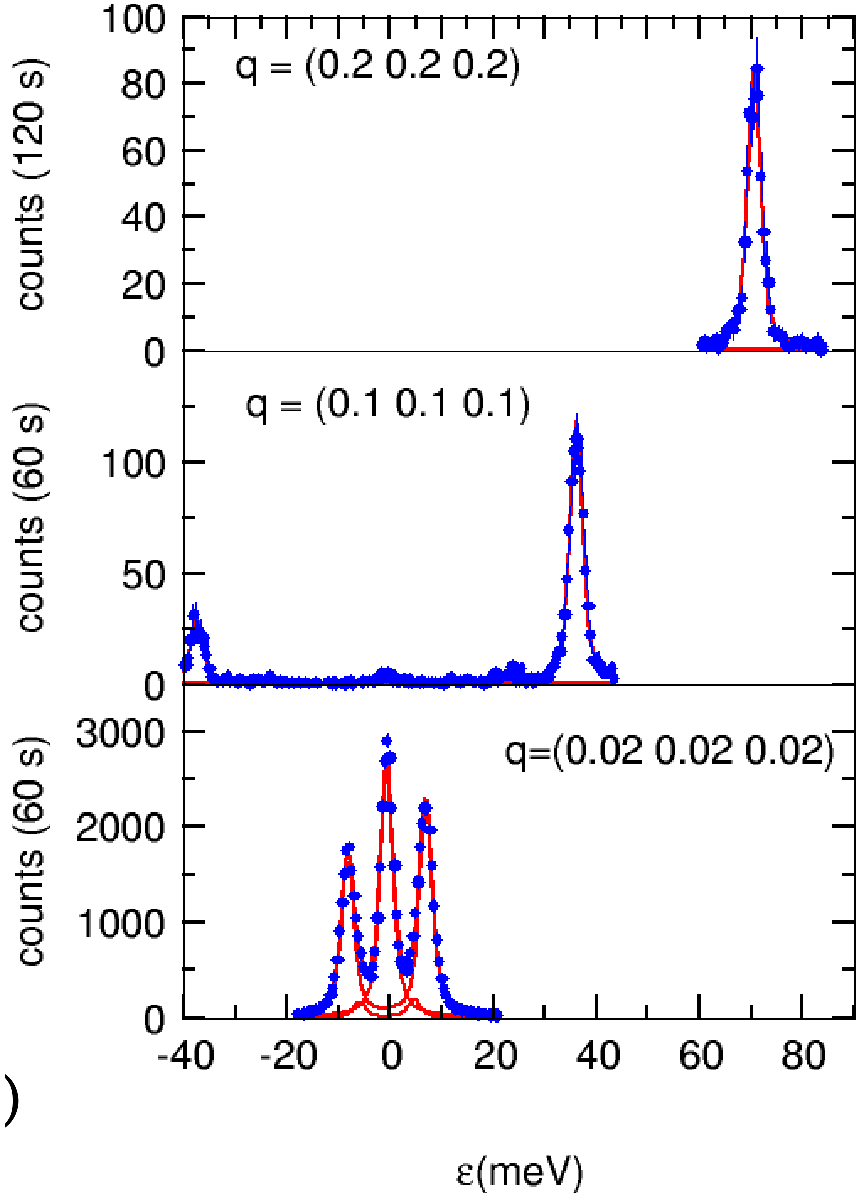
Intensity is scattered when

$\hbar\omega_i - \hbar\omega_f = \hbar\omega_{ph}$

but now I can change also

$\hbar k_i - \hbar k_f = \hbar Q$

and follow a dispersion



M. d’Astuto and M. Krisch JDN **10** (2010)
R. Verbeni, *et al.. RSI* **79** (2008)

Dispersion with neutrons & X-rays

Energy of the phonon line :

→ Phonon frequency

Here an example using X-rays (neutrons would be the same)

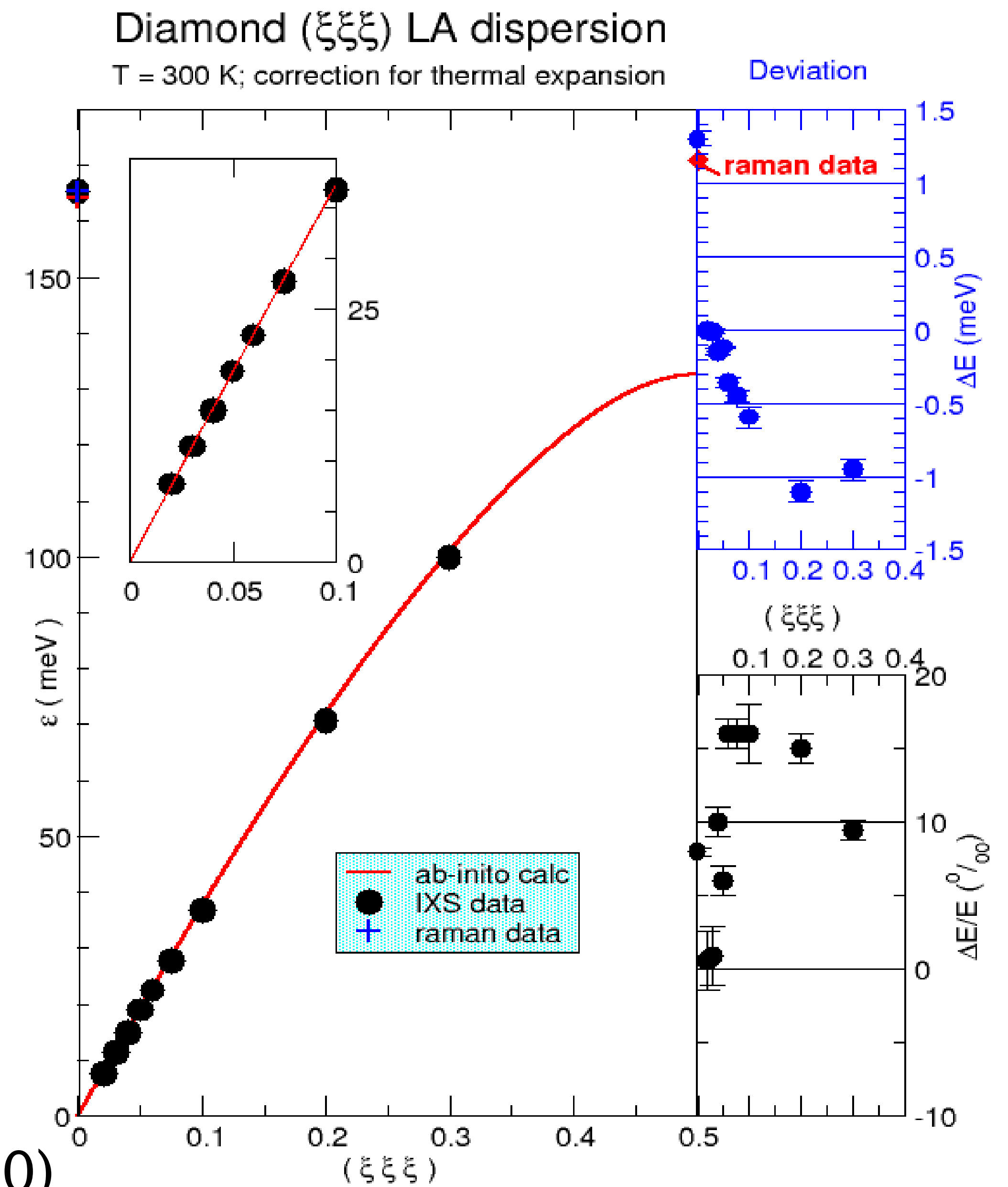
Intensity is scattered when

$\hbar\omega_i - \hbar\omega_f = \hbar\omega_{ph}$

but now I can change also

$\hbar k_i - \hbar k_f = \hbar Q$

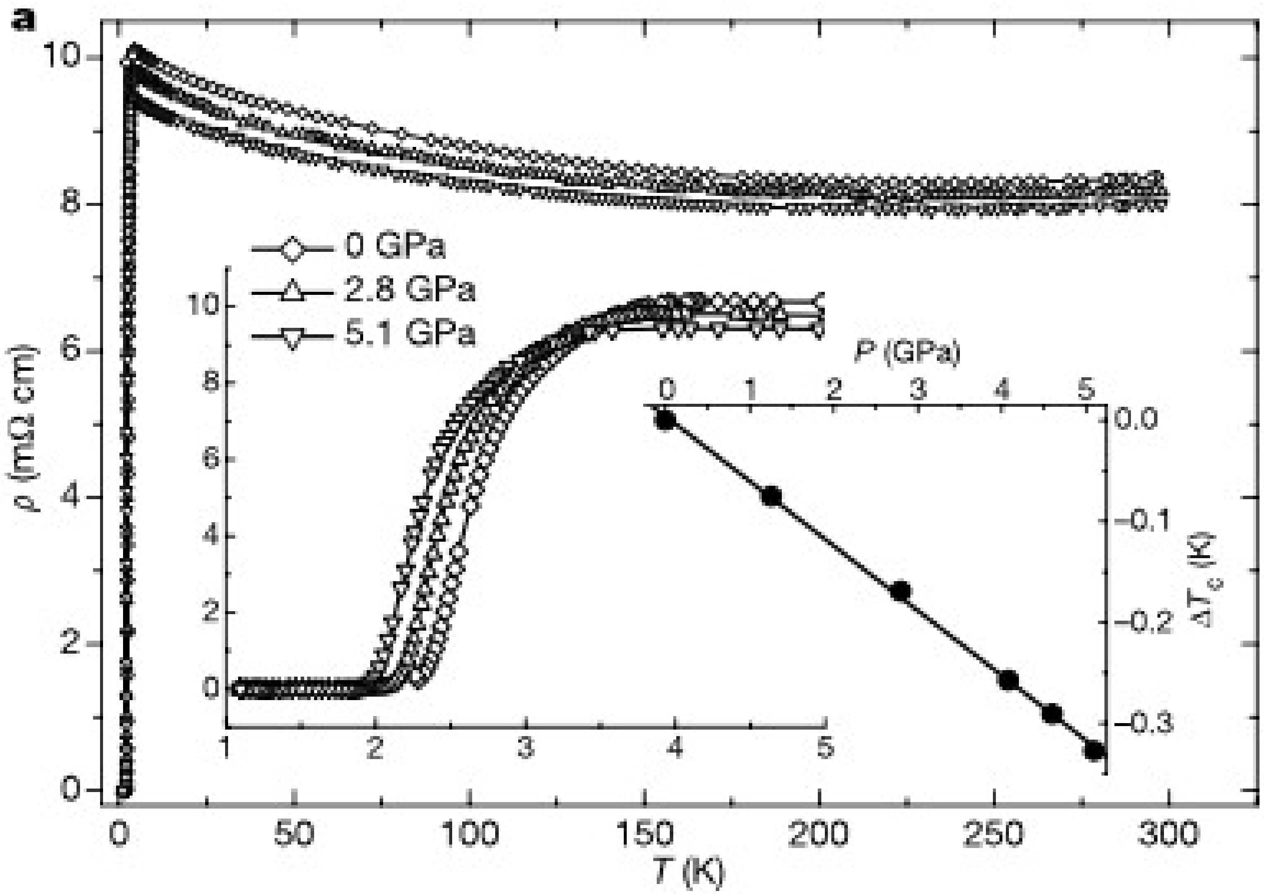
and follow a dispersion



M. d'Astuto and M. Krisch JDN **10** (2010)
R. Verbeni, *et al.. RSI* **79** (2008)

Diamond superconductivity

Boron doped diamond is superconductor at 4 K
E. A. Ekimov, *et al.*, *Nature* **428** (2004)



...and up to 11 K depending on doping level
X. Blase, *et al.*, *Nat. Mater.* **8** (2009)

A high Tc for impurity doping

Electron - phonons interactions and superconductivity in a nutshell

Superconductivity basic idea:

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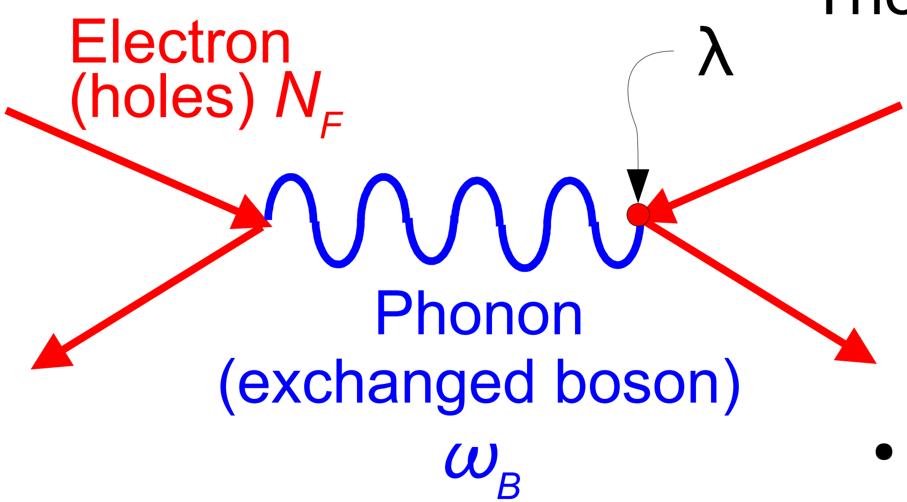
Reciprocal space



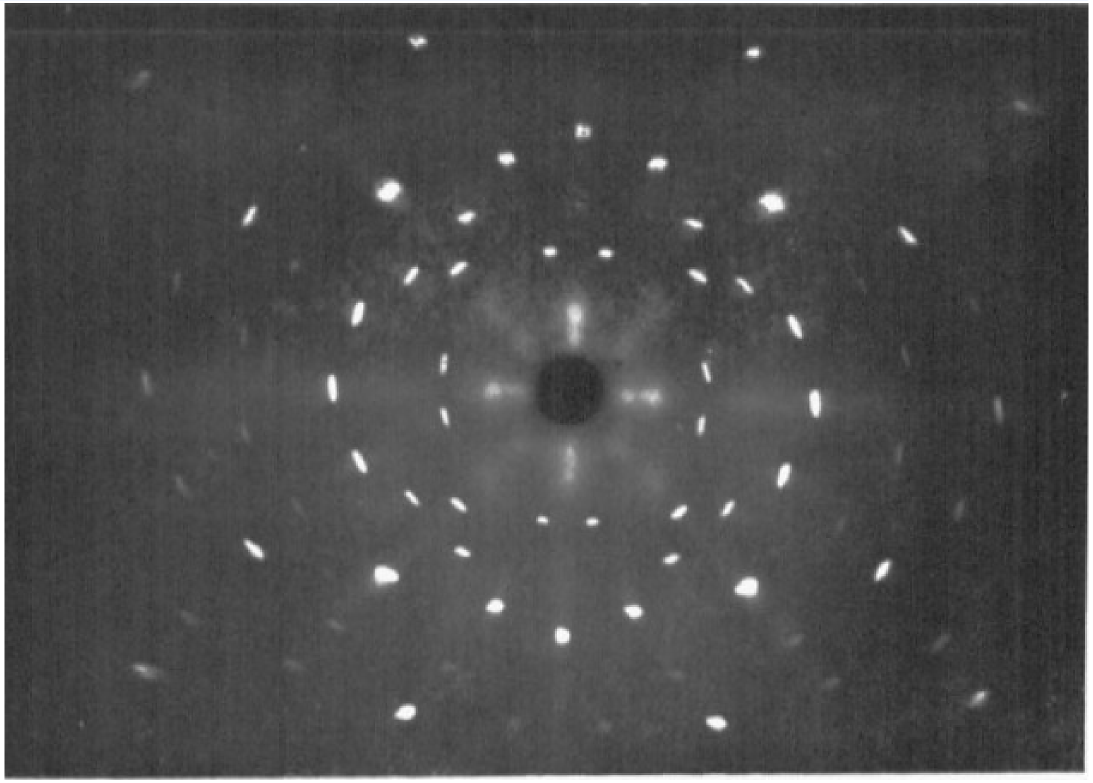
The transition temperature (Tc) is function of:

- the boson frequency (ω_B);
- the interaction strength (λ);
- the electron density @ Fermi surface (N_F).

Thermal diffuse scattering (Faxen-Waller Scattering)

Inelastic X-ray Scattering aka Thermal Diffuse Scattering

J. Laval: “The crystalline diffusion of x-rays may be envisaged as resulting from the Bragg reflections, with a change in frequency, on the level waves of thermic agitation” *Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences* **214** (1942)

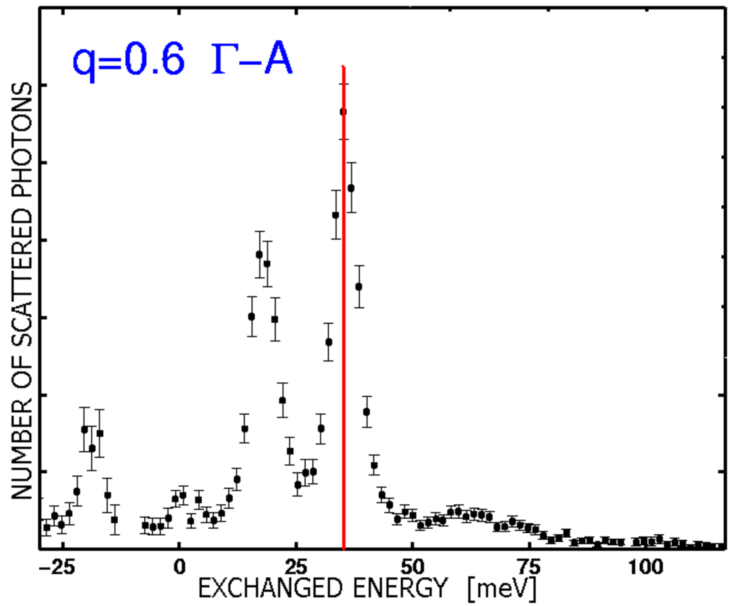


Stationary crystal of NaCl, direct radiation from Mo target along cube-axis direction; 2½-hour exposure, room temperature.
K. Lonsdale *Rep. Prog. Phys.* **9** (1942)

Phonon parameters from inelastic scattering

Energy of the phonon line :

→ Phonon frequency



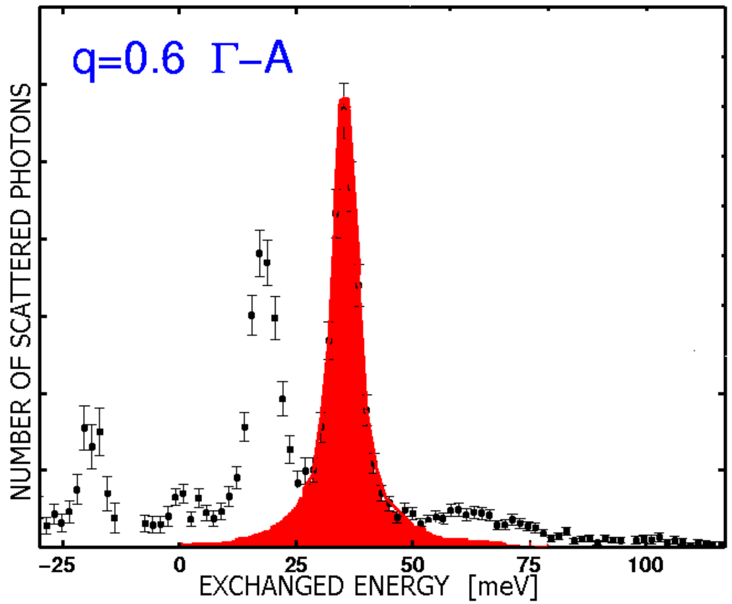
Phonon parameters from inelastic scattering

Energy of the phonon line :

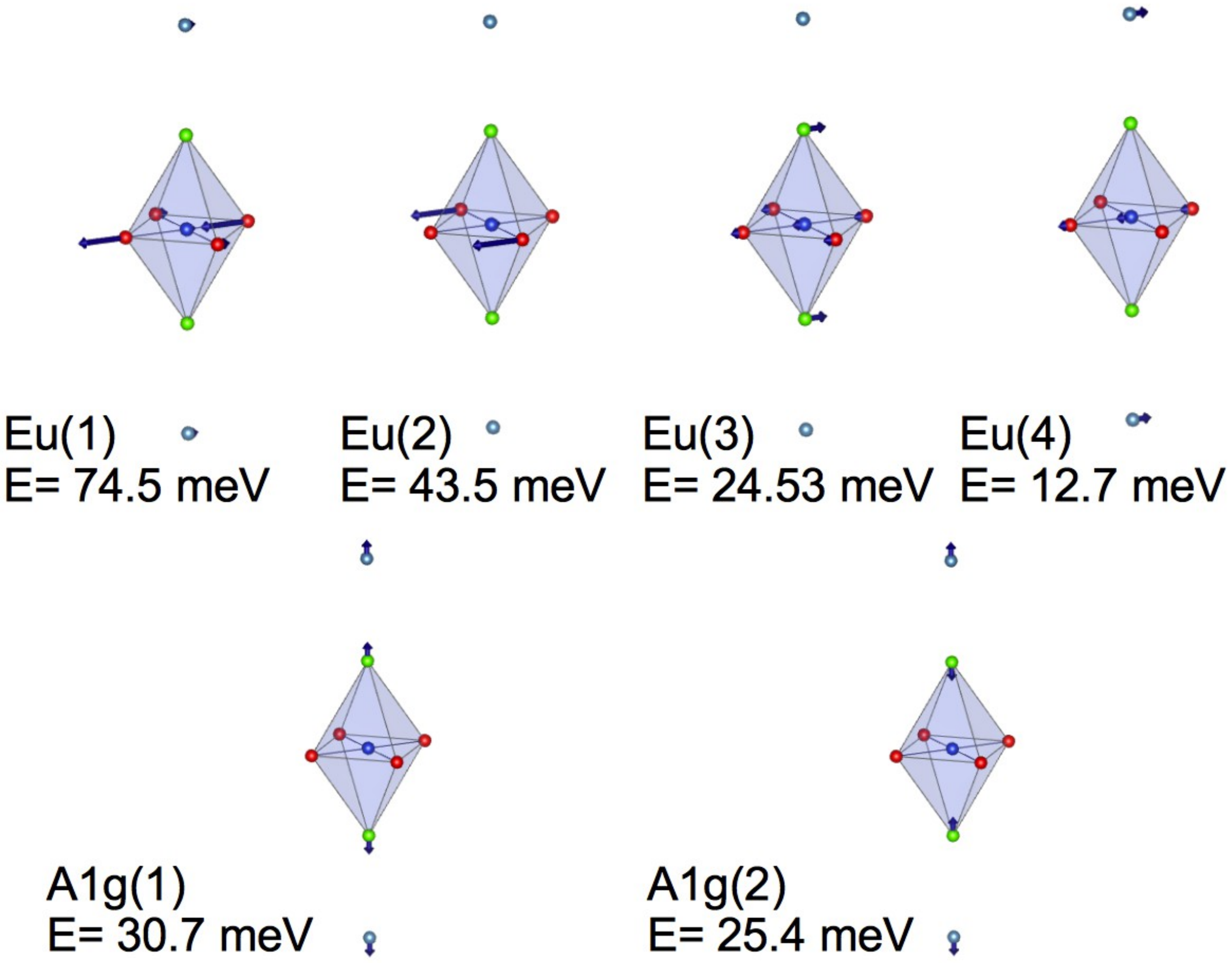
→ Phonon frequency

Intensity of the phonon line :

→ Phonon eigenvectors



Phonon dispersion in $Ca_{2-x}CuO_2Cl_2$

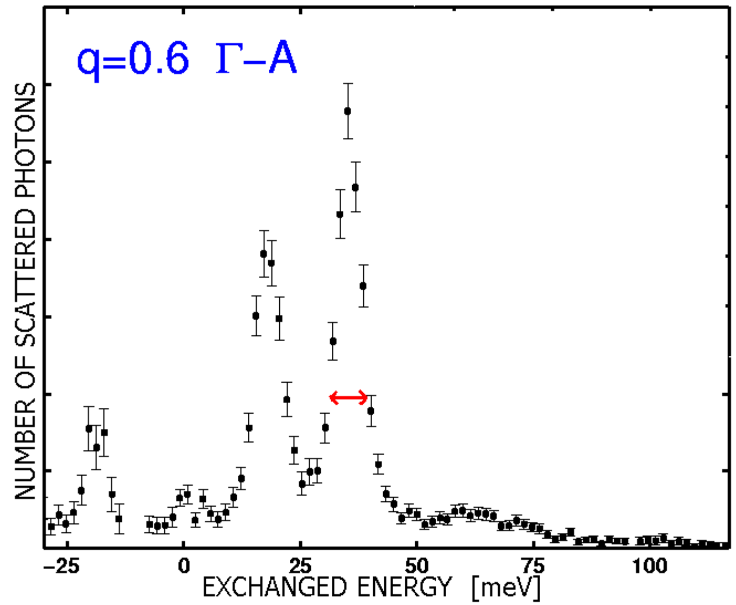


d'Astuto *et al. PRB* **88** (2013)

Phonon parameters from inelastic scattering

Phonon linewidth :

→ Phonon life-time + instrument resolution



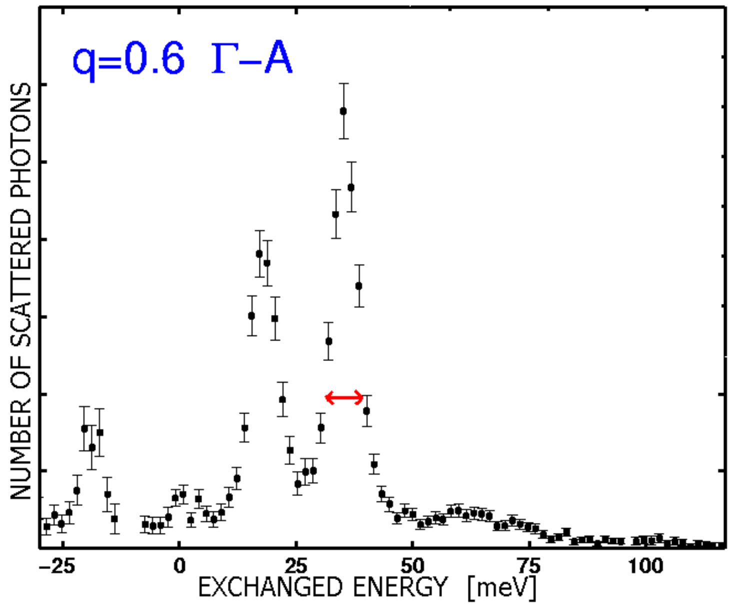
Phonon parameters from inelastic scattering

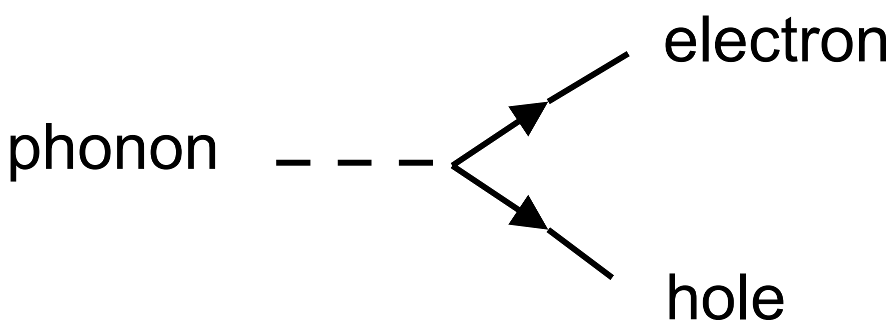
Phonon linewidth :

→ **Phonon life-time** + instrument resolution

Decay of a phonon in an electron-hole pair

→ Due to the electron-phonon coupling





Phonon parameters from inelastic scattering

Phonon linewidth :

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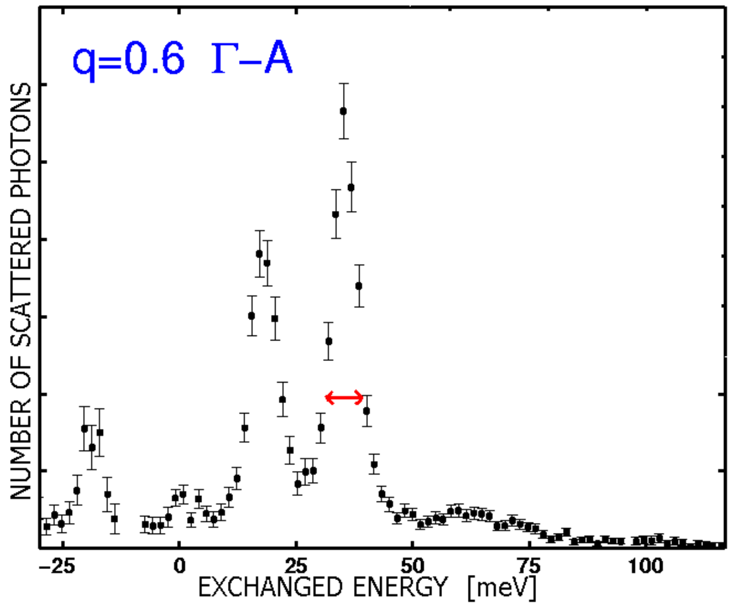
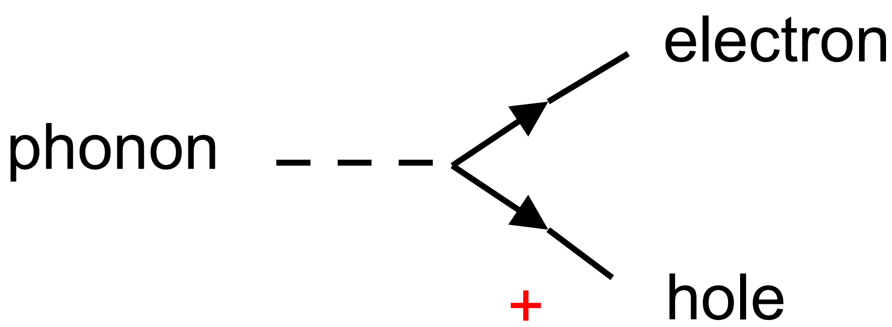
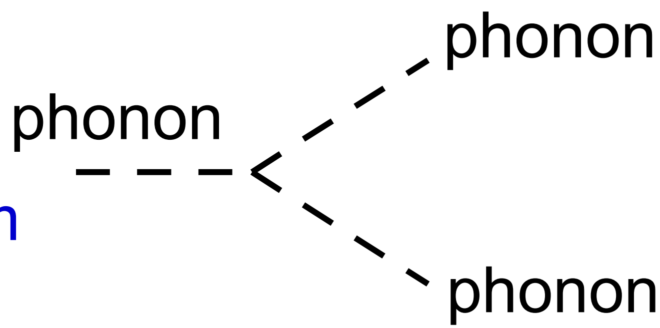


→ Decay of a phonon in an electron-hole pair
Due to the electron-phonon coupling



→ Anharmonicity: decay of a phonon in two phonons conserving energy and momentum

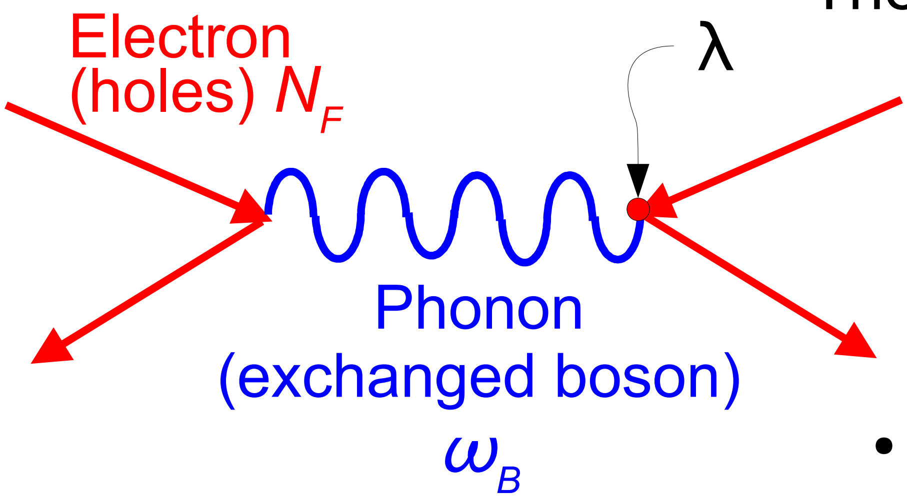


Electron - phonons interactions and superconductivity in a nutshell

Superconductivity basic idea:

creation of "Cooper pairs" ⇨ "bosonic" charge carriers

Reciprocal space



The transition temperature (Tc) is function of:

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- the interaction strength (λ);
- the electron density @ Fermi surface (N_F).

Inelastic X-ray Scattering

Thermal diffuse scattering comes from phonons: very strong yield

Comparable to neutron:

$r_0 = e^2/m_e c^2 \sim b$

$$\frac{\partial^2\sigma}{\partial\Omega\partial E} = \left[r_0^2(\hat{\epsilon}_i \cdot \hat{\epsilon}_f)^2\right]\left[\frac{k_i}{k_f}\sum_{I,F} P_I |\langle F|\sum_k f_k(Q) e^{i\vec{Q}\cdot\vec{R}_k}|I\rangle|^2 \delta(E - E_f - E_i)\right]$$

$$f_k(\vec{Q}) = -1/e \int d\vec{r}\, e^{i\vec{Q}\cdot\vec{r}_j} \rho_k(\vec{r})$$

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These two replaced by b_k for neutrons
(See yesterday lectures by Jean Daillant and Claire Colin)

Inelastic X-ray Scattering

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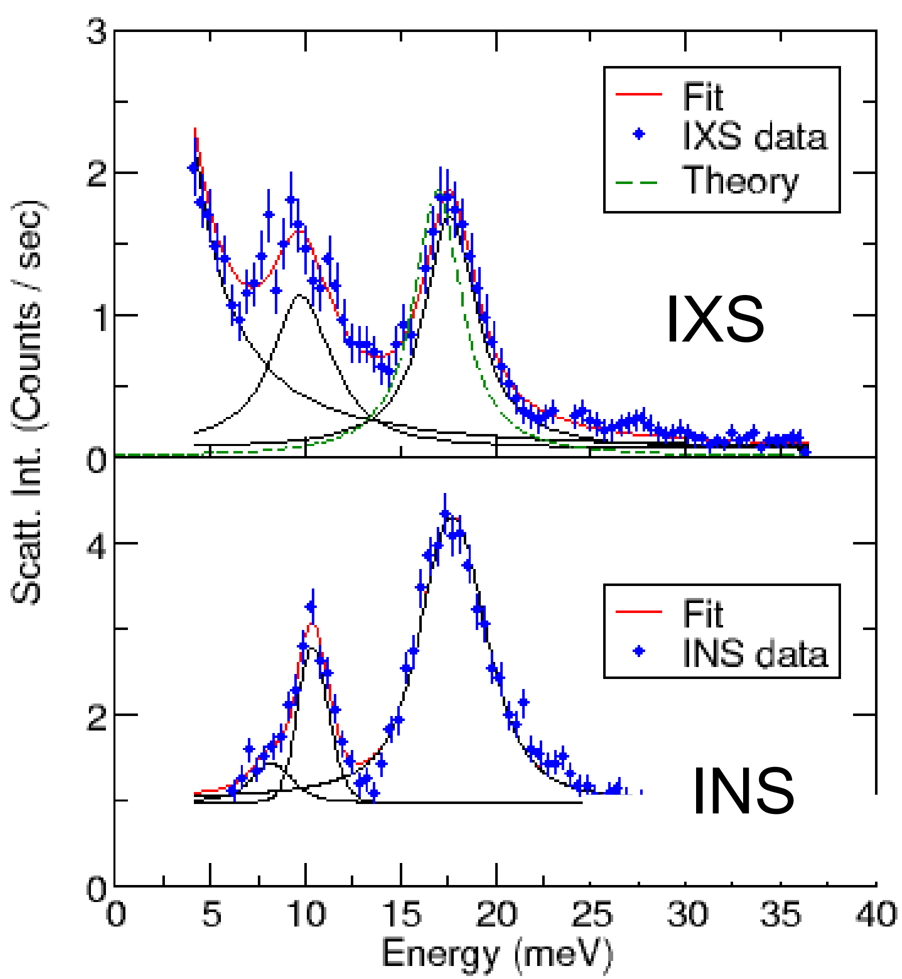
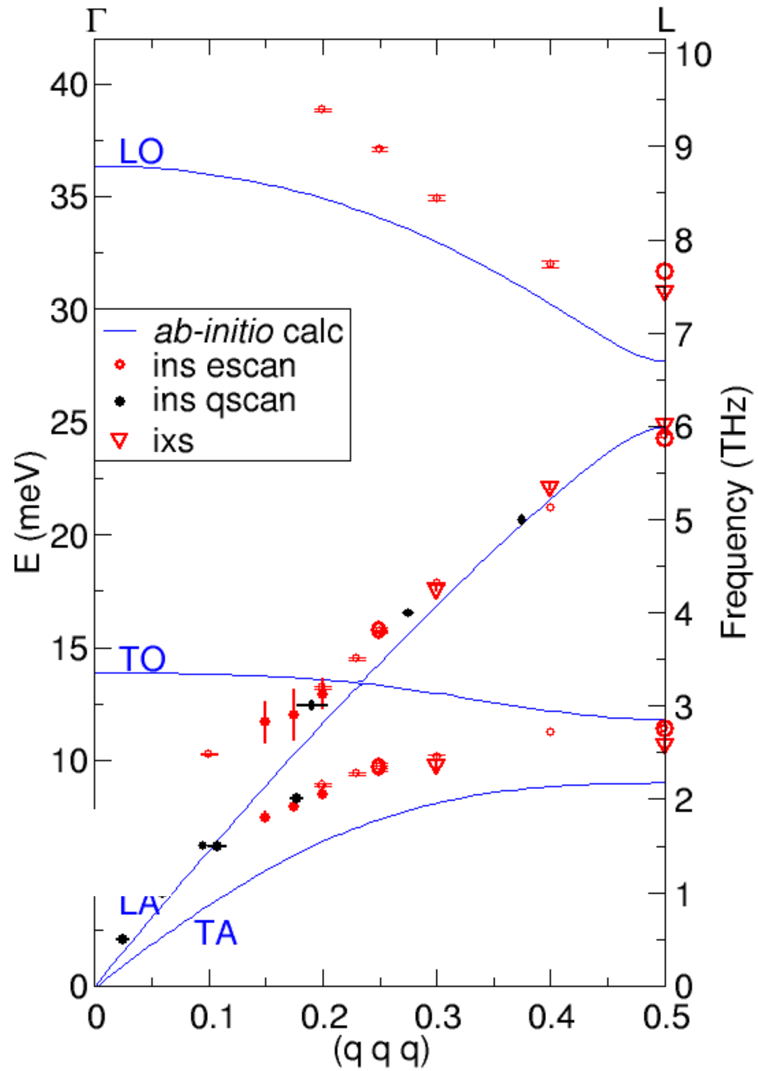
(Optic photon) Raman scattering completely different (change of polarisability)

INS vs IXS example: superconductivity in CaC_6



c-axis phonon dispersion in CaC_6



M. d'Astuto et al. PRB **81** (2010)

Inelastic X-ray Scattering

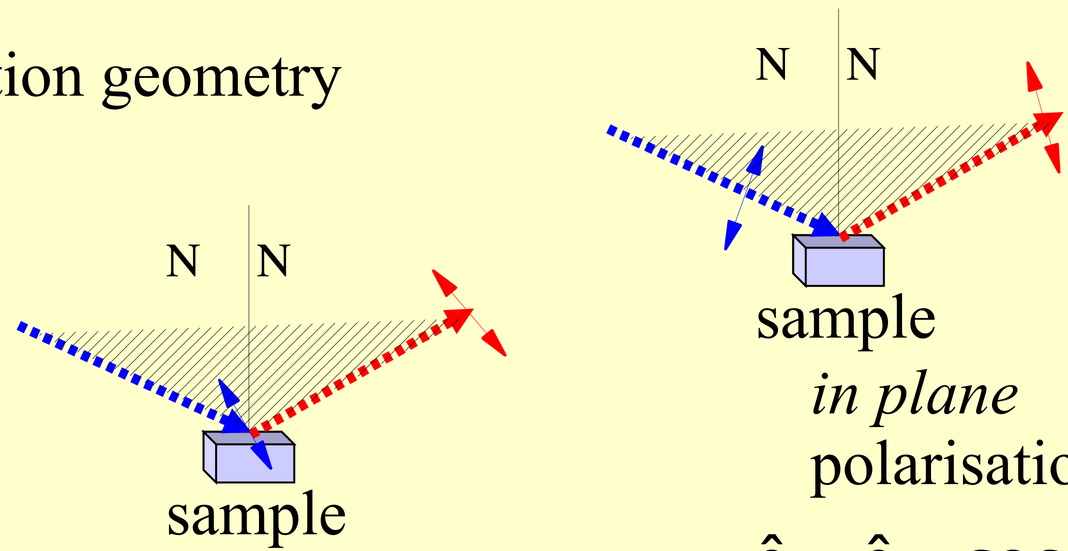
Thermal diffuse scattering comes from phonons: very strong yield

Comparable to neutron:

$r_0 = e^2/m_e c^2 \sim b$

$$\frac{\partial^2\sigma}{\partial\Omega\partial E} = \left[r_0^2(\hat{\epsilon}_i \cdot \hat{\epsilon}_f)^2\right]$$

Reflection geometry



out of plane polarisation $\hat{e}_i \,.\, \hat{e}_f = 1$

in plane polarisation $\hat{e}_i \,.\, \hat{e}_f = \cos(\vartheta)$

Inelastic X-ray Scattering

Thermal diffuse scattering comes from phonons: very strong yield

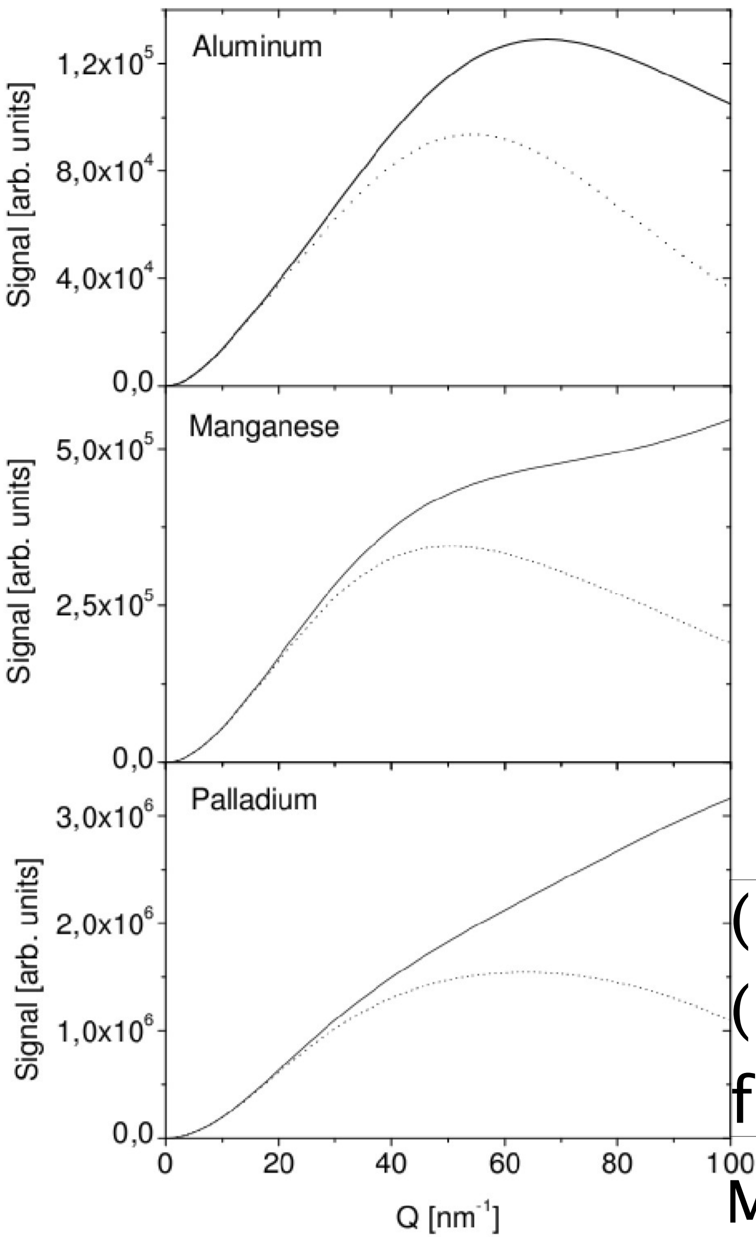
Comparable to neutron:

$r_0 = e^2/m_e c^2 \sim b$

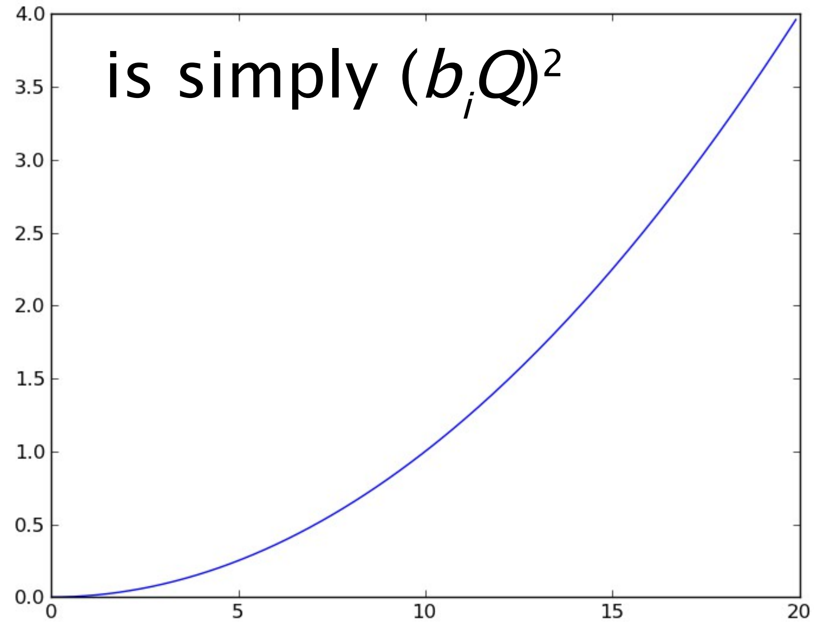
$$\frac{\partial^2\sigma}{\partial\Omega\partial E} = \left[r_0^2(\hat{\epsilon}_i \cdot \hat{\epsilon}_f)^2\right]\left[\frac{k_i}{k_f}\sum_{I,F} P_I |\langle F| \sum_k f_k(Q) e^{i\vec{Q}\cdot\vec{R}_k} |I\rangle|^2 \delta(E - E_f - E_i)\right]$$

$$\sim \vec{Q} \cdot \hat{e}_k^n(\vec{q})$$

For X-ray:



For neutrons:



is simply $(b_i Q)^2$

$(f_i(Q)Q)^2$ (solid line) and
$(f_i(Q)Q)^2\cos2(ts)$ (dashed line)
for 22 keV x-rays

M. d'Astuto and M. Krisch JDN **10** (2010)

Inelastic X-ray Scattering

Thermal diffuse scattering comes from phonons: very strong yield

Comparable to neutron:

$r_0 = e^2/m_e c^2 \sim b$

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$$\sim \vec{Q} \cdot \hat{e}_k^n(\vec{q})$$

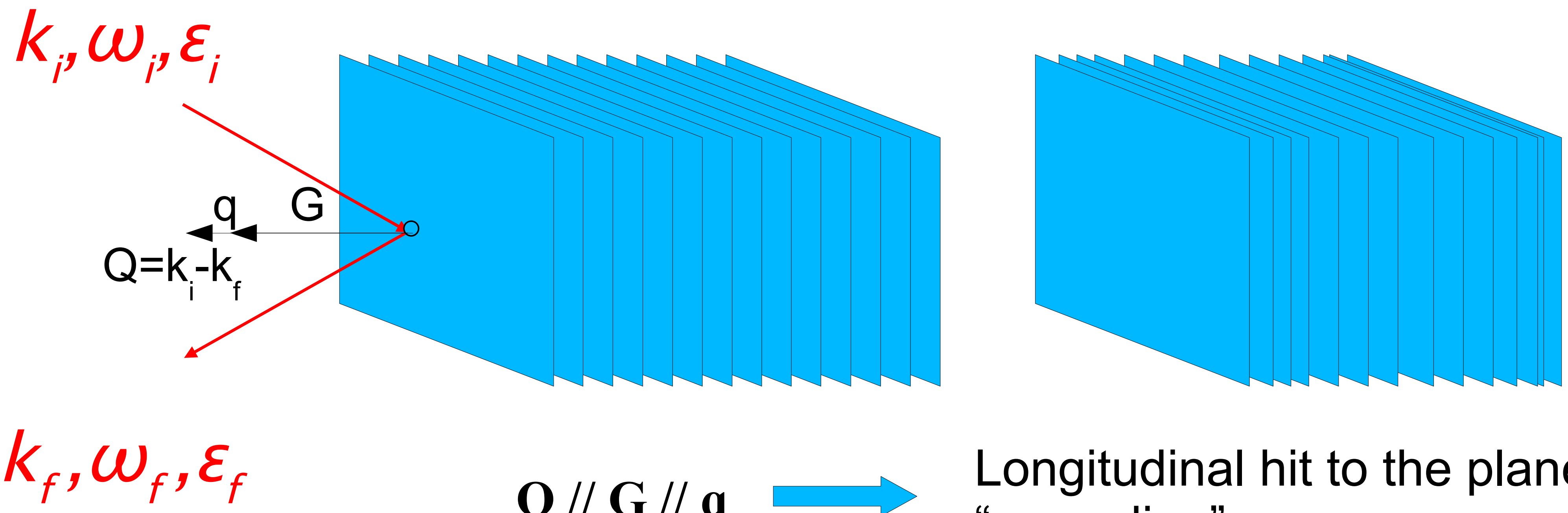
Inelastic Scattering: kinematic

$$\hbar\omega_i - \hbar\omega_f = \hbar\omega_{ph}$$

$$\vec{Q} \cdot \hat{e}_k^n(\vec{q})$$

$$\mathbf{Q} = \mathbf{G} + \mathbf{q}$$

$$\hbar k_i - \hbar k_f = \hbar Q$$



$\mathbf{Q}$ // $\mathbf{G}$ // $\mathbf{q}$ → Longitudinal hit to the planes "accordion"

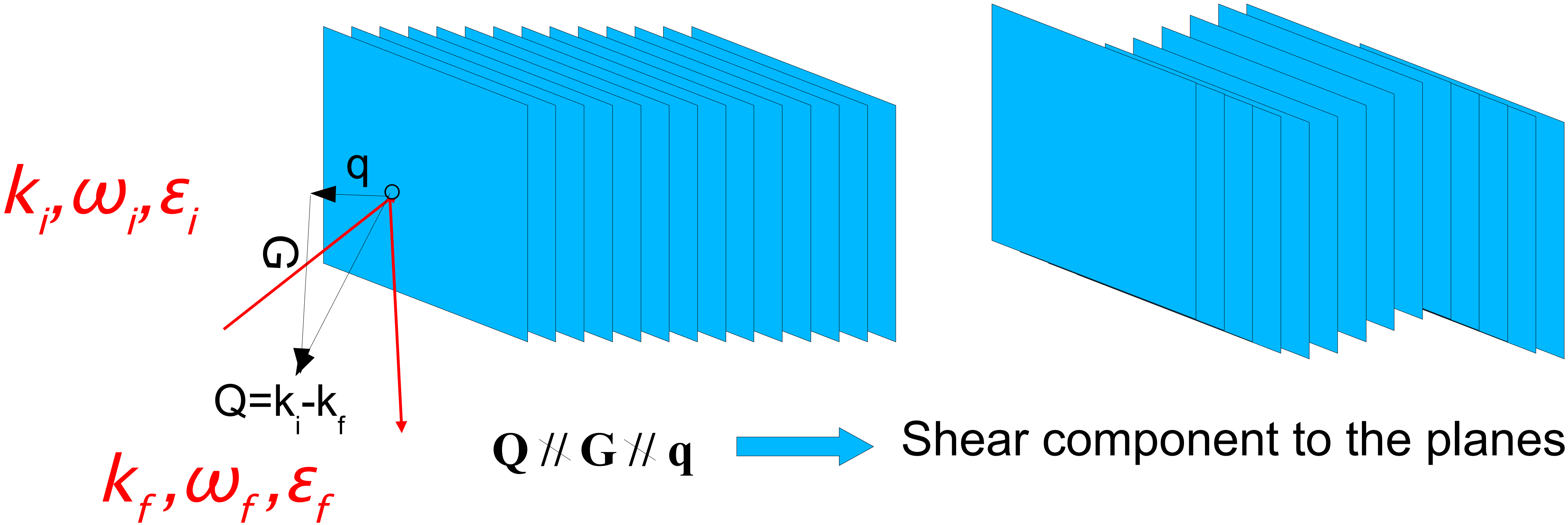
Inelastic Scattering: kinematic

$$\hbar\omega_i - \hbar\omega_f = \hbar\omega_{ph}$$

$$\vec{Q} \cdot \hat{e}^n_k(\vec{q})$$

$$\mathbf{Q} = \mathbf{G} + \mathbf{q}$$

$$\hbar k_i - \hbar k_f = \hbar Q$$



$\mathbf{Q} \not\parallel \mathbf{G} \not\parallel \mathbf{q}$ → Shear component to the planes

Spectroscopies with synchrotron and neutrons

neutrons

Several types of spectrometer:

- *3-axis*
  - *backscattering*
- *time-of-flight*
- *spin-echo*
- *plus coupled ones (3-axis/spin-echo)*

synchrotron light sources

Too many types, I'll focus on:

- *3-axis Rowland geometry*
  - *backscattering*
  - *soft X-ray*

Spectroscopies with synchrotron and neutrons

neutrons

Several types of spectrometer:

- *3-axis*
  - *backscattering*
- *time-of-flight*
- *spin-echo*
- *plus coupled ones (3-axis/spin-echo)*

neutrons

Neutron in - neutron out

- *inelastic scattering*

interaction with nuclei
(this lecture)
&
electron's spin
(lecture II)

Spectroscopies with synchrotron and neutrons

neutrons

Several types of spectrometer:

- *3-axis*
  - *standard (meV resolution)*
  - *backscattering (eV resolution)*
- *time-of-f lght*
- *spin-echo*
- *plus coupled ones (3-axis/spin-echo)*

synchrotron light sources

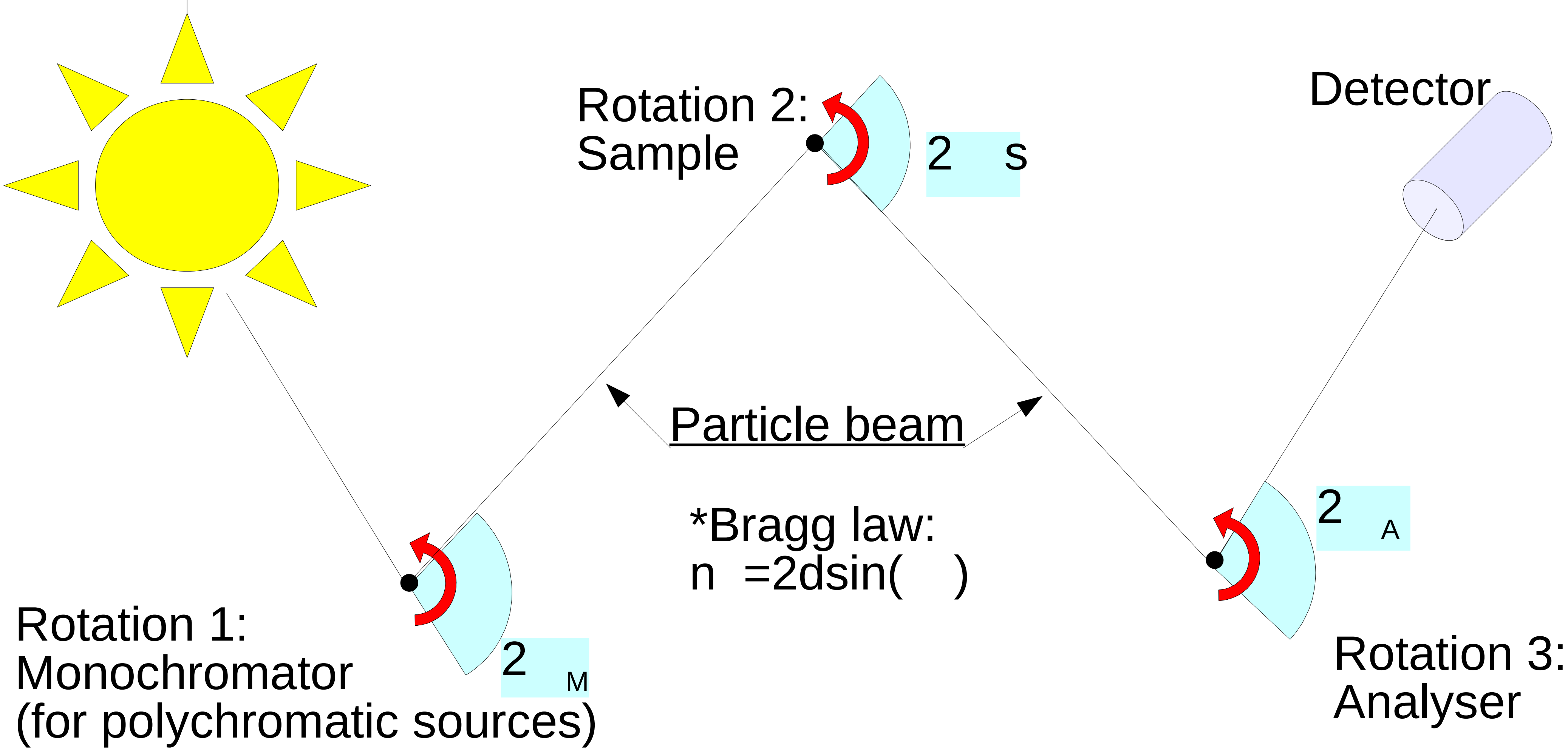
Too many types, I'll focus on:

- *3-axis Rowland geometry*
  - *backscattering (phonons)*
  - *soft X-ray (magnons)*

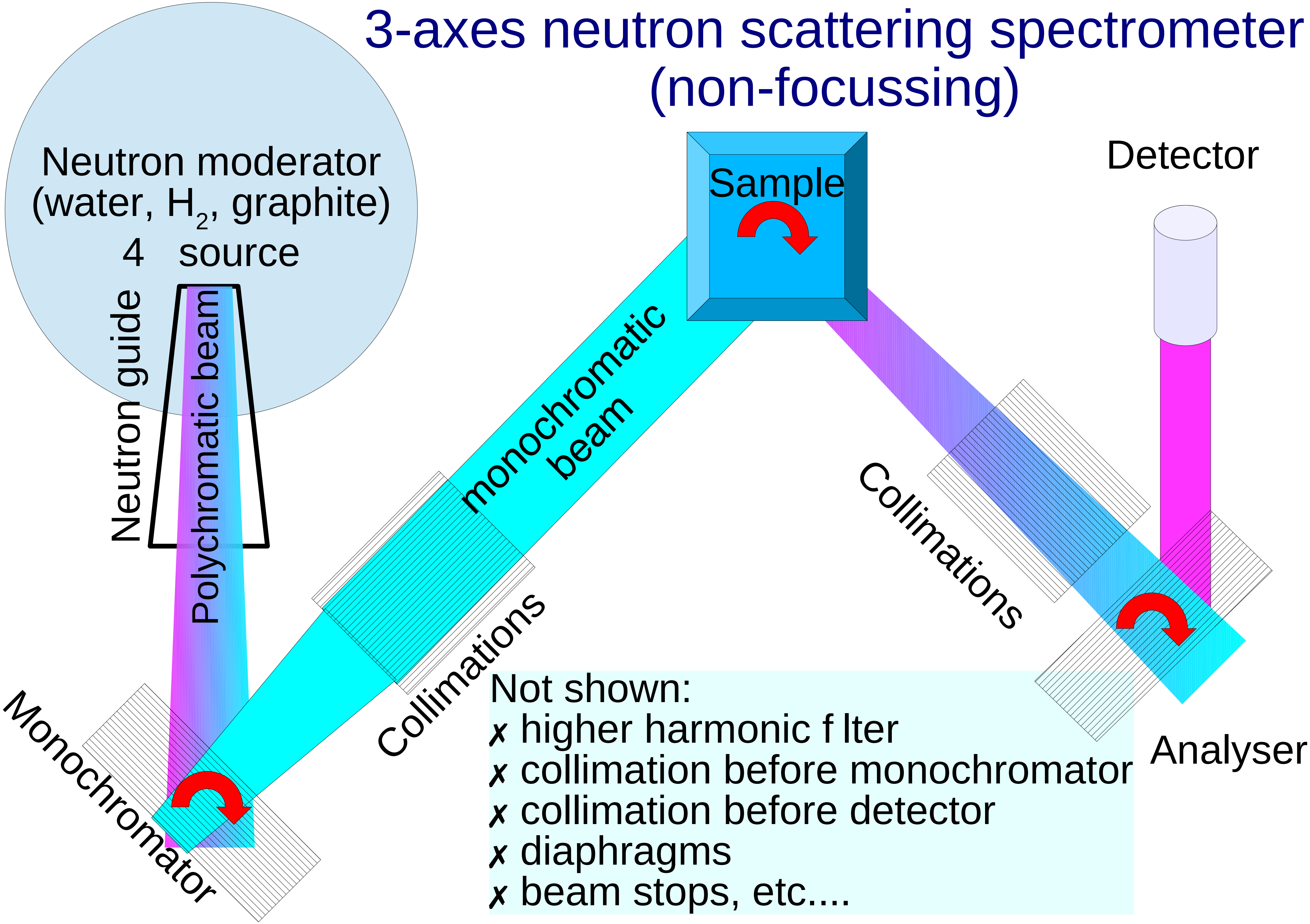
A source
(LASER, lamp,
nuclear reactor, spallation,
synchrotron...)

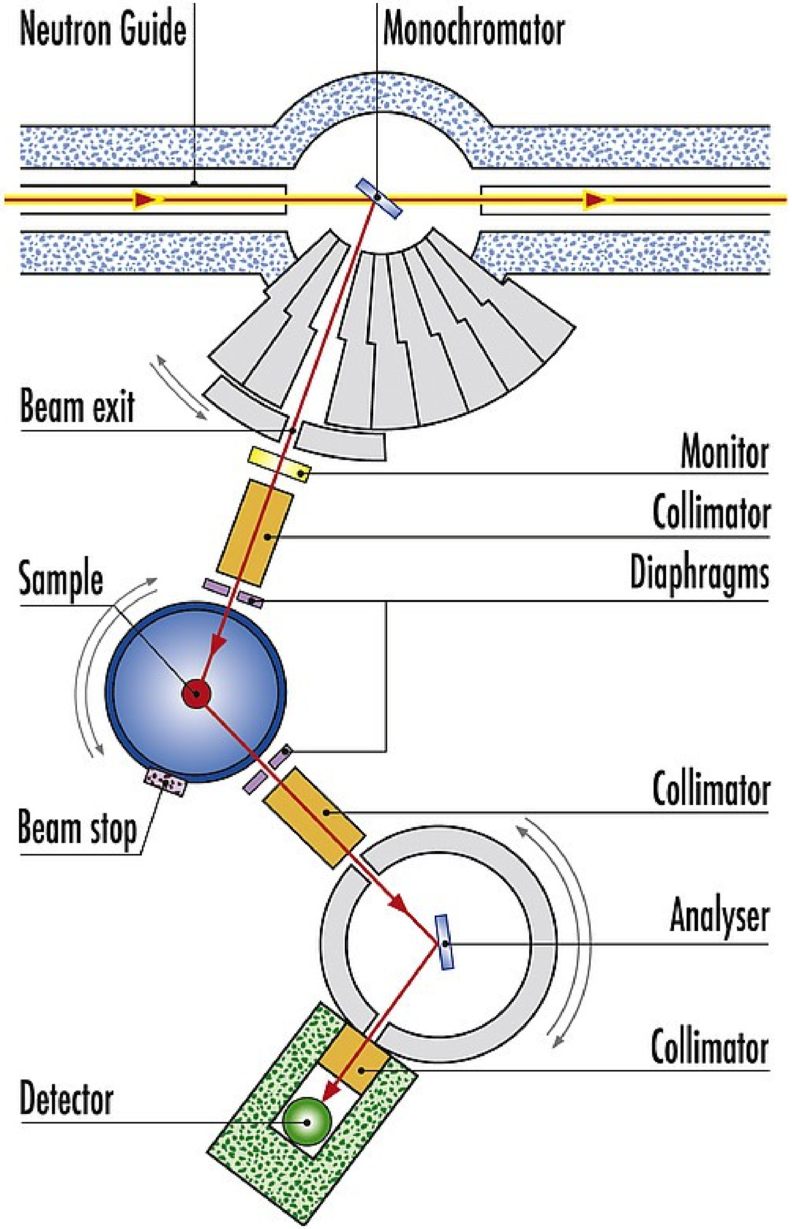
3-axes spectrometer general

Use 3 times the Bragg law*:
- ✔ for monochromator and analyser, to select the energy
- ✔ for the sample, to select the wave-vector



3-axes neutron scattering spectrometer (non-focussing)





IN3 instrument layout
(ILL, Grenoble, France)

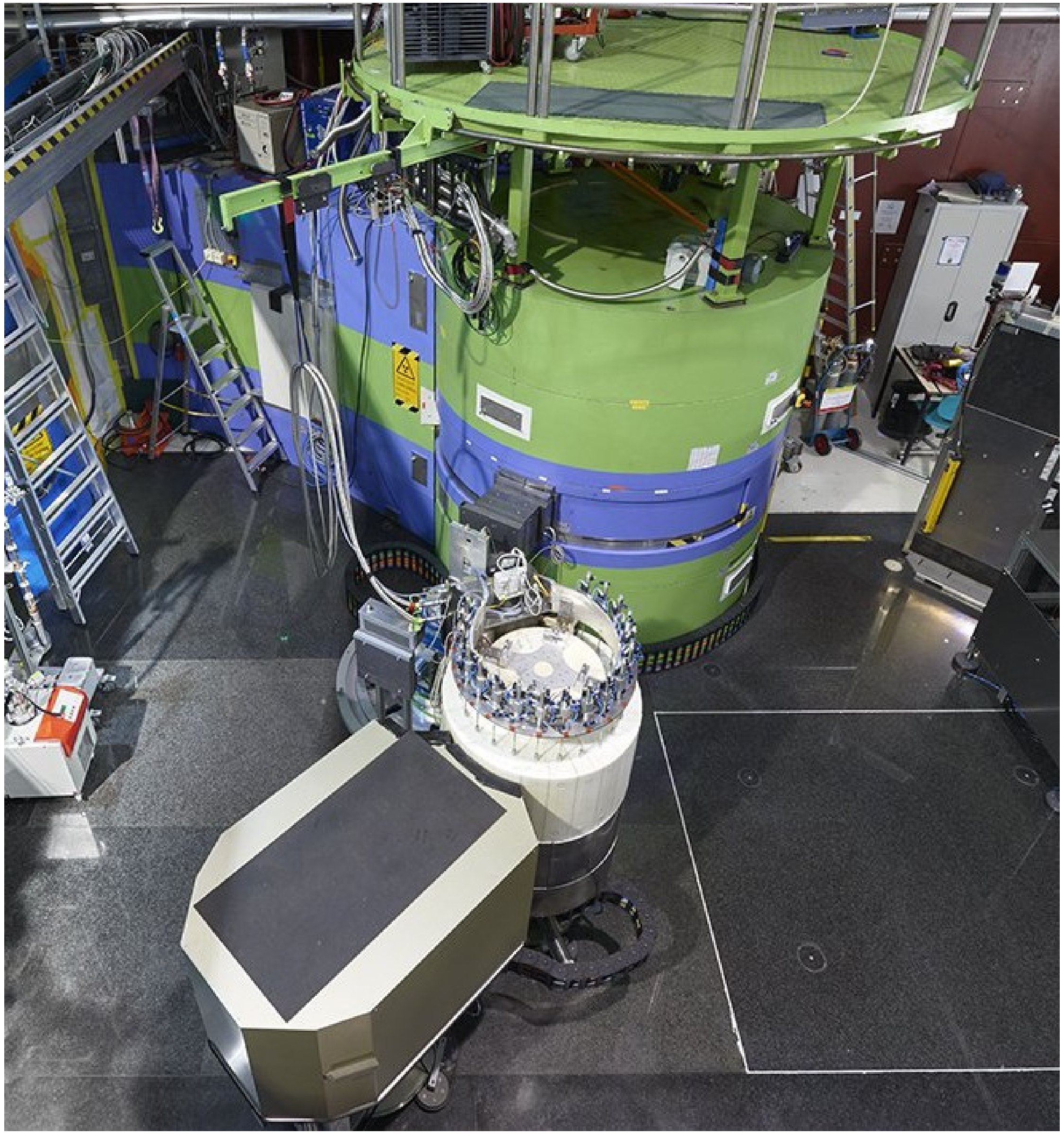


Image of PANDA at FRM-II
(Garching, Germany)

Inelastic X-ray Scattering development

- Thermal diffuse scattering known from ~ 1942 (Laval, Lonsdale, Born)

- 3-axes X-ray spectrometer known from ~ 1930 (DuMond and Kirkpatrick)

- Inelastic Neutron Scattering spectrometer build 1956 @ Chalk River by Brockhouse

- Why Inelastic X-ray Scattering came only >> 1990 ?

Inelastic X-ray Scattering development

- Thermal diffuse scattering known from ~ 1942 (Laval, Lonsdale, Born)

- 3-axes X-ray spectrometer known from ~ 1930 (DuMond and Kirkpatrick)

- Inelastic Neutron Scattering spectrometer build 1956 @ Chalk River by Brockhouse

- Why Inelastic X-ray Scattering came only >> 1990 ?

For a thermal neutron of 14 meV (160 K) k=2.662 $Å^{-1}$
for meV resolution $\Delta E/E \sim 1$

Inelastic X-ray Scattering development

- Thermal diffuse scattering known from ~ 1942 (Laval, Lonsdale, Born)

- 3-axes X-ray spectrometer known from ~ 1930 (DuMond and Kirkpatrick)

- Inelastic Neutron Scattering spectrometer build 1956 @ Chalk River by Brockhouse

- Why Inelastic X-ray Scattering came only >> 1990 ?

For a photon with 1 Å wave-length I have ~12 keV energy
for meV resolution $\Delta E/E \sim 10^{6}$–10^{7}

Inelastic X-ray Scattering development

I need high resolving power: meV resolution with keV particles
$\Delta E/E \sim 10^6$
for photon wave-vector: $\Delta k/k \sim 10^6$

Possible with perfect crystals, large scattering angle:

from Bragg law $(\Delta k/k) = \cot\vartheta\ \delta\vartheta$ (large scattering angle)
from dynamical scattering theory $\delta Q/Q = 16\pi r_0 |f(Q)|/(Q^2V)$

Large Q small width (~ 1/d) → large E (Burkel Peisl Dorner 1986 HASYLAB)

Problem: flat, perfect crystals → small $\delta\vartheta$

Solution → undulator at 3d generation synchrotron

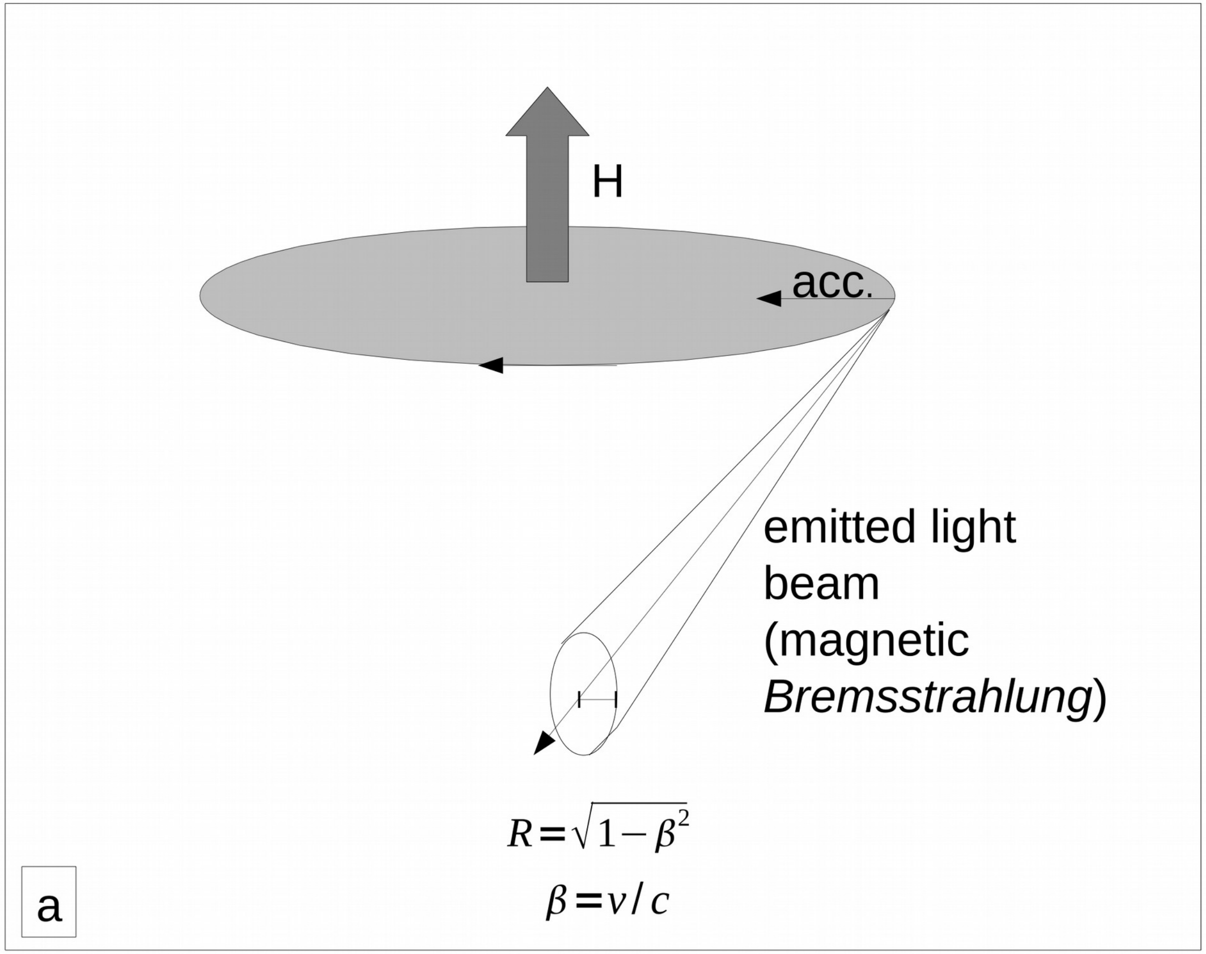
Inelastic X-ray Scattering development

Solution → undulator at 3d generation synchrotron

Reflection	E(keV)	ΔE	Ref.
(7 7 7)	13.8	4.9	Sette and Krisch (1994)
(8 8 8)	15.8	3.8	Schwoerer–Bohning (1994)
(9 9 9)	17.8	2.4	Masciovecchio et al (1996)
(11 11 11)	21.8	1.3	Schwoerer–Bohning (1994)
(13 13 13)	25.7	0.45	Verbeni et al (1996)
(16 16 16)	31.6	0.28	ESRF (1995)
(17 17 17)	33.6	0.28	Krisch (1997)

Inelastic X-ray Scattering development

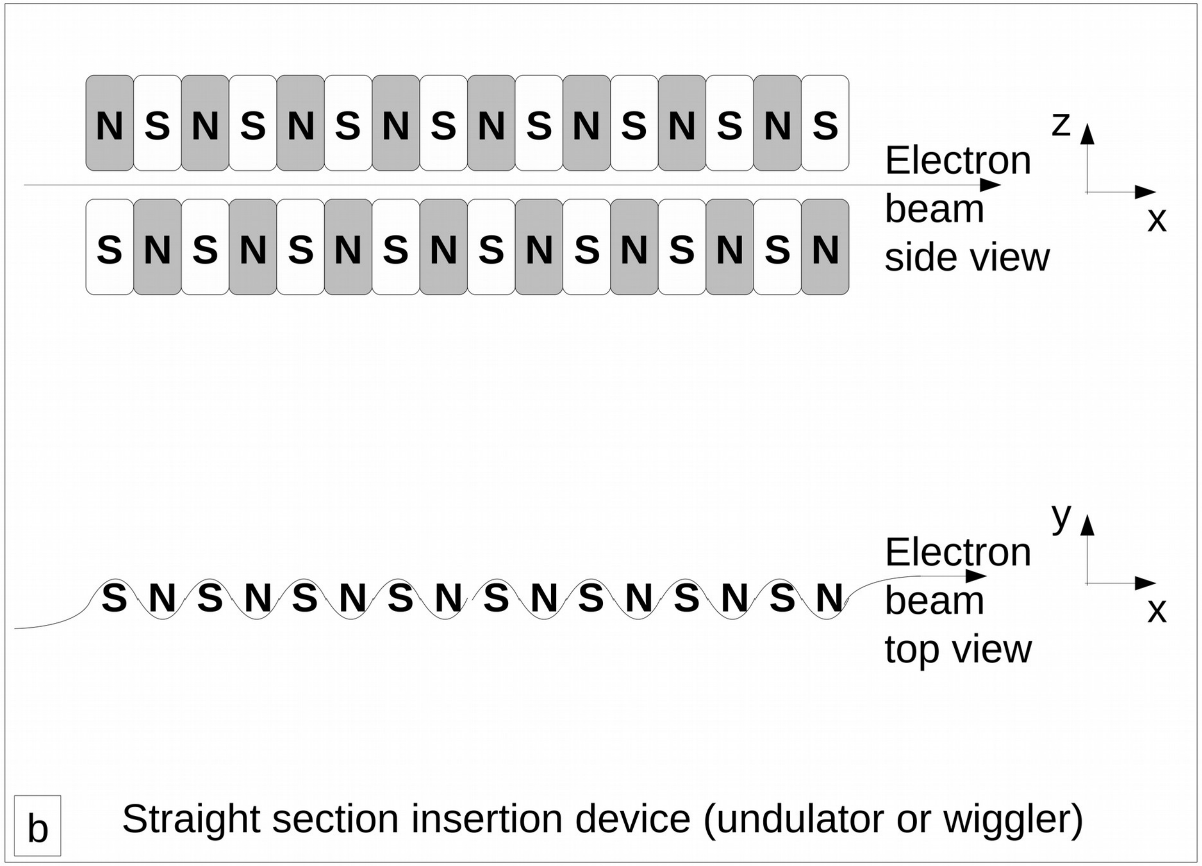
Solution ➡ undulator at 3d generation synchrotron



M. d'Astuto and M. Krisch JDN **10** (2010)

Inelastic X-ray Scattering development

Solution ➡ undulator at 3d generation synchrotron

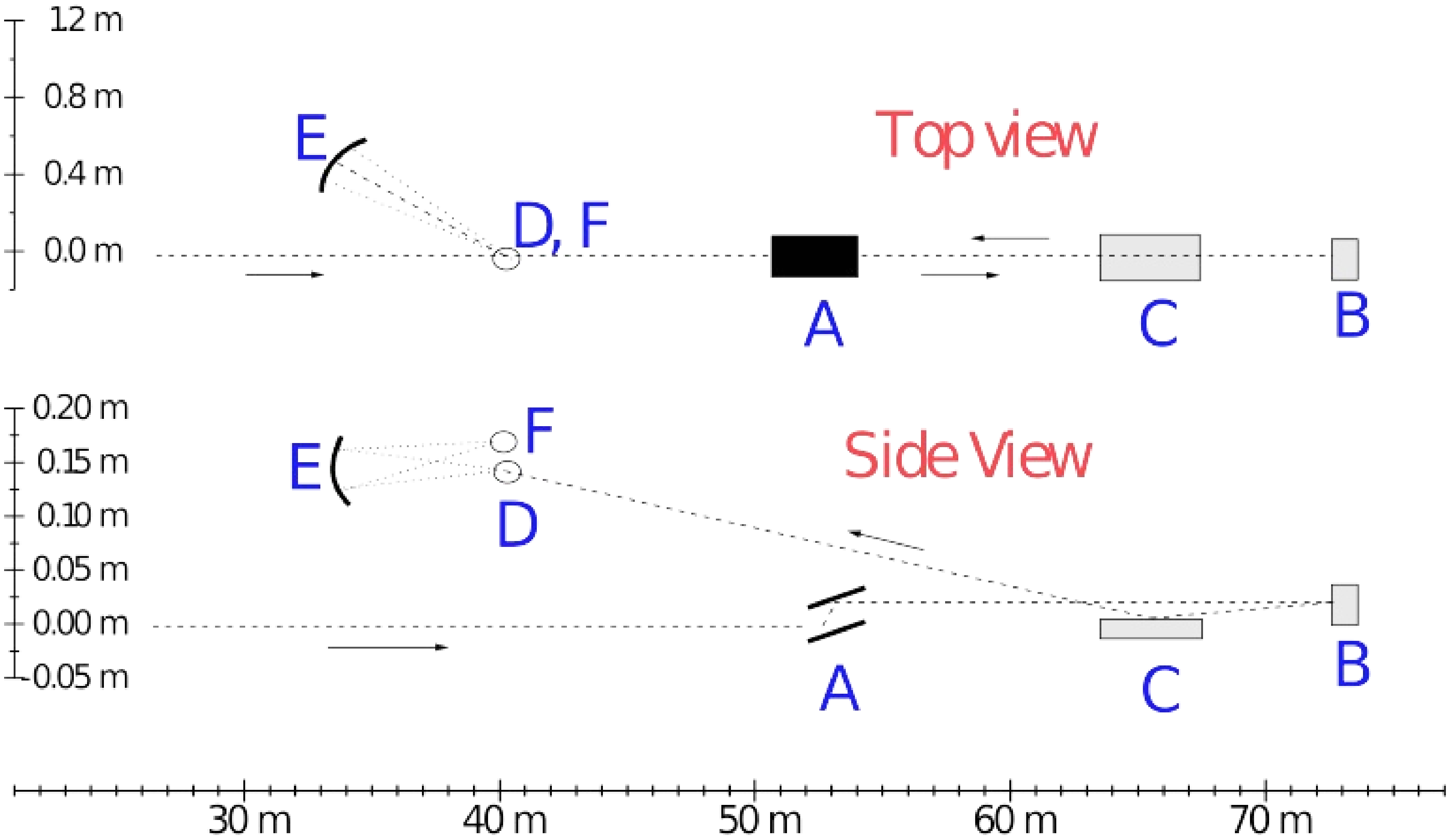


Straight section insertion device (undulator or wiggler)

M. d'Astuto and M. Krisch JDN **10** (2010)

Inelastic X-ray Scattering development

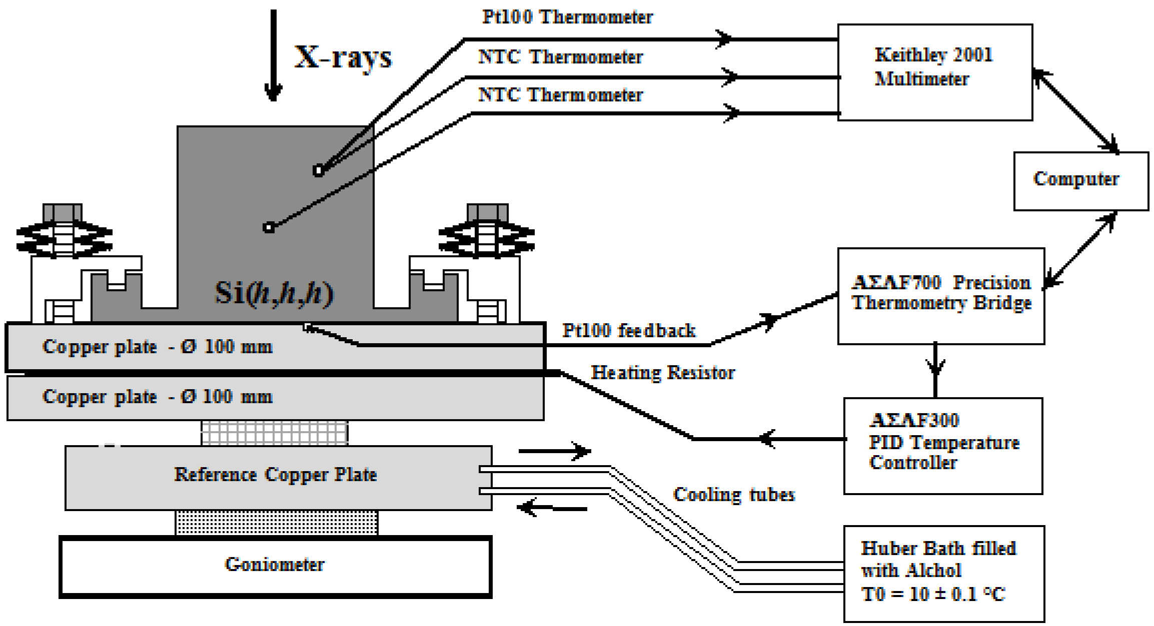
Solution ➡ undulator at 3d generation synchrotron



M. d'Astuto and M. Krisch JDN **10** (2010)

Inelastic X-ray Scattering development

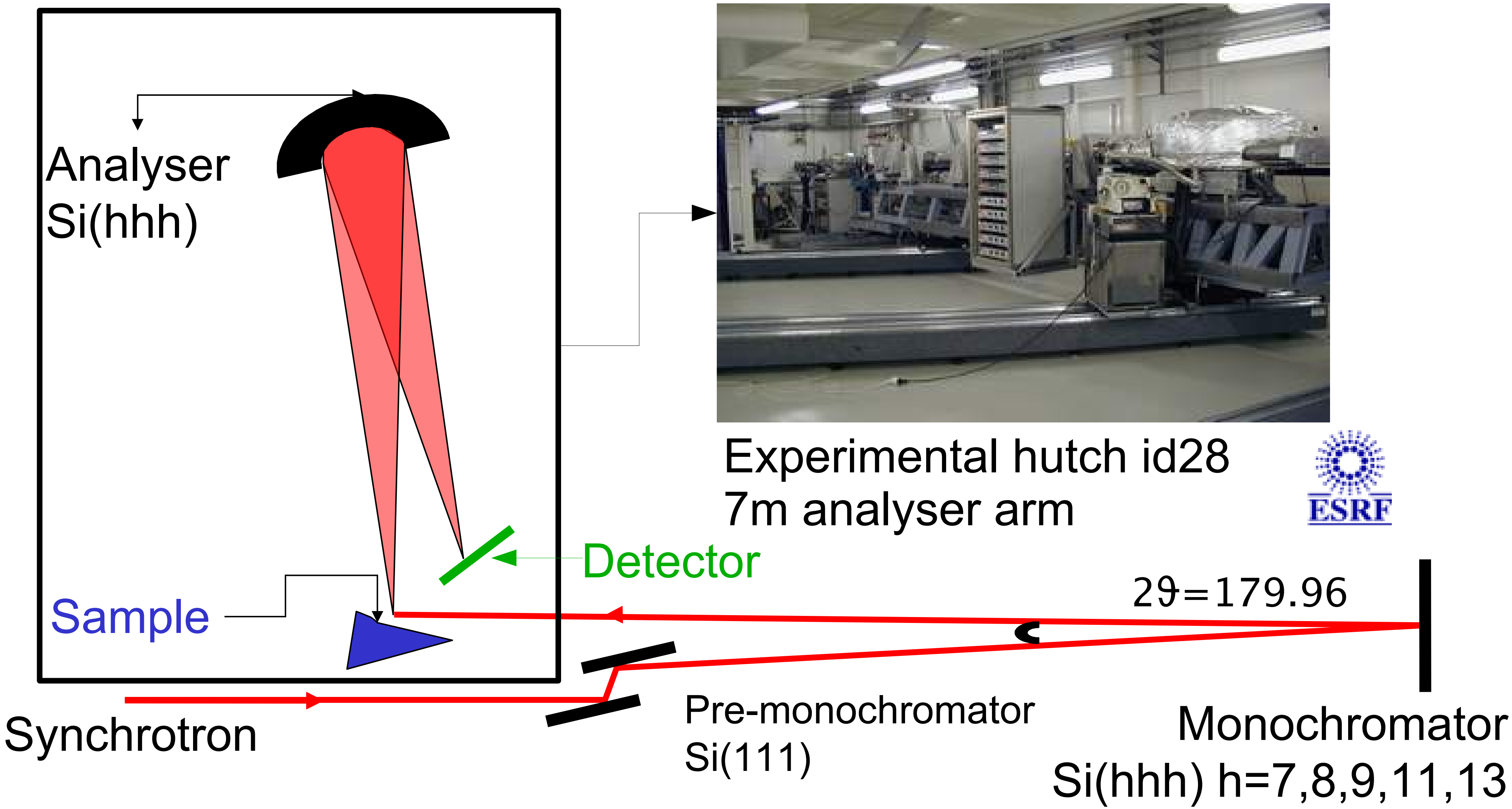
Solution ➡ high resolution, perfect crystal, monochromator



with temperature scan: $n\lambda=2d(T)\sin(\vartheta)$

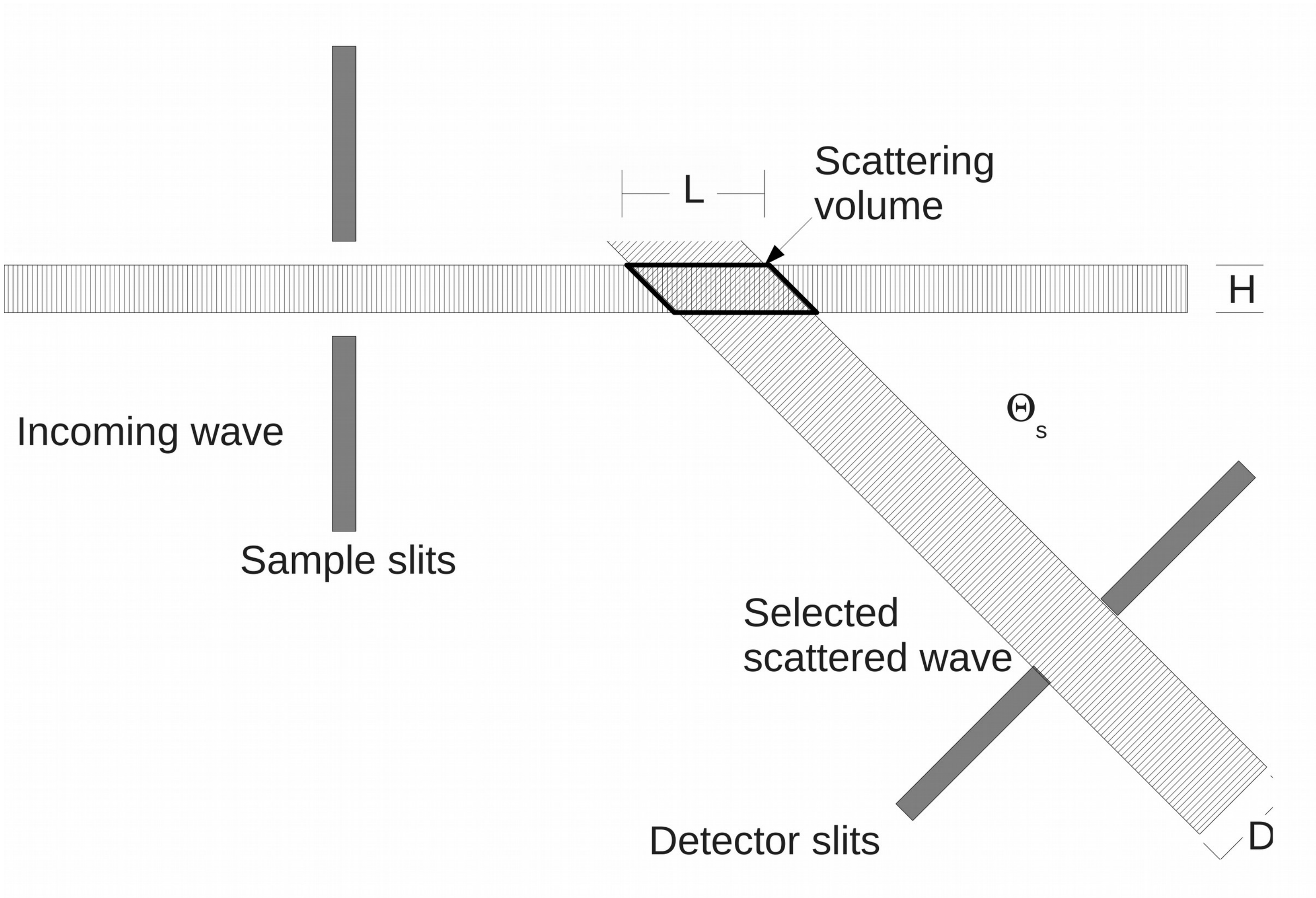
M. d'Astuto and M. Krisch JDN **10** (2010)
R. Verbeni, M. d'Astuto, *et al.. Review of Scientific Instruments*, **79** (2008)

Backscattering Inelastic X-ray Spectrometer



Focus 250x250 μm² - 25x90 μm² very high Q resolution

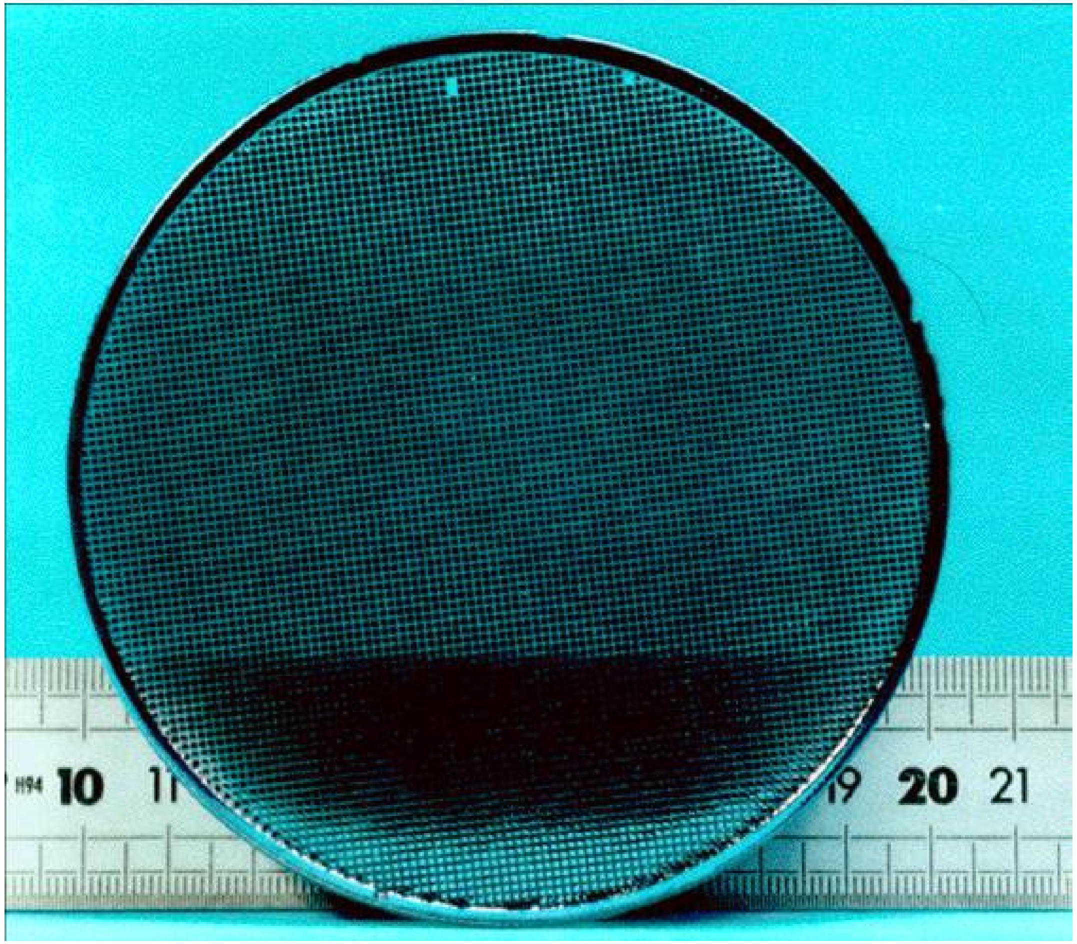
Inelastic X-ray Scattering development



M. d'Astuto and M. Krisch JDN **10** (2010)

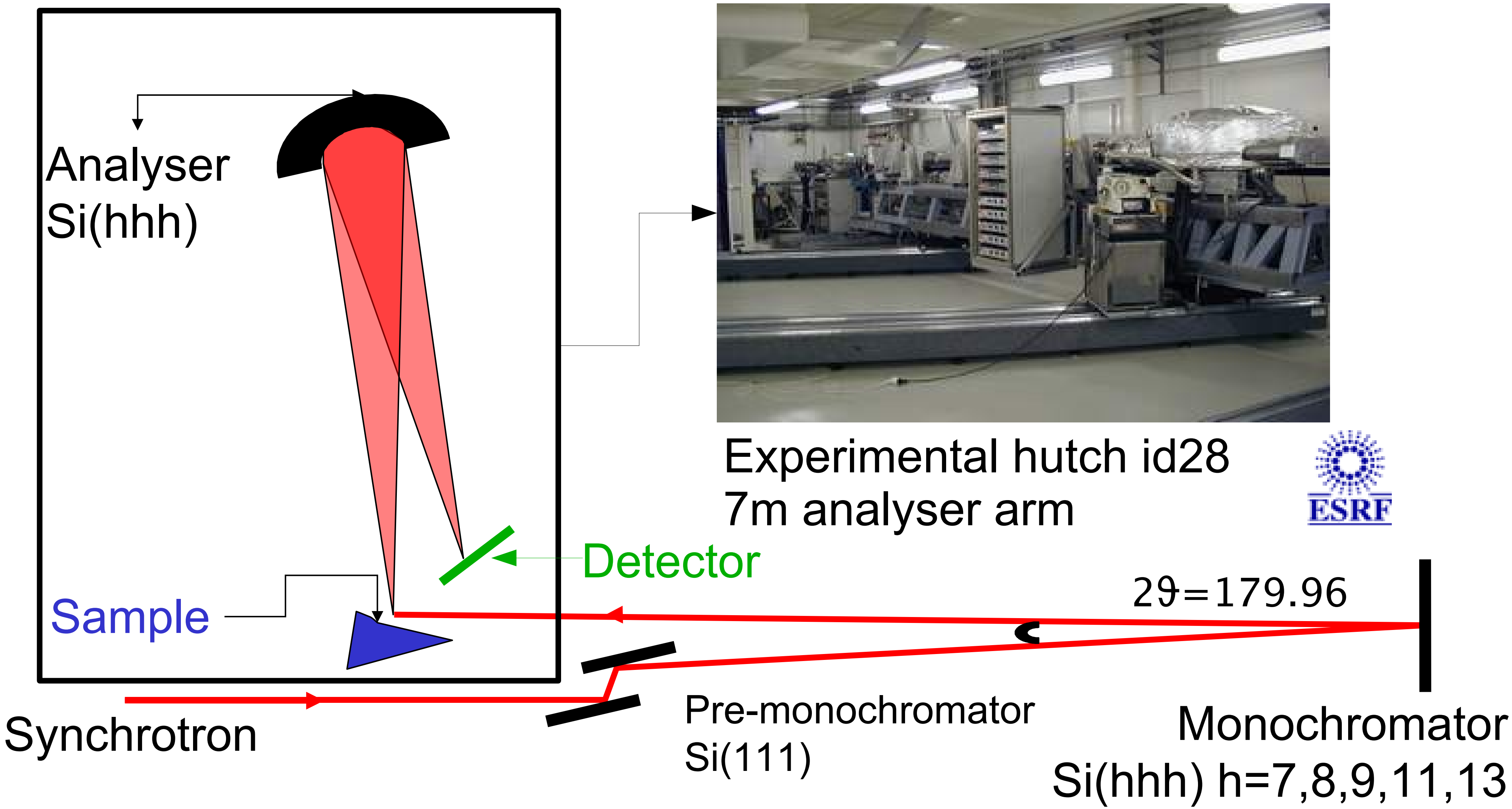
Inelastic X-ray Scattering development

Problem → scattered photons at 4π !
Solution → diced analysers



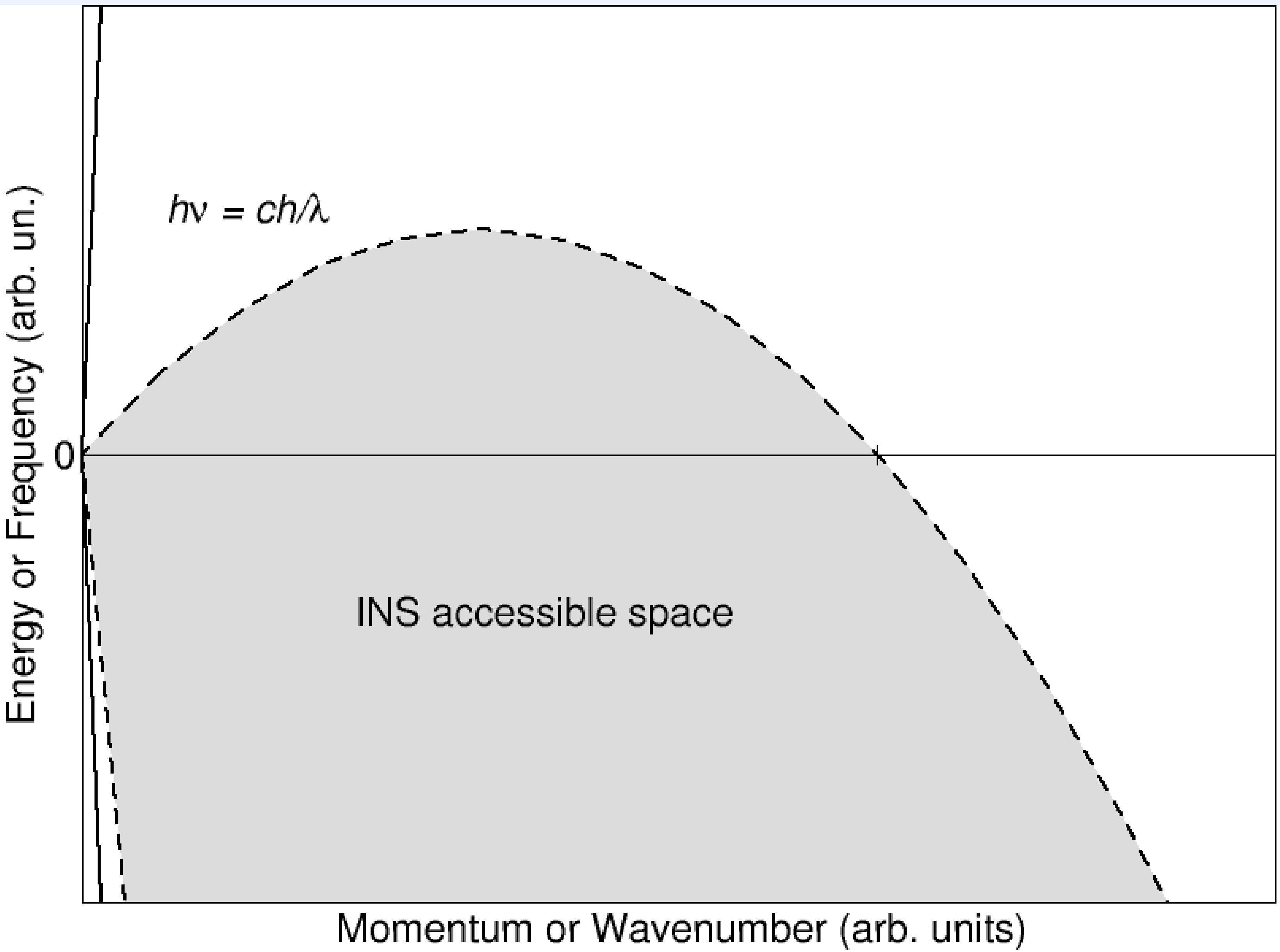
M. d'Astuto and M. Krisch JDN **10** (2010)

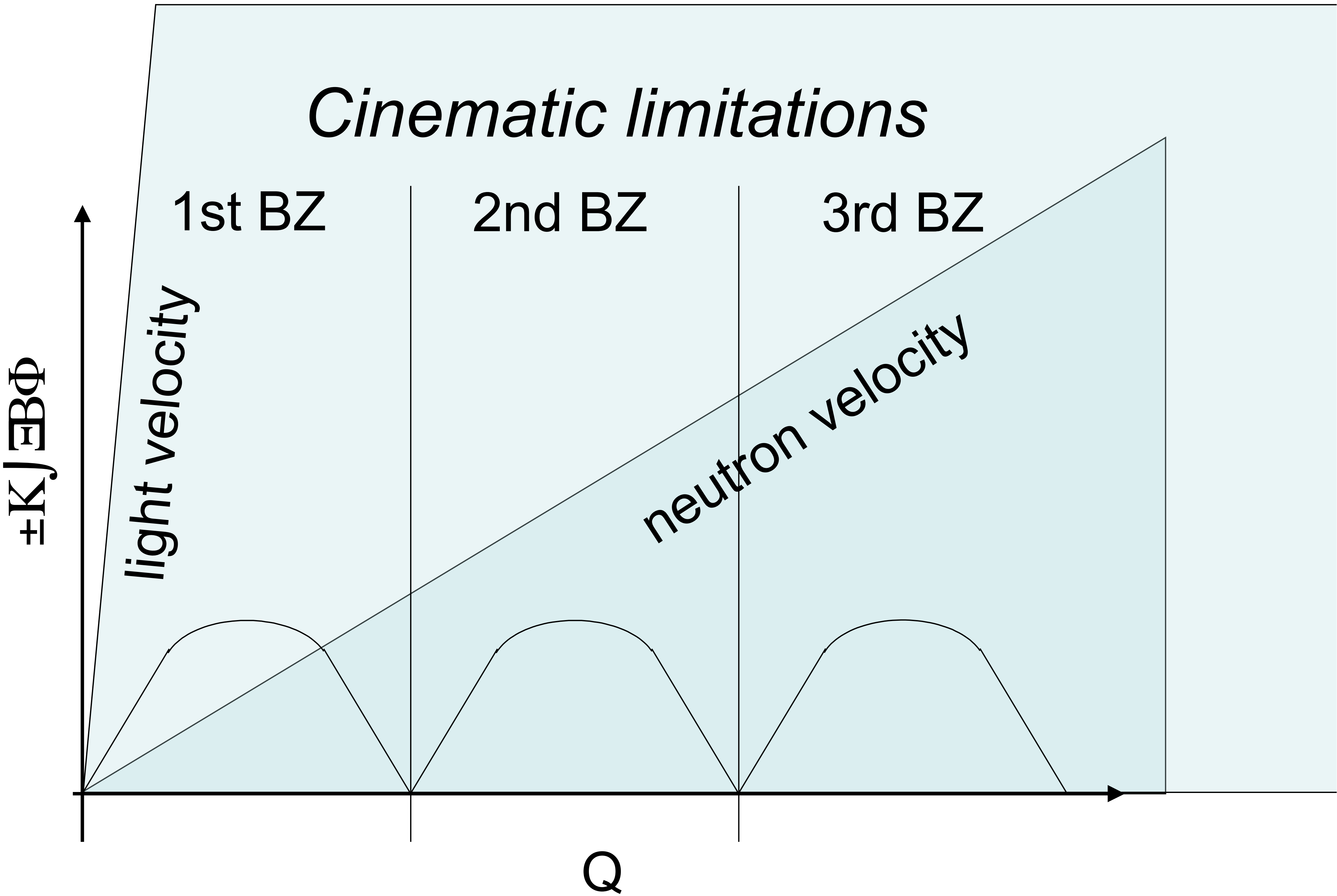
Backscattering Inelastic X-ray Spectrometer



Focus 250x250 μm² - 25x90 μm² very high Q resolution

Momentum space access: neutrons and photons




Cinematic limitations
1st BZ
2nd BZ
3rd BZ
light velocity
neutron velocity
Q

Inelastic X-ray Scattering advantage

Advantage for crystalline systems:

- small single crystals;
- high (Q,E) resolution;
- constant (Q,E) resolution volume

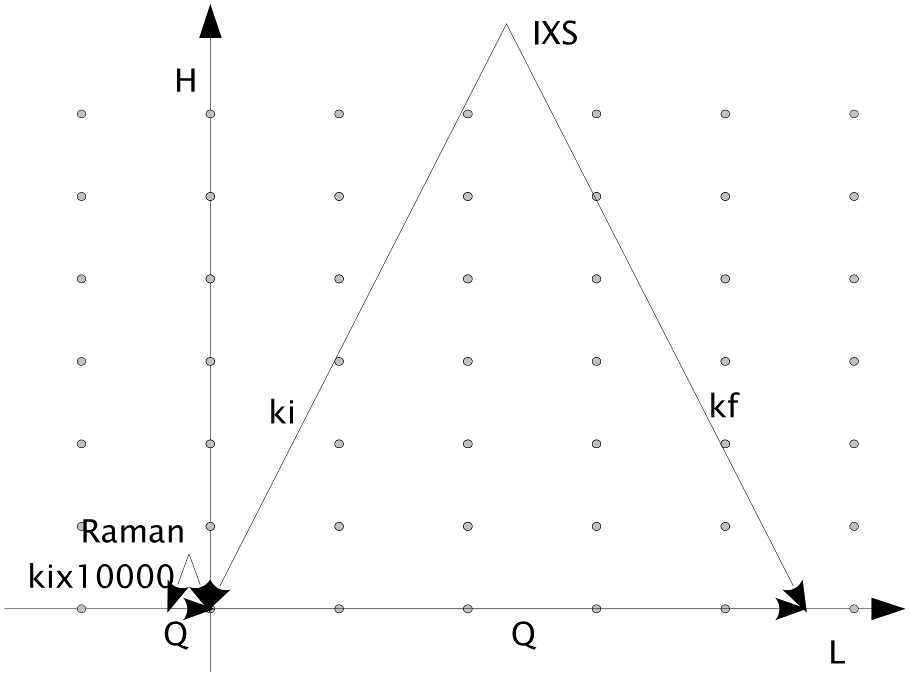
M. d’Astuto and M. Krisch JDN **10** (2010)

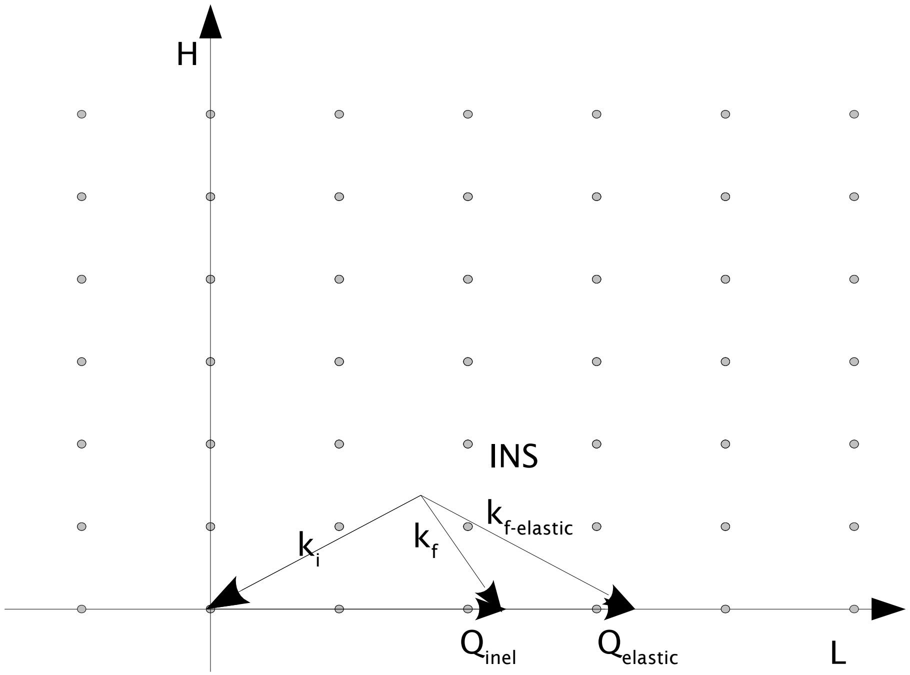
Scattering vectors for typical incident energies:

2.5 eV visible light (green);

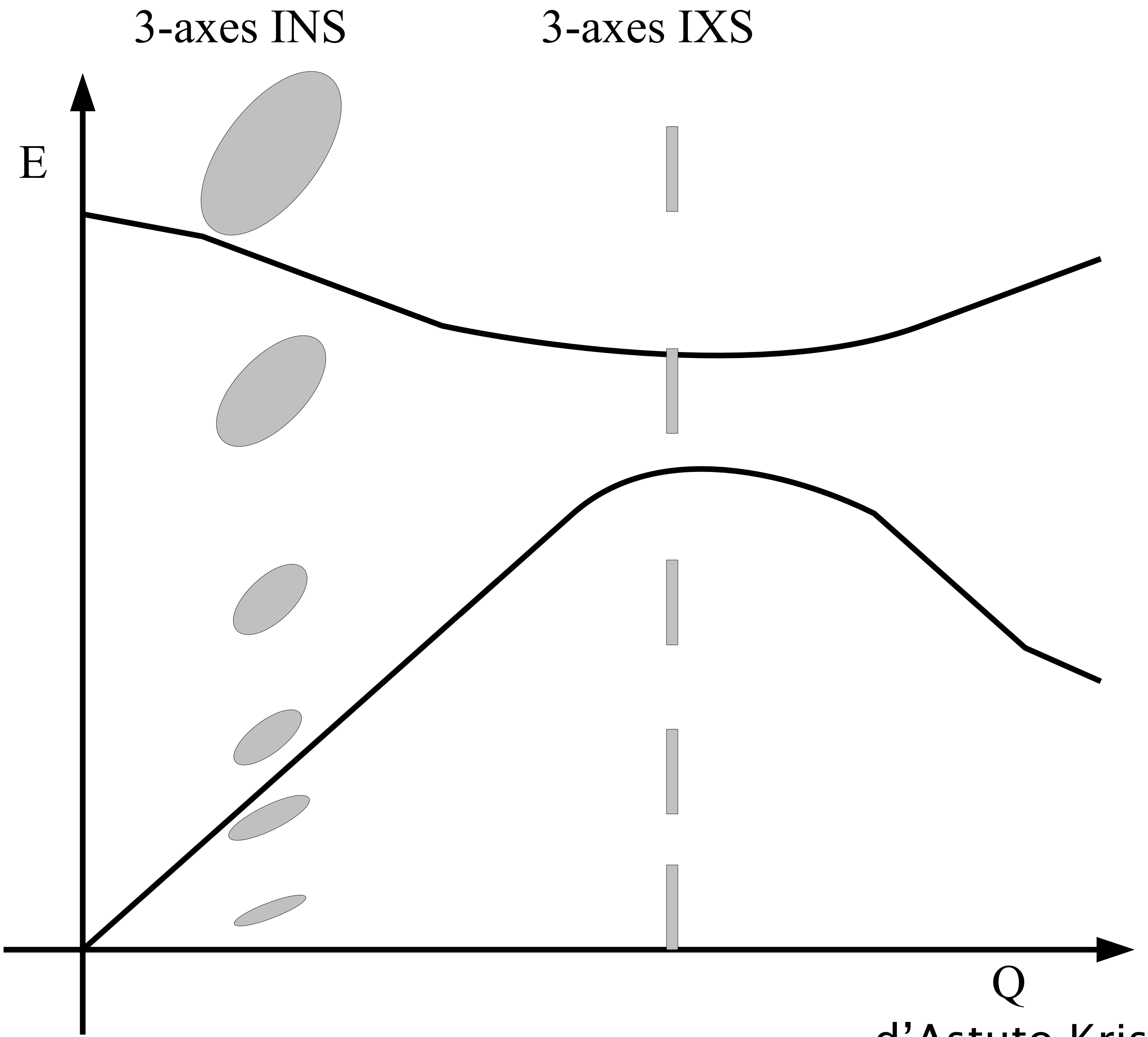
17793 eV X-ray from Si(999);

14 meV neutrons (tuned to best graphite filter windows).



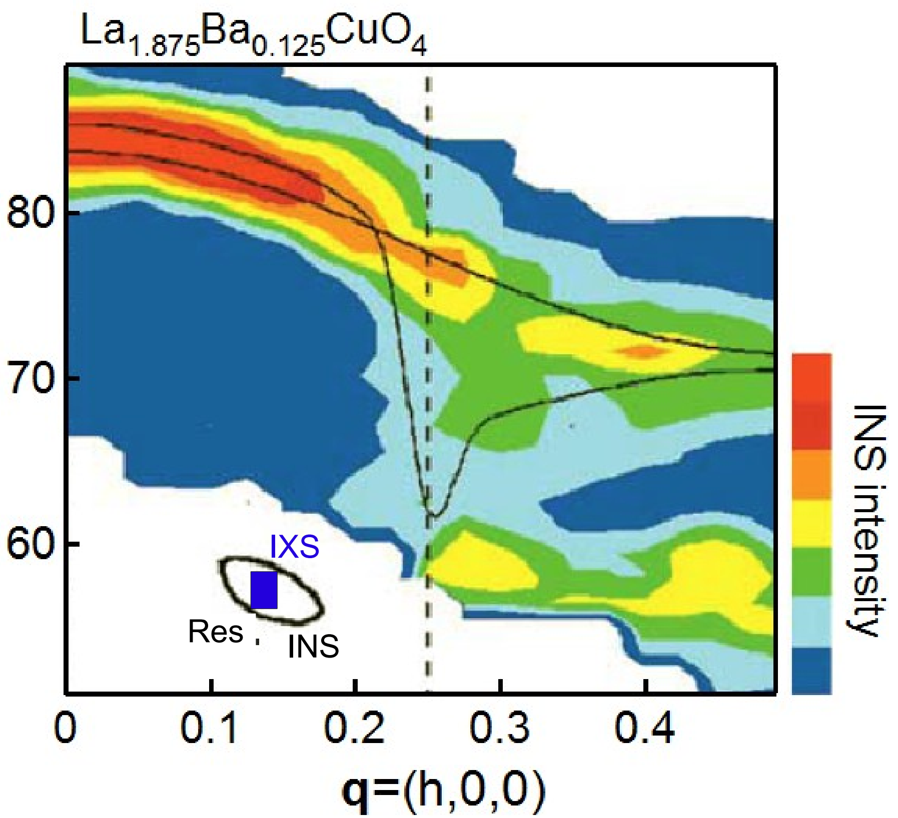


M. d'Astuto and M. Krisch JDN **10** (2010)

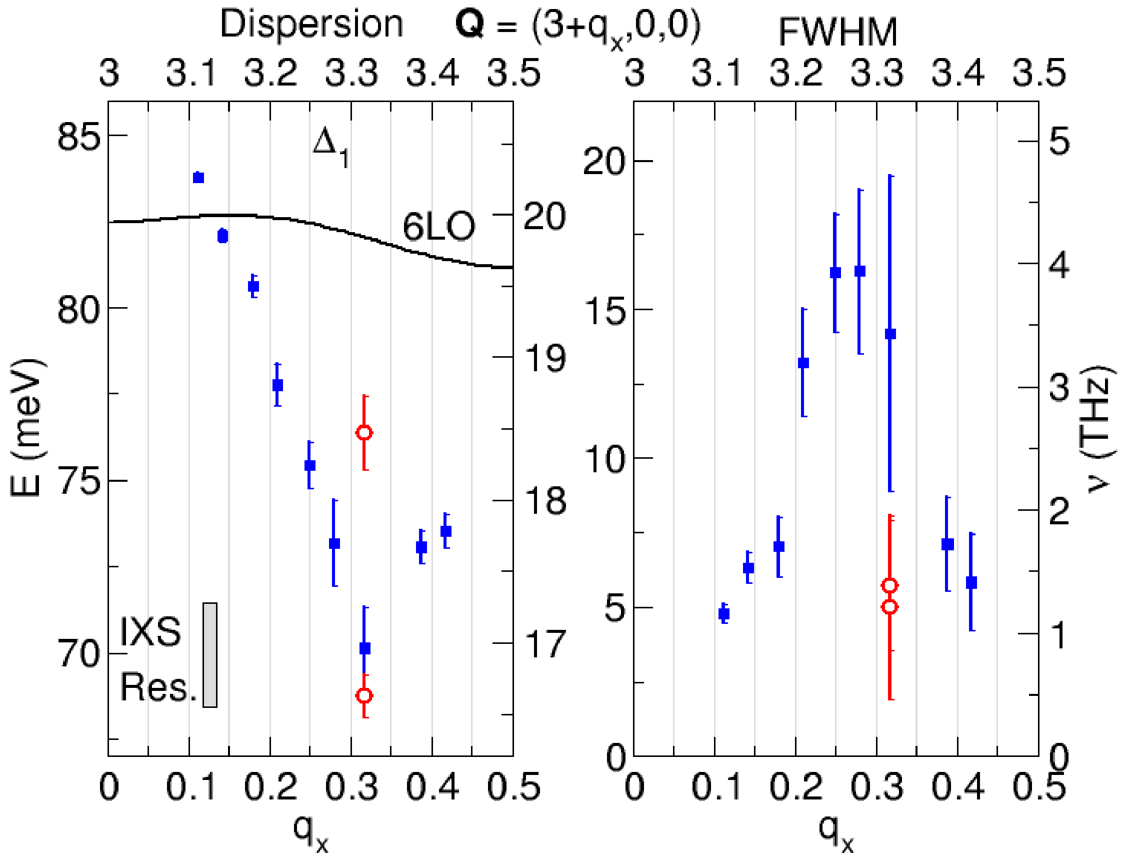


d’Astuto Krisch JDN **10** (2010)

Bond stretching modes in cuprates superconductors



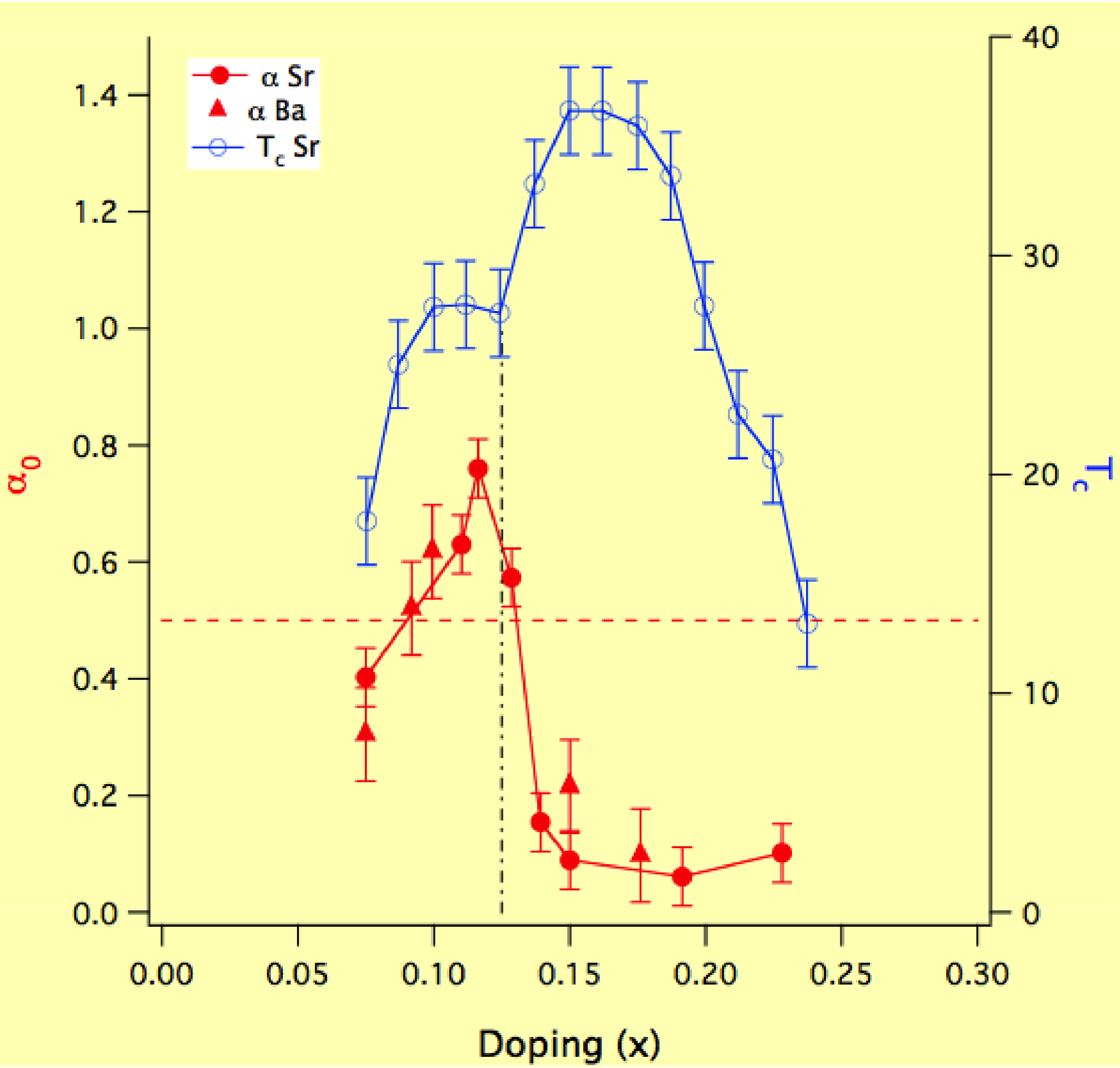
Inelastic Neutron scattering data x=0.125
Reznik *et al.* *Nature* **440** (2006)



Inelastic X-ray scattering data x=0.14
d'Astuto *et al.* *PRB* **78** (2008)

Cupratesphase diagram

$La_{2-x}M_xCuO_4$ (M=Sr, Ba)



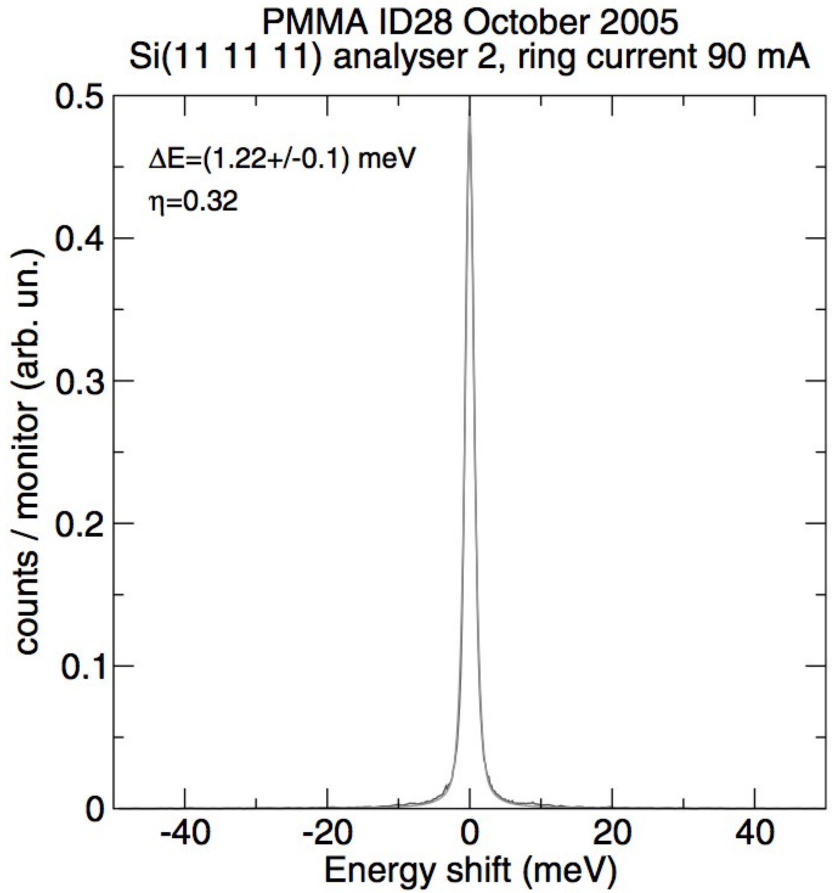
M. K. Crawford, *et al. Science* **250** (1990)
P.G. Radaelli *et al. PRB* **49** (1994)

Inelastic X-ray Scattering drawback

Energy resolution is not Gaussian (pseudo-voigt line-shape), so:

- bad contrast high/low energy

- worst case at the Zone Centre: no possible measurements close to a Bragg point



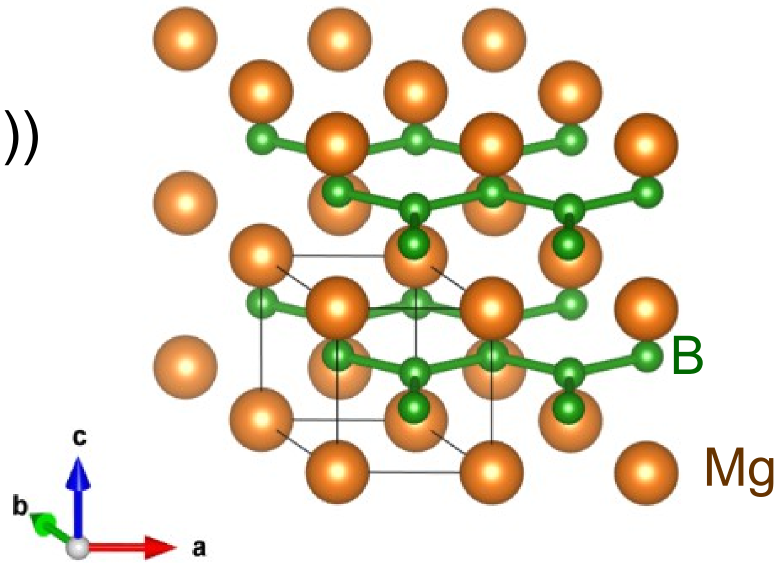
M. d'Astuto and M. Krisch JDN **10** (2010)
C. Masciovecchio, *et al. Nucl. Instrum. Meth. B*, **111** (1996)

Inelastic X-ray Scattering summary

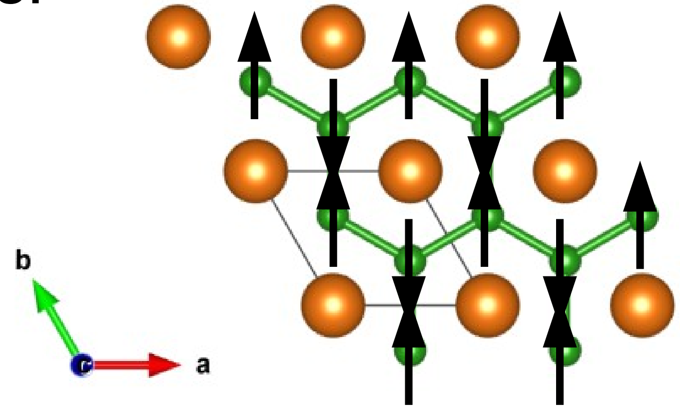
	neutrons	X-rays	Section
Phonons	yes	yes	2.1
Magnons	yes	no	2.1
Scattering	coherent + incoherent	coherent only	2.1
Coherent cross section*(barns)	1 – 30	$10^1 - 10^4$	2.1
Typical penetration depths	cm	0.01 – 1 mm	2.1, see Fig. 3
Spot size on the sample	cm	30 – 300 μm	3.3
Kinematic limitations	yes	no	2.2
λ/n contaminations	yes	no	2.2
Energy resolution	5 – 1% of E_i	5.5 – 1.5 meV	3.3, see Tab. 1
Typical collimation			
incident	1°	0.0045°	3.3
scattered	1°	0.2°	3.4

Superconductivity in MgB_2

39 K superconductivity in MgB_2
(Nagamatsu *et al. Nature* **410** (2001))



seems well explained by a coupling of E2g modes:



with σ and π Boron p-bands along Γ – A (*i.e.*, parallel to c*):
(Choi *et al. Nature* **418** (2002))

Isotopic effect in MgB_2: anharmonic E2g mode?

"Anomalous isotopic effect" :
(Hinks *et al. Nature* **411** (2001))

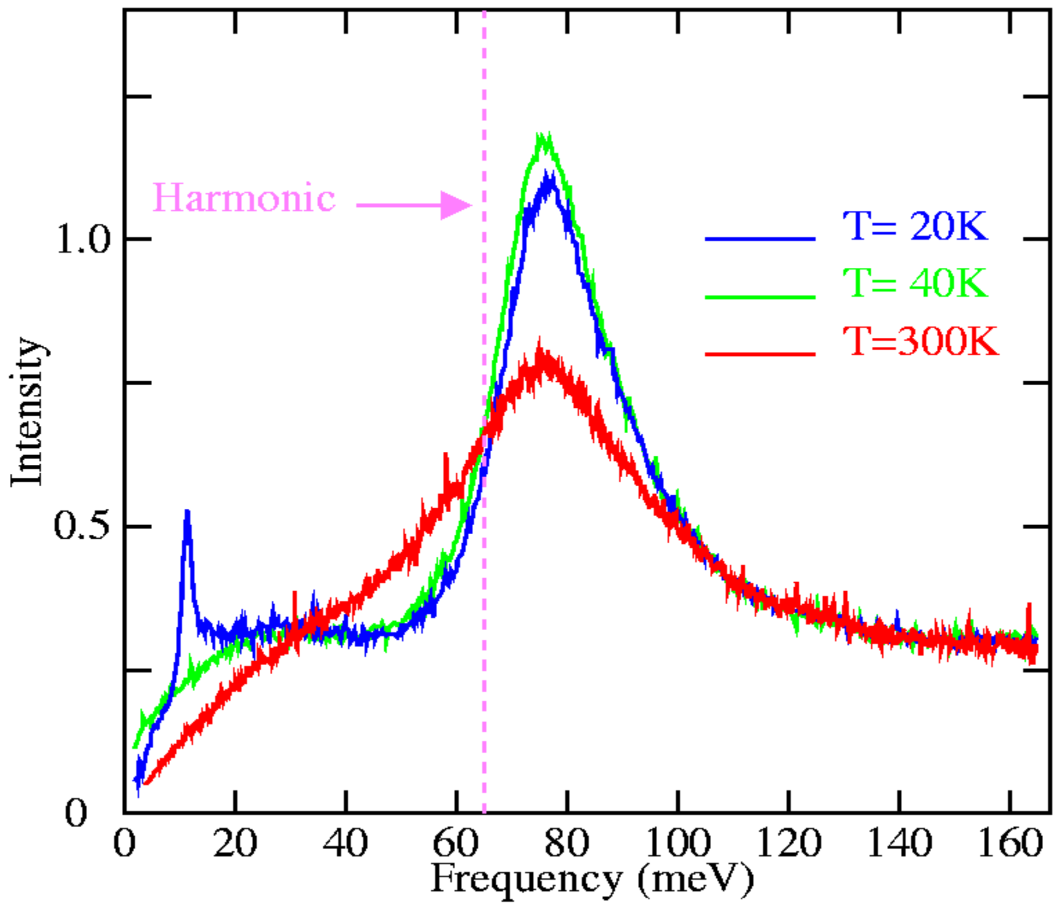
$$T_c \propto \omega_{ph} \propto \frac{1}{\sqrt{M_i}} = M_i^{-\alpha}$$

$\alpha_{BCS} \sim 0.50$

α_B	0.31(1) +
α_{Mg}	0.02(1) =
α_{tot}	0.33(2)

Possible explanation: large anharmonicity of E2g mode
Suggested by phrozen-phonon *ab-initio* calculation
(Yildirim *et al. PRL* **87** (2001))
Apparently confirmed in early Raman results.
Quilty *et al, PRL* **88** (2002)

Raman in MgB_2: anharmonic E2g mode?



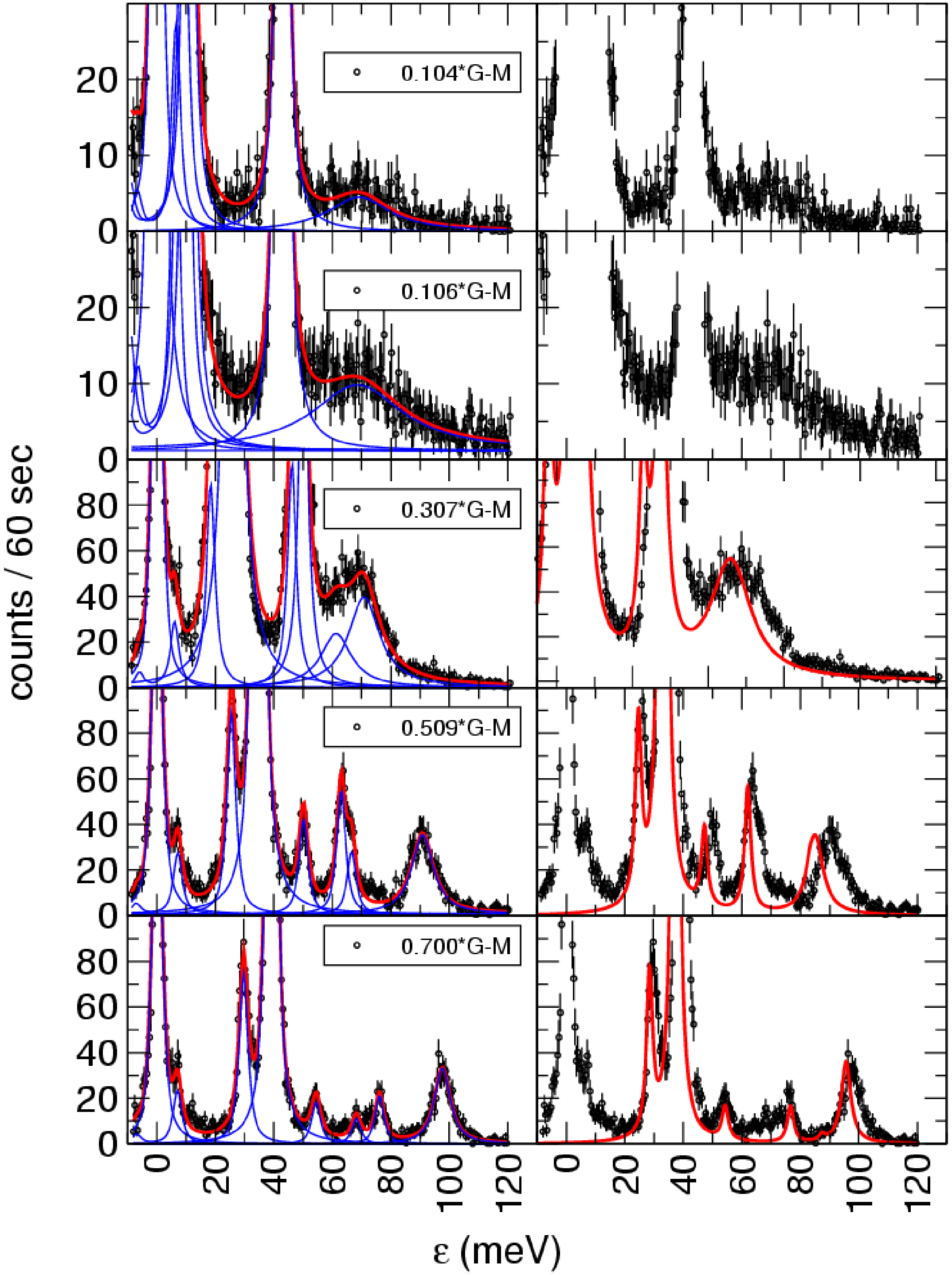
- The Raman Shift is about 10 meV (18%) higher
- Broadening is double at 300K than the IXS one
- Linewidth temperature dependence

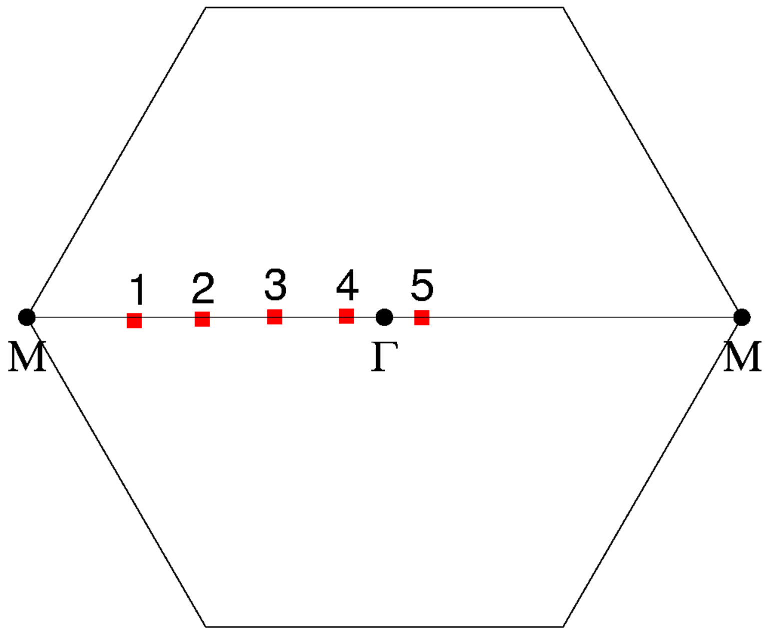
Raman scattering seems to indicate large anharmonic effects

Quilty *et al*, *PRL* **88** (2002)

Inelastic scattering spectroscopy with neutrons and X-rays for superconductivity – Matteo d'Astuto 2019

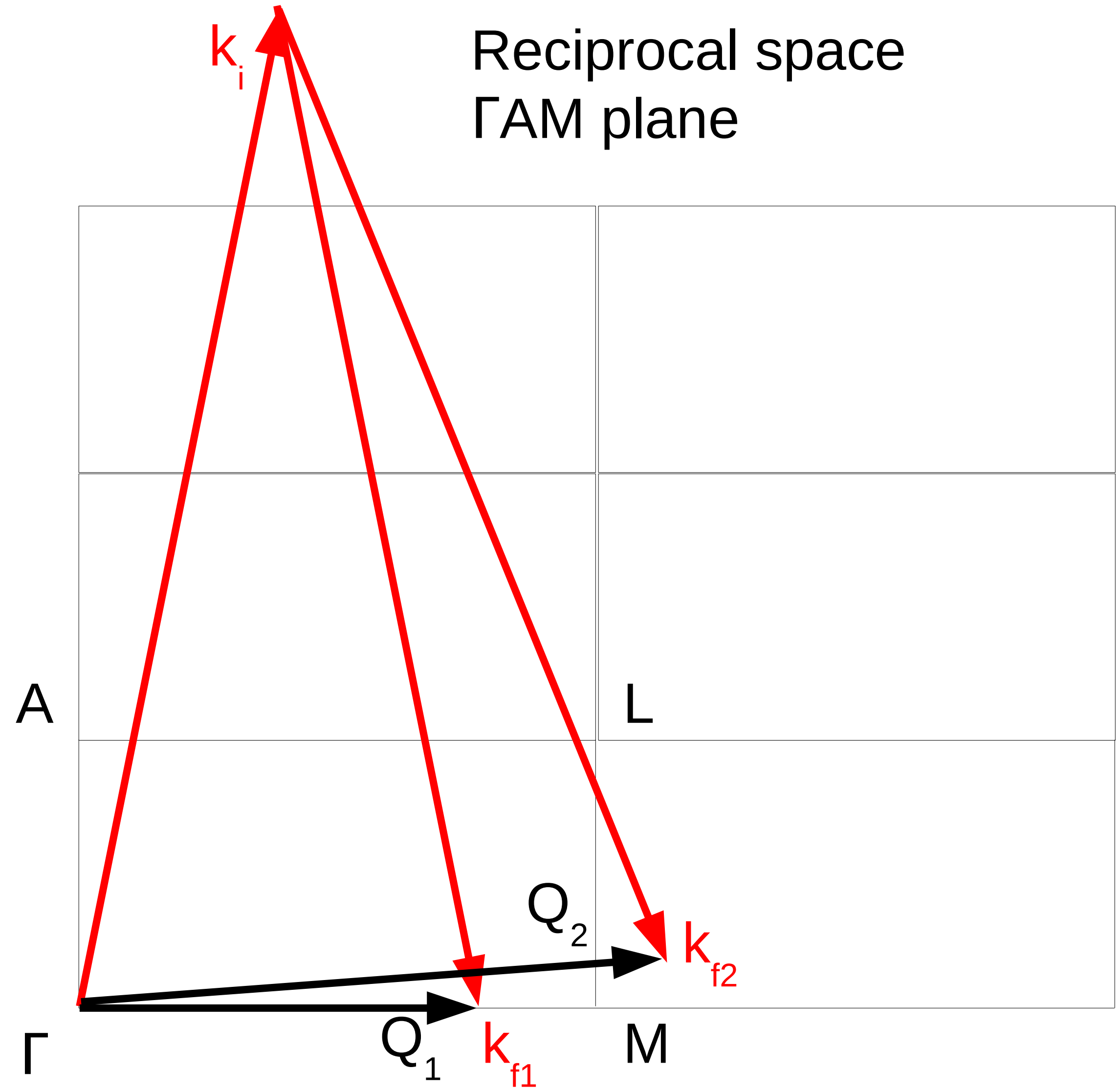
IXS in MgB_2

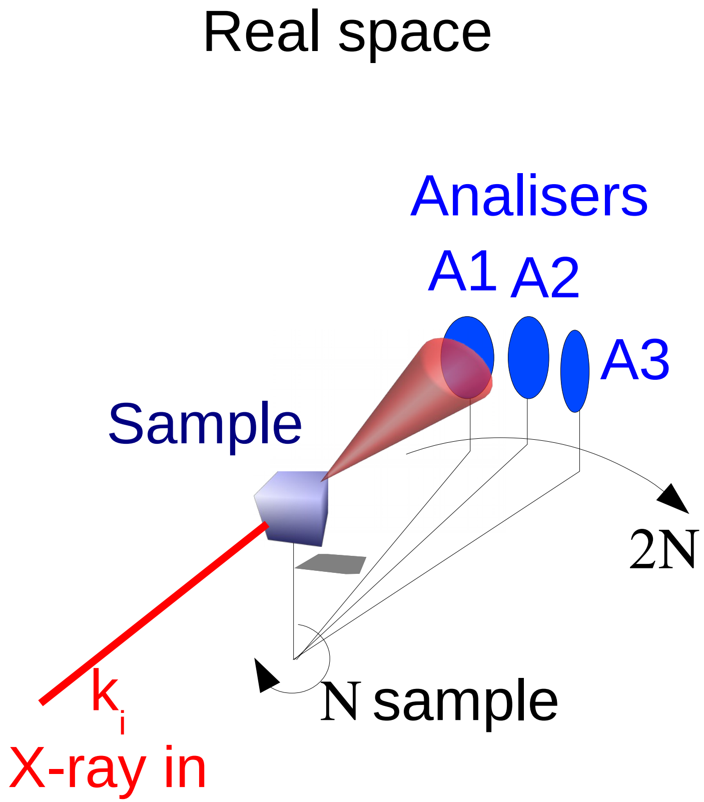




d'Astuto, *et al. PRB* **75** (2007)

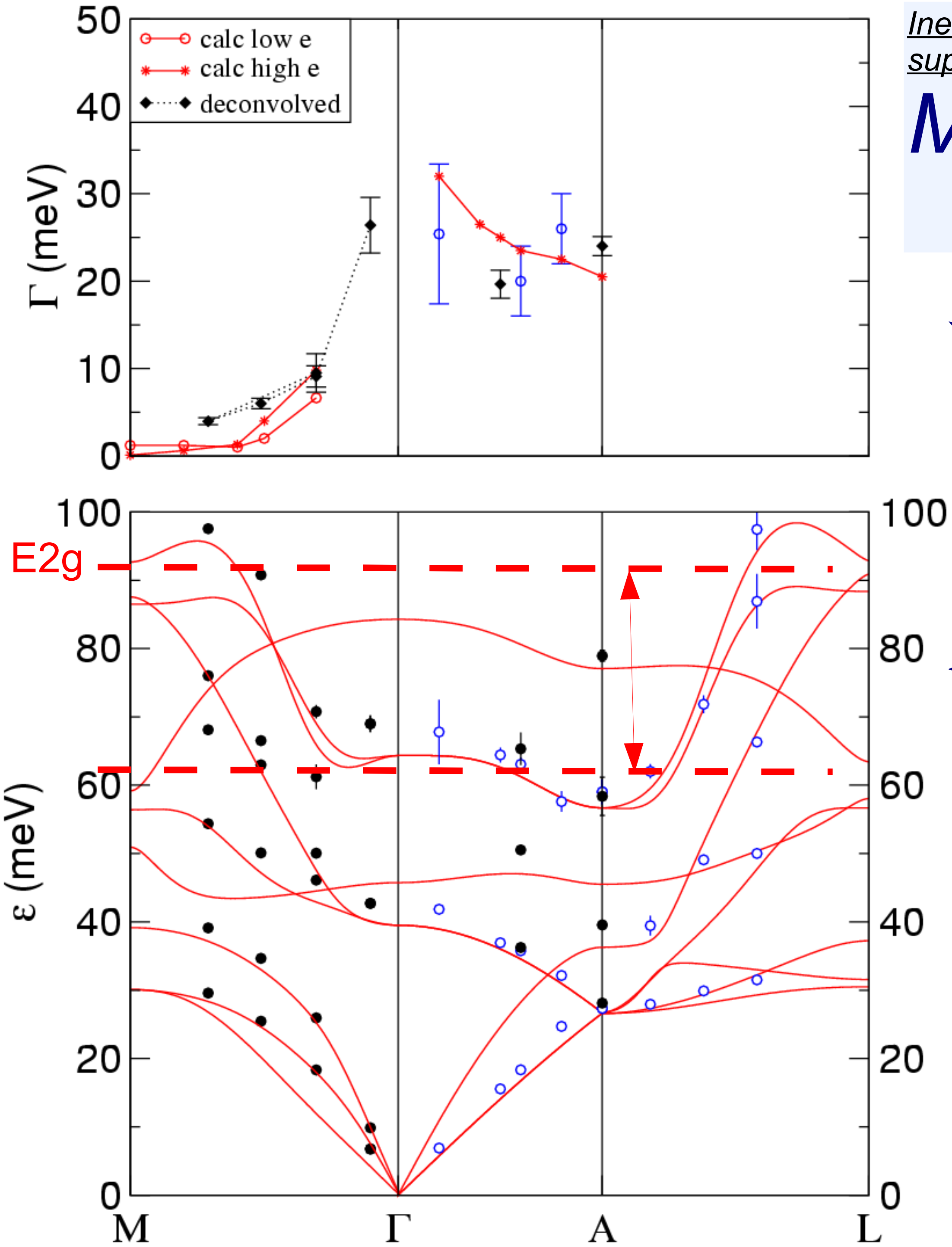
Multianalyser system at ID28 (ESRF)





Inelastic scattering spectroscopy with neutrons and X-rays for superconductivity – Matteo d'Astuto 2019

MgB_2 phonon dispersion

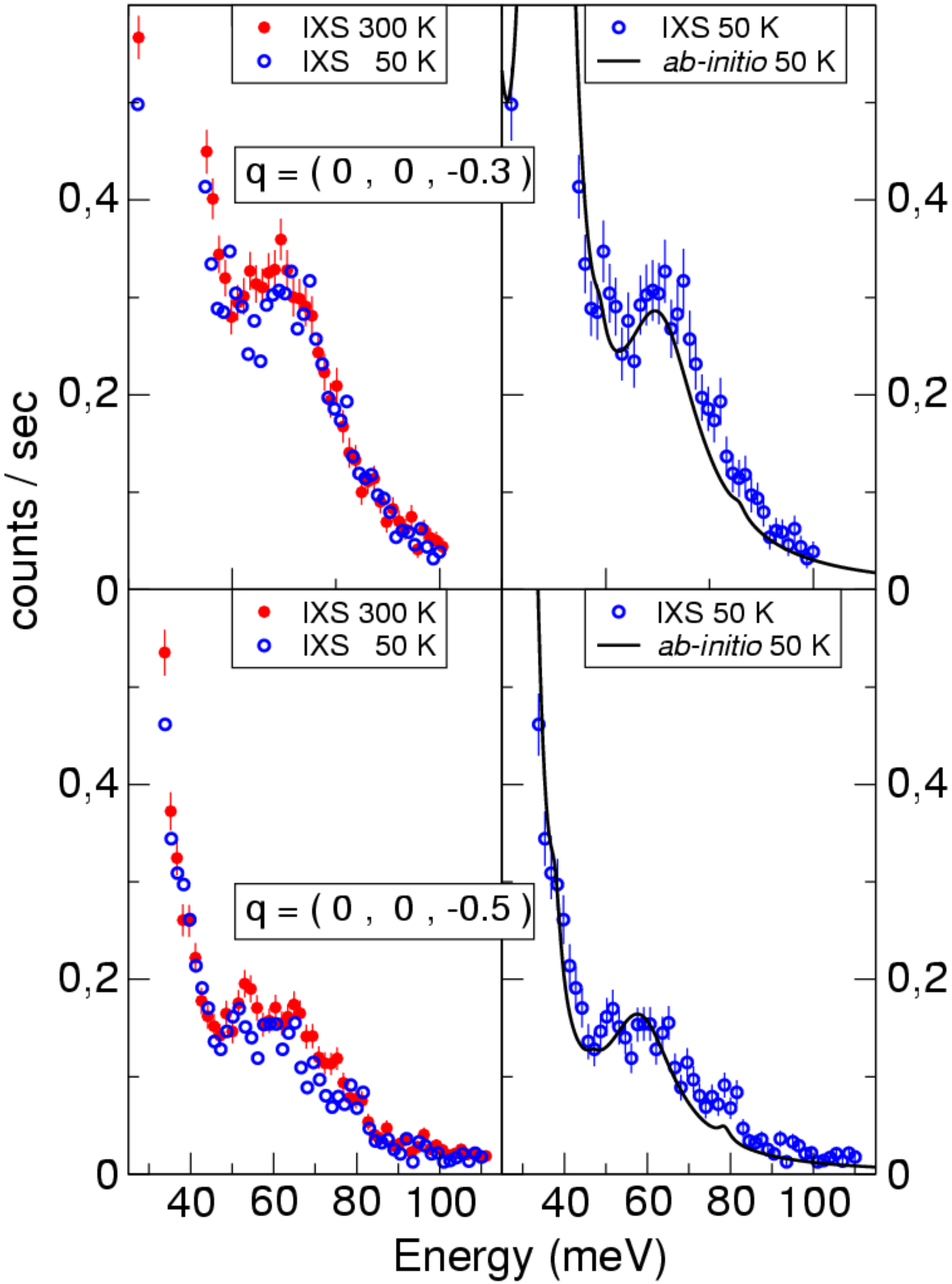


Width :
high res.IXS data ◆
low res. IXS data
Theory

Energy :
high res. IXS data ●
low res. IXS data
Theory

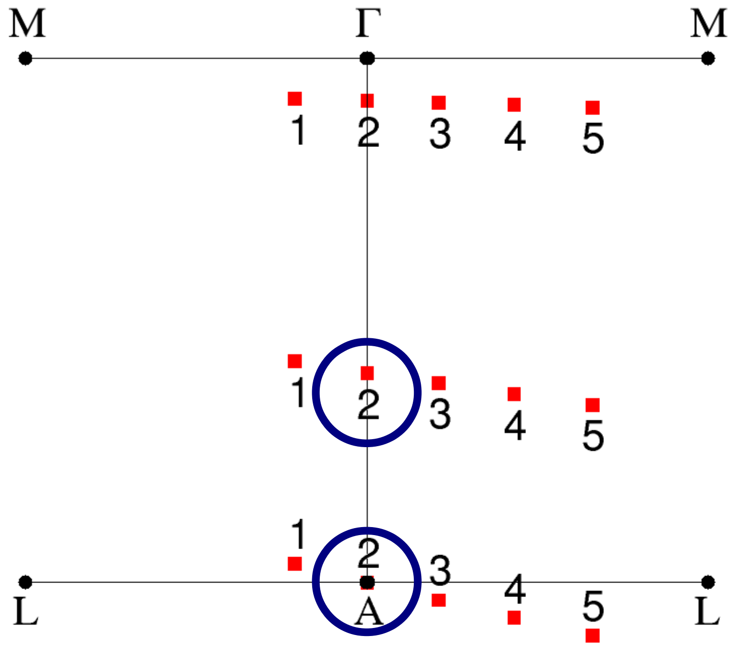
d'Astuto, Calandra, Reich *et al.* *PRB* **75** (2007)

A. Shukla *et al.* *PRL* **90** (2003)



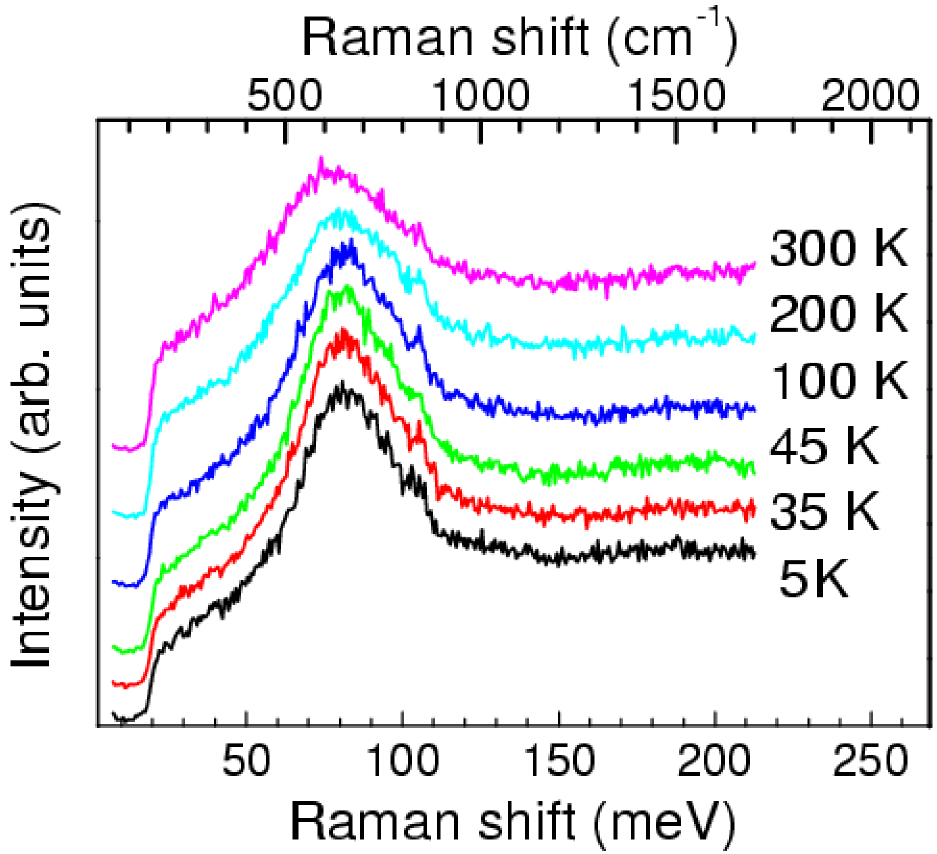
MgB_2 E2g vs T

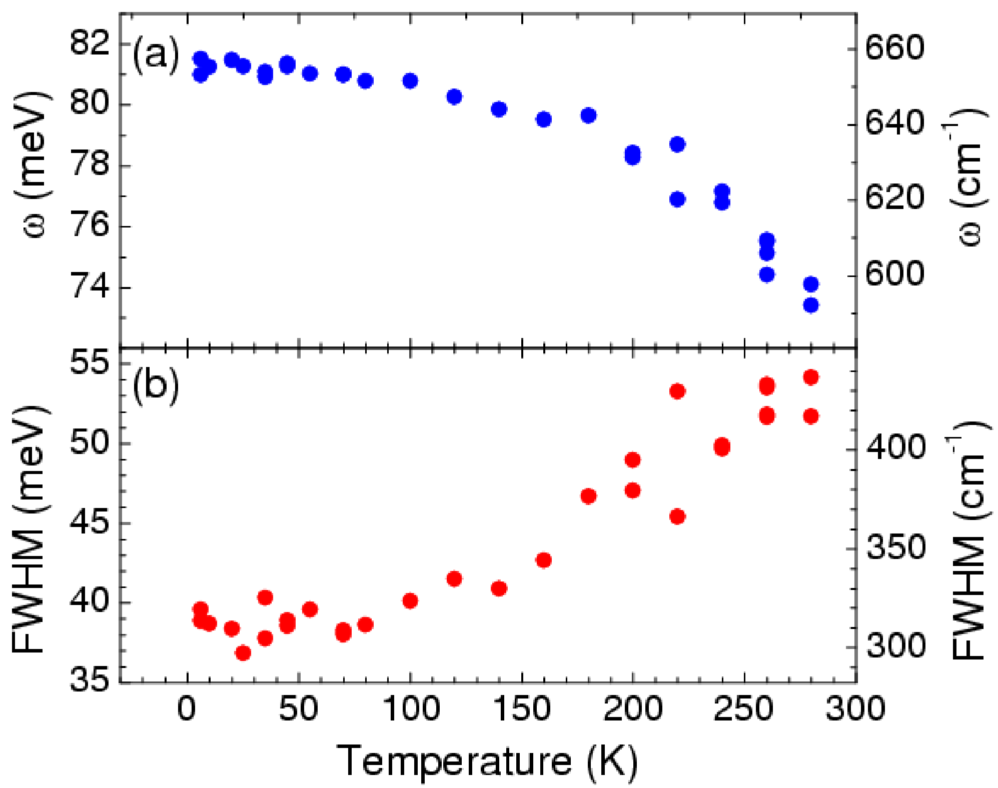
No T variation for E2g T and ≥ from 300 to 50 K.



d'Astuto, Calandra, Reich *et al.* *PRB* **75** (2007)

Raman scattering, dynamical effects?





d'Astuto, Calandra, Reich *et al. PRB* **75** (2007); Cappelluti *PRB* **73** (2006)

Raman shift ω(T) ↘ T ➡ Not an anharmonic effect !

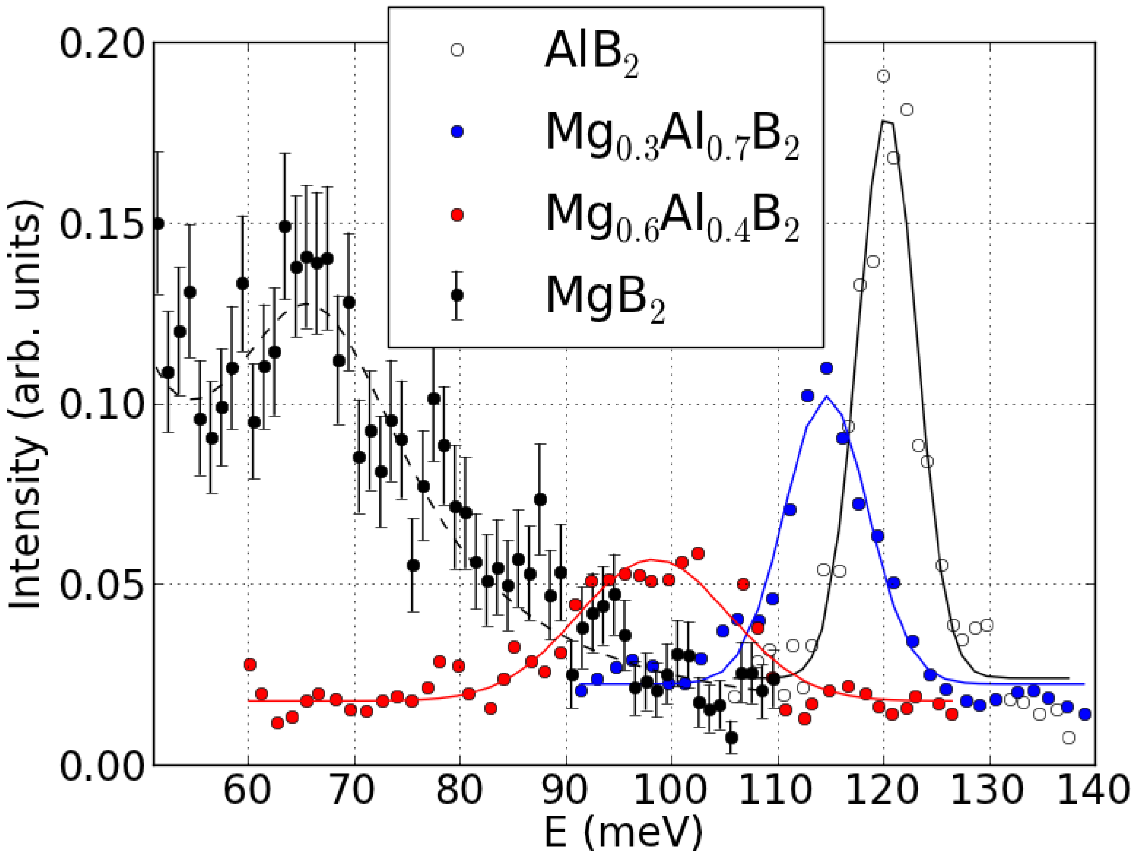
$Mg_{1-x}Al_xB_2$ dispersion and broadening

- Broadening disappears for x=0.5
- Tc vanish for x=0.5
- Dispersions : mix of MgB_2 and AlB_2 fit with IXS data

Renker *et al.* *PRL* **88** (2002) 067001

De la Peña-Seaman *et al.* *PRB* **79** (2009)

IXS energy scan at 0.4 Γ - A



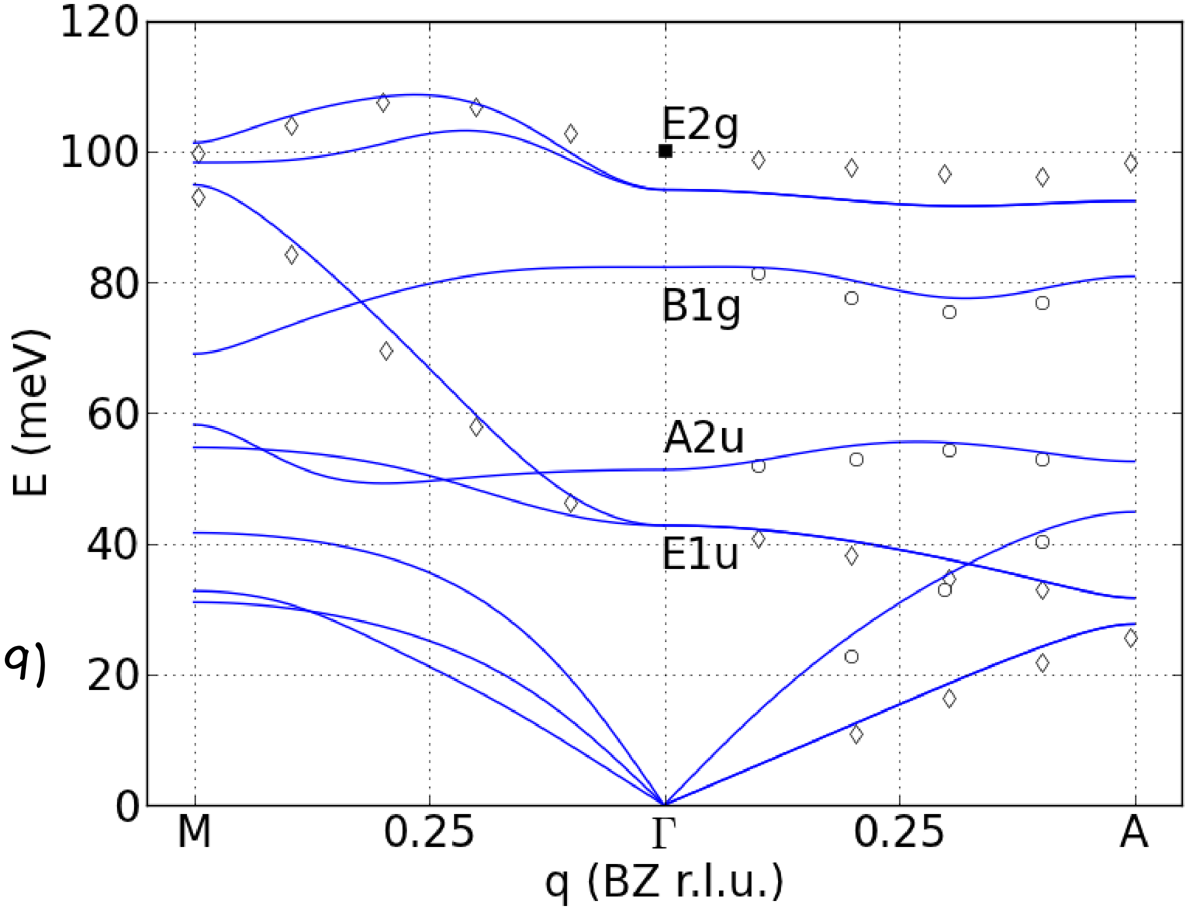
d'Astuto *et al.* *PRB* **93** (2016)

$Mg_{1-x}Al_xB_2$ dispersion and broadening

- Broadening disappears for x=0.5
- Tc vanish for x=0.5
- Dispersions :
  mix of MgB_2 and AlB_2
  fit with IXS data

Renker *et al.* *PRL* **88** (2002) 067001
De la Peña-Seaman *et al.* *PRB* **79** (2009)

Dispersion x~0.4 IXS data and VCA calculations

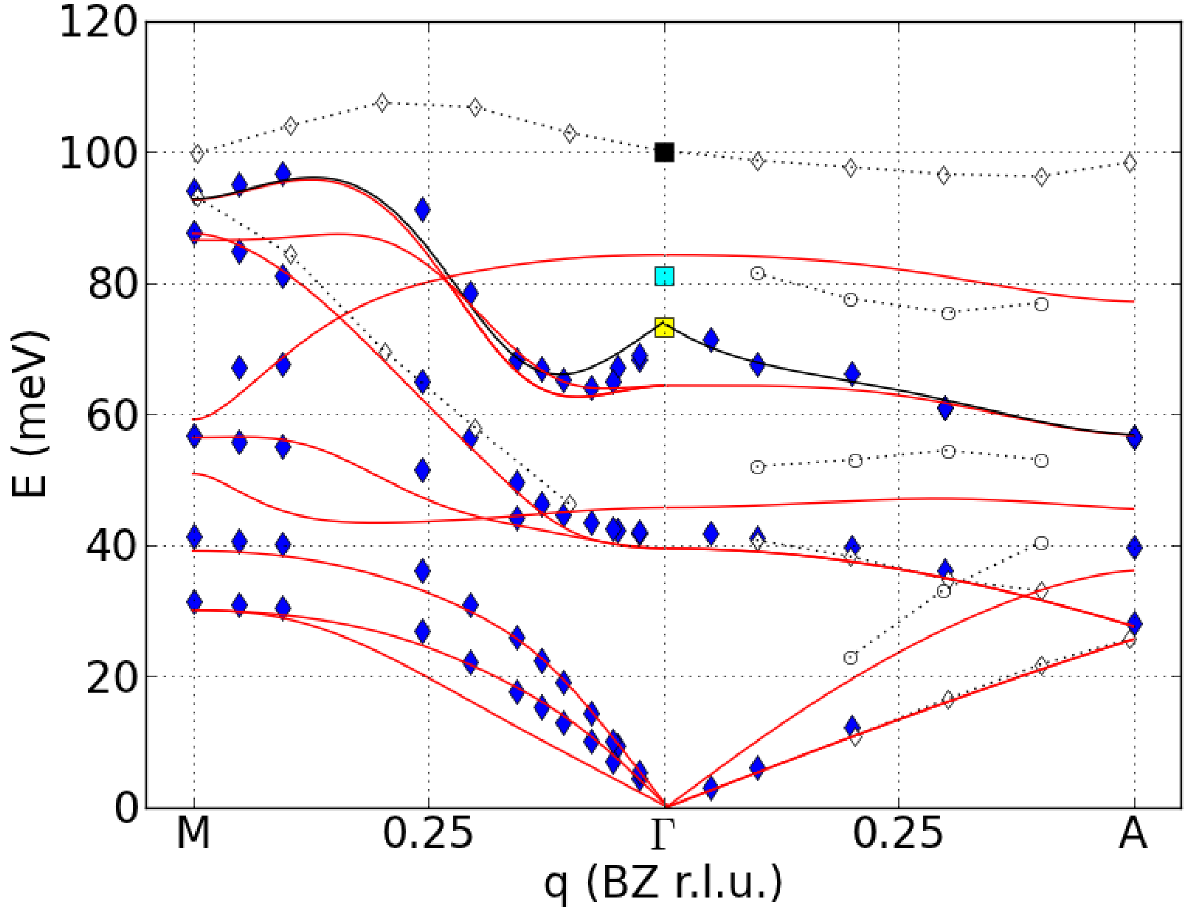


d'Astuto *et al.* *PRB* **93** (2016)

MgB_2 anomaly at Γ

- E2g mode bends up towards Γ for q<0.1 (BZ units)
- highlighted on new high q-resolution experiment
- consistent with Raman via a (very) fast dispersion at zone centre

MgB_2 Dispersion, Raman and IXS data, DFT calculations



d'Astuto *et al.* *PRB* 93 (2016)

Landau damping effect

Anomalous dispersions bends up toward the Brillouin Zone Centre

non-adiabatic effect in layered metals if:

$$|\mathbf{q} \cdot \mathbf{v}_F| \ll \omega$$

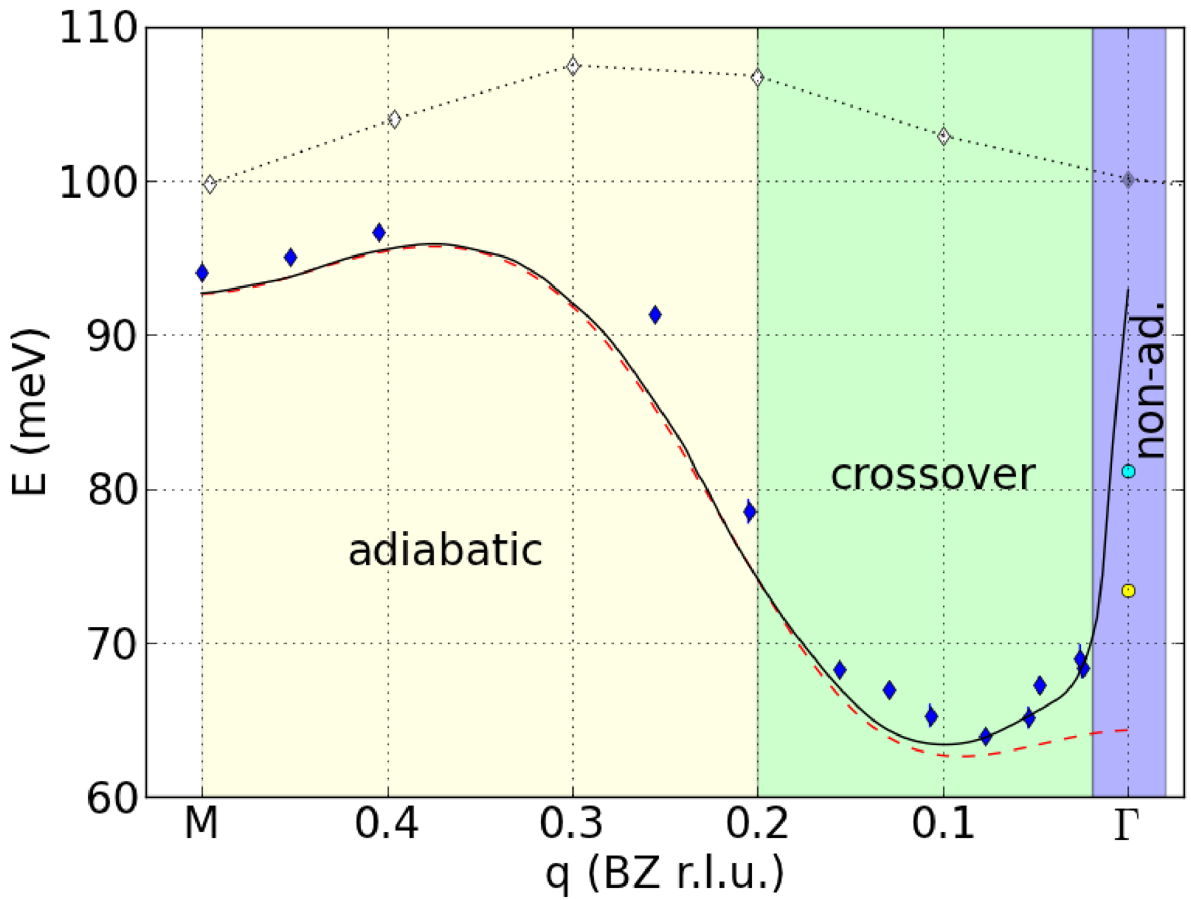
and

$$\omega \gg 1/\tau$$

Calandra, *et al. PhysicaC 456 (2007)*

Saitta, *et al. PRL* 100 (2008)

MgB2 Dispersion, Raman and IXS data, DFT calculations



d'Astuto *et al. PRB* 93 (2016)