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H4.SMR/1013-33

SCHOOL ON THE USE OF SYNCHROTRON RADIATION
IN SCIENCE AND TECHNOLOGY:
"John Fuggle Memorial"

3 November - 5 December 1997

Miramare - Trieste, Italy

Inelastic X-Ray Scattering I

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Inelastic X-Ray Scattering

1. Introduction and IXS from Collective Ion Excitations

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A) General introduction

B) IXS from collective ion excitations

1) Theoretical background

2) X-rays versus neutrons

3) Experimental principles

4) Examples

- Water and Ice
- Glasses (glycerol, v-SiO_2, Orthoterphenyl)
- liquid lithium

- crystalline myoglobin
- crystalline SiO_2
- crystalline CdTe at 7.5 GPa

- Neon at 0.3 GPa

C) Summary

Inelastic X-ray Scattering

The two lectures on inelastic x-ray scattering should allow the audience to get a feeling of what can be done with this technique. The necessary theoretical background is layed out only to the extent that is nessary for the general understanding of the phenomena, while many examples are given in order to show to which type of problems inelastic x-ray scattering can be applied. The purpose of this short note is a further illustration of the transparency copies and provision of a literature list (for sure incomplete). Due to the limited time available the two lectures can not give a complete overview covering every aspect. Consequently the selection reflects my personal preference, and to a certain extent my own research interest. I apologize for the inconsistencies in the nomenclature, i.e. the use of q and Q for the momentum transfer in the scattering process.

The first lecture provides a general introduction to the technique, and then focuses on inelastic x-ray scattering (IXS) from collective ion excitations. This branch of IXS, only developped in the last 10 years, has made tremendous advances, thanks to the availability of 3. generation synchrotron sources and important improvements in instrumentation. It has become an established technique, complementary and sometimes superior to inelastic neutron scattering (INS). The experimental observable is the dynamical structure factor $S(Q,\omega)$, which describes the atomic density fluctuations spectrum. The best known example are phonons in single crystals, and the experimental determination of phonon dispersion curves has been an important research field of inelastic neutron scattering. With respect to INS, IXS has the following advantages: (i) at a given momentum transfer Q essentially unlimited energy transfer (all the phonon branches can be measured with the same instrument) with constant instrumental resolution; (ii) study of crystals which are only available in small sizes; (iii) Study of systems under extreme thermodynamic conditions (high/low temperature; high pressure). In particular aspect (i) makes IXS very powerful for the study of the high frequency dynamics of liquids, glasses and gases in a region of the Q-ω space, not accessible by INS, as will be illustrated by the examples given in the lecture. One important omission in the first lecture concerns x-ray inelastic scattering, utilizing the Mössbauer effect, which as well has made important progress in the past few years.

The second lecture deals with inelastic scattering from electronic excitations. Here I will concentrate only on the aspects closely related to core spectroscopies, in particular to x-ray absorption spectroscopy (XAS). Consequently, non-resonant valence electron excitations and Compton scattering will not be discussed. The first part of the lecture deals with resonant IXS (RIXS) (often called as well resonant Raman scattering (RRS)), where the incident energy is tuned to an absorption edge of the element under study, and the core-hole, created in the absorption process, is filled by an electron from a shallower core level or the filled part of the valence band under emission of an x-ray. For excitation energies above the absorption edge the process is the

well known x-ray fluoresence. It will be shown that RIXS allows to identify absorption channels which can not be separated by XAS, how intratomic electronic correlations can be studied and utilized, and how the resonant enhancement can be used to reveal weak spectral features. In particular, the complementarity of RIXS with respect to XAS and x-ray magnetic circular dichroism (XMCD) in the study of magnetic materials will be discussed. The second part of the lecture deals with non-resonant IXS from core electron excitations, as well called inelastic Raman scattering (IRS). In this case, the relation to XAS is even closer than in the case of RIXS. As a matter of fact, under certain conditions IRS and XAS yield the same result. IRS allows to perform soft x-ray absorption studies in the hard x-ray regime. This has advantages in the study of systems which are not compatible with an ultra-high vacuum environment, necessary in the soft x-ray regime. Moreover, by varying the momentum transfer Q, the electric dipole selection rule, defining the final state symmetry which can be reached in an absorption process, is relaxed and, for example, electric monopolar transitions become possible.

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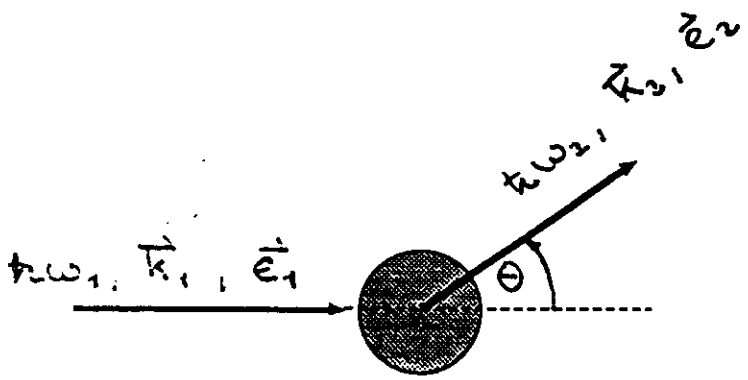
Scattering Process



Ground State $|I\rangle$ ⟶ Interaction between photon field and electrons ⟶ Final State $|F\rangle$

- Energy Transfer: $\hbar\omega = \hbar\omega_1 - \hbar\omega_2$
- Momentum Transfer: $\vec{q} = \vec{k}_1 - \vec{k}_2$

for $\omega << \omega_1$: $q = 2k_1 \sin(\Theta/2)$

- Cross section for events leading to photons with momentum $\vec{k}_2$, (to be observed within a solid angle $\Delta\Omega$), and energy $\hbar\omega_2$ (with resolution $\Delta\hbar\omega_2$).

Interaction Hamiltonian

$$H_{int} = \frac{e}{m_e c} \sum_j \left(\frac{e}{2c} \vec{A}_j^2 + \vec{A}_j \vec{p}_j \right) \qquad \text{(non relativistic)}$$

$\vec{A}_j$: Vector potential of the electromagnetic field

$\vec{p}_j$: Momentum operator of the electron

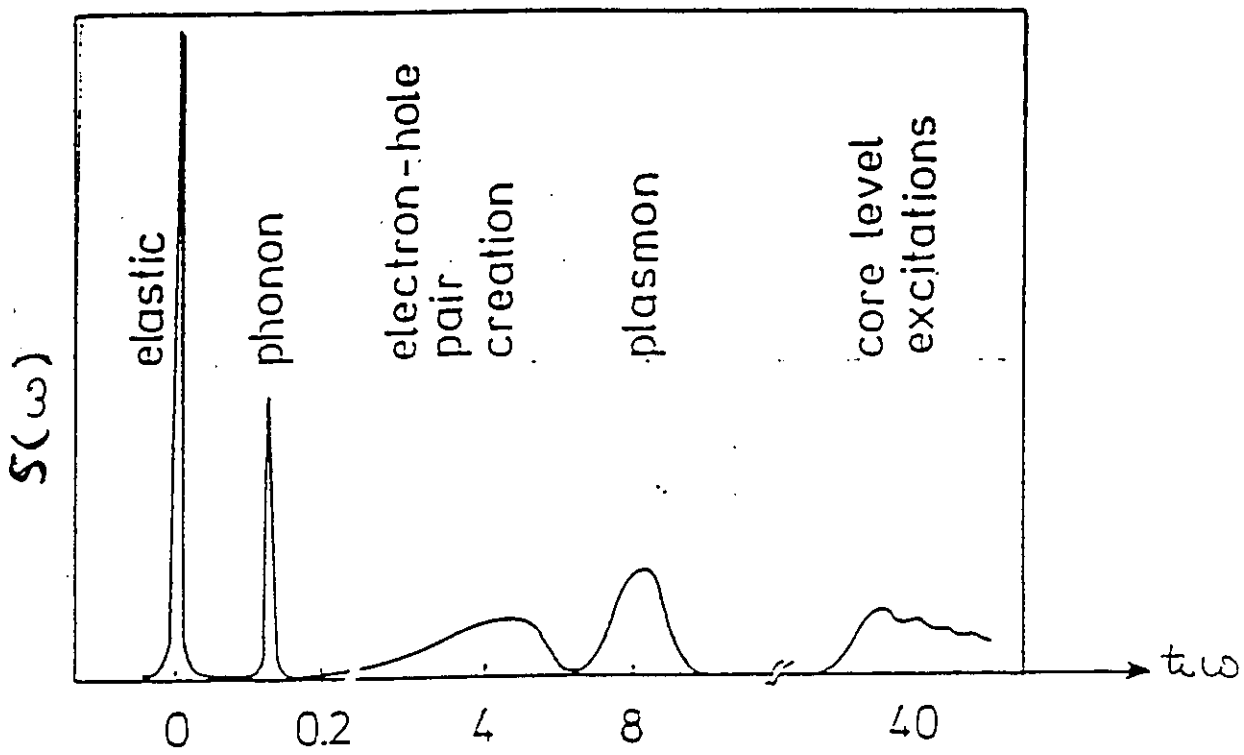
Lowest order perturbation theory (Fermi's Golden Rule)

Double differential cross section

$$\frac{d^2\sigma}{d\Omega d\omega_2} = r_0^2 \frac{\omega_2}{\omega_1} \sum_{I,F} \left| \left\langle F \left| \Sigma_j e^{i(\vec{k}_2 - \vec{k}_1)\vec{r}_j} \right| I \right\rangle (\vec{e}_1 \cdot \vec{e}_2) + \frac{1}{m_e} \sum_N \frac{\left\langle F \left| \vec{e}_2 \cdot \Sigma_j \vec{p}_j e^{-i\vec{k}_2 \vec{r}_j} \right| N \right\rangle \left\langle N \left| \vec{e}_1 \cdot \Sigma_j \vec{p}_j e^{i\vec{k}_1 \vec{r}_j} \right| I \right\rangle}{E_I - E_N + \hbar\omega_1 + 0.5 i \Gamma_N} \right|^2$$

$$\delta(E_F - E_I - \hbar\omega)$$

Inelastic X-ray Scattering



1) Collective ion excitations: $qd \approx 1$ (d: interionic distance); $\hbar\omega$: phonon energy

2) Valence electron excitations: $qr_c \approx 1$ (r_c: interparticle distance); $\hbar\omega$: free-electron plasma frequency

3) Inner shell excitations: $qa < 1$ (a: inner electron shell radius); $\hbar\omega$: electron binding energy

4) Compton scattering: $qr_c >> 1$; $\hbar\omega >>$ binding energy

5) Resonant Raman Scattering: $\hbar\omega_1 \sim E_{abs}$, $\hbar\omega_2 \sim E_{fl}$

Application versus experimental needs

Inelastic x-ray scattering is a weak process:

=> extract as many photons of the desired energy as possible out of the source. (Monochromator)

=> energy analysis + collect some solid angle Ω. (Analyser)

Tunability of the momentum transfer.

Selection of the polarization.

1) Collective ion excitations (phonons):

$\hbar\omega_1$: 10 - 20 keV
$\Delta\hbar\omega$: 1-10 meV

2) Valence electron excitations:

$\hbar\omega_1$: 10 keV
$\Delta\hbar\omega$: 0.3 - 3 eV

3) Non-resonant Raman scattering

$\hbar\omega_1$: 10 keV
$\Delta\hbar\omega$: 1 eV -> (0.1 eV) K-hole lifetime of light elements

4) Resonant Raman scattering:

$\hbar\omega_1$: 0.5-15 keV tunable to K-,L and M-edges of interest
$\Delta\hbar\omega$: 0.1 -1 eV $\approx$ lifetime of final state core-hole

Inelastic X-ray Scattering from collective ion excitations

$$\frac{d^2\sigma}{d\omega_2 d\Omega} = r_o^2 \frac{\omega_2}{\omega_1} \left| \langle F | \Sigma_j e^{i\vec{Q}\vec{r}_j} | I \rangle \right|^2 \hat{e}_1 \hat{e}_2 \, \delta(E_F - E_I)$$

$$r_o^2 \frac{\omega_2}{\omega_1} \left| \langle F_N | \langle I_e | \Sigma_j e^{i\vec{Q}\vec{R}_j} \Sigma_i e^{i\vec{Q}\vec{r}_i} | I_e \rangle | I_N \rangle \right|^2 \hat{e}_1 \hat{e}_2 \, \delta(E_F - E_I)$$

$$r_o^2 \frac{\omega_2}{\omega_1} \left| \langle F_N | f_Q \Sigma_j e^{i\vec{Q}\vec{R}_j} | I_N \rangle \right|^2 \hat{e}_1 \hat{e}_2 \, \delta(E_F - E_I)$$

Adiabatic Approximation: Factorization of electronic and ionic wavefunction.

Electrons are left in their ground state, $|I_e\rangle$

Observation of collective ion excitations, $|I_N\rangle \rightarrow |F_N\rangle$

$$\frac{d^2\sigma}{d\omega_2 d\Omega} = r_o^2 \frac{\omega_2}{\omega_1} \left(\vec{e}_1 \cdot \vec{e}_2 \right) \left| f(\vec{Q}) \right|^2 S(\vec{Q}, \omega)$$

Thomson term: Coupling of the charge to the electromagnetic field.

Dynamical structure factor $S(\vec{Q},\omega)$: Properties of the scattering sample, independently of the perturbing electromagnetic field.

"When a crystal is irradiated with X-rays, the processes of photoelectric absorption and fluorescence are no doubt accompanied by absorption and emission of phonons. The energy changes involved are however so large compared with phonon energies that information about phonon spectrum of the crystal cannot be obtained in this way. The same is true for Compton scattering."[1] W.Cochran, 1966.

1 W. Cochran, in "Phonons" ed. by R.W.H. Stevenson, Oliver and Boyd, London (1966).

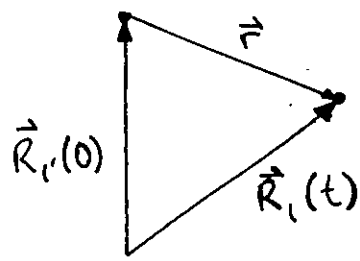
Physical meaning of $S(\vec{Q},\omega)$

$S(\vec{Q},\omega)$ is the space and time Fourier transform of the pair correlation function $G(\vec{r},t)$.

$$S(\vec{Q},\omega) = \frac{1}{2\pi\hbar}\int G(\vec{r},t)\exp\left(i\left(\vec{Q}\vec{r} - \omega t\right)\right)d\vec{r}dt$$

with:

$$G(\vec{r},t) = \frac{1}{N}\sum_{l,l'}\int\left\langle\delta\left(\vec{r}' - \vec{R}_{l'}(0)\right)\delta\left(\vec{r}' + \vec{r} - \vec{R}_{l}(t)\right)\right\rangle d\vec{r}'$$



$G(\vec{r},t)$ is the probability to find two different particles at positions $\vec{R}_{l'}(t=0)$ and $\vec{R}_{l}(t)$, separated by the distance $\vec{r}$ and the time intervall t.

- Relation between momentum transfer $\vec{Q}$ and λ_c, a distance describing the *spatial inhomogeneity* of the scattering system.

- Relation between scattering events at different times: Relation between energy transfer $\hbar\omega$ and the *characteristic resonance frequencies* of the system.

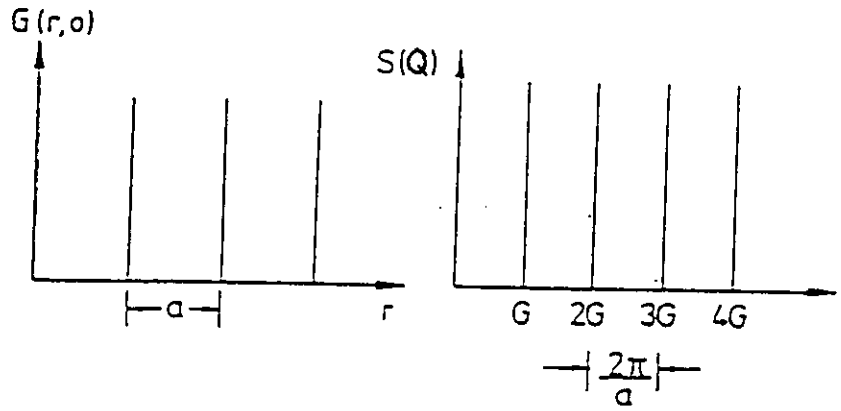
Determination of the atomic density fluctuations spectrum $S(\vec{Q}, \omega)$

The static structure factor $S(\vec{Q})$

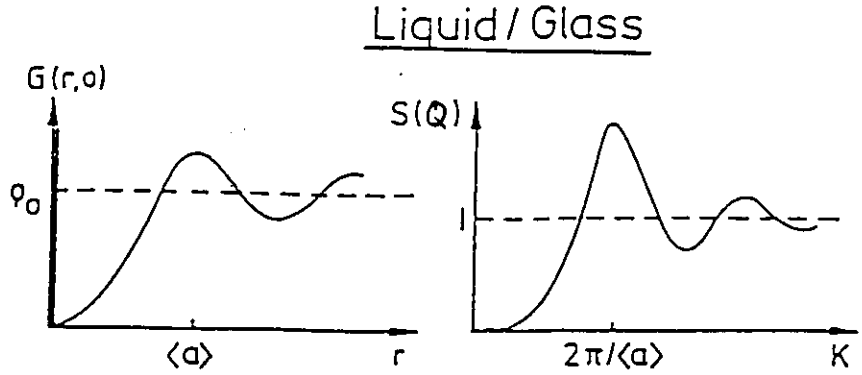
$$S(\vec{Q}) = \int S(\vec{Q},\omega)\,d(\hbar\omega) = \frac{1}{2\pi\hbar}\int G(\vec{r},0)\exp(i\vec{Q}\vec{r})\,d\vec{r}$$

t = 0 => Snapshot of the pair correlation function.

A) Crystal



B) Liquid/Glass



There is no distinction between a liquid and a glass!

The dynamic structure factor $S(\vec{Q},\omega)$

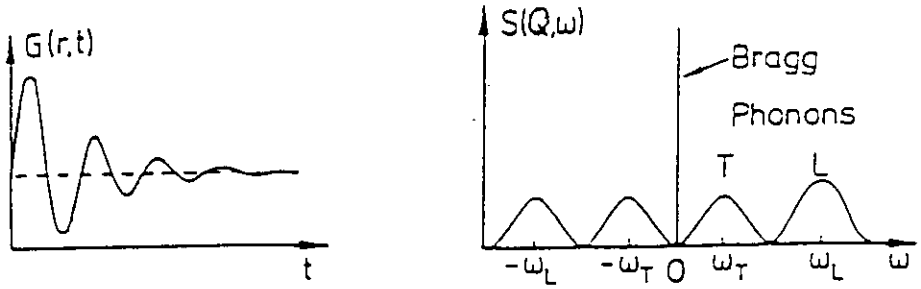
A) Crystal

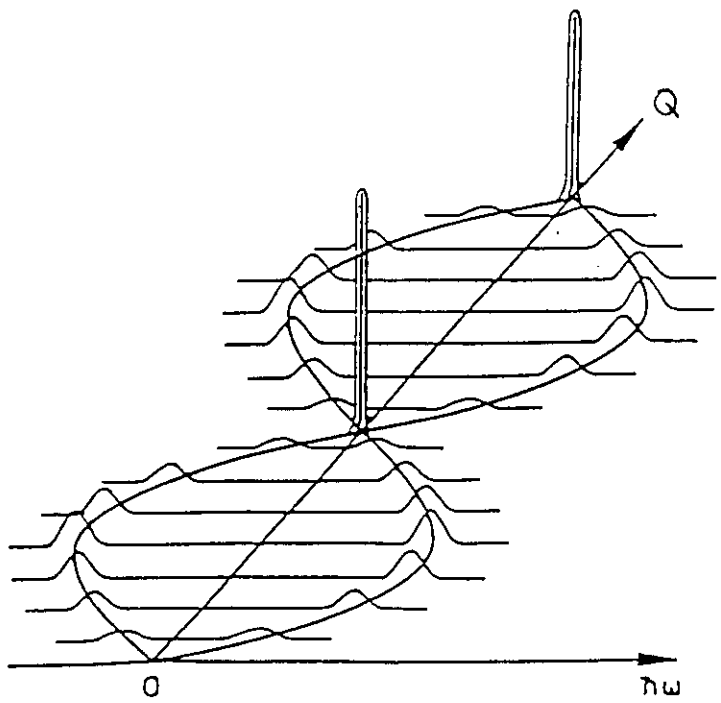
- ideal crystal: harmonic motion of atoms about their equilibrium position.
=> Harmonic oscillations of $G(\vec{r},t)$.

-real crystal: anharmonic effects.
=> damped oscillations of $G(\vec{r},t)$.

$S(\vec{Q},\omega)$:

- Elastic intensity only at the Bragg peaks.
- phonons, eventually with a certain width Γ due to the damping.





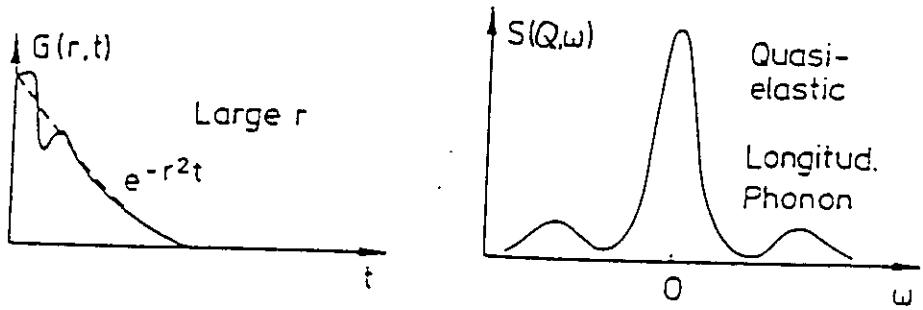
B) Liquids

- Loss of correlation after particle collisions.
=> Exponential decay of $G(\vec{r},t)$, where τ denotes a typical memory or collision time.

- For large $\vec{r}$ ($\vec{r}$ >> interatomic distances, $\vec{Q}=2\pi/\vec{r}$) and $t << \tau$ ($t = 2\pi/\omega$) correlation prevails.
=> Damped oscillations of $G(\vec{r},t)$.

$S(\vec{Q},\omega)$:

- Elastic intensity due to exponential decay of $G(\vec{r},t)$.
- phonon-like excitations (compressional modes, sound propagation)



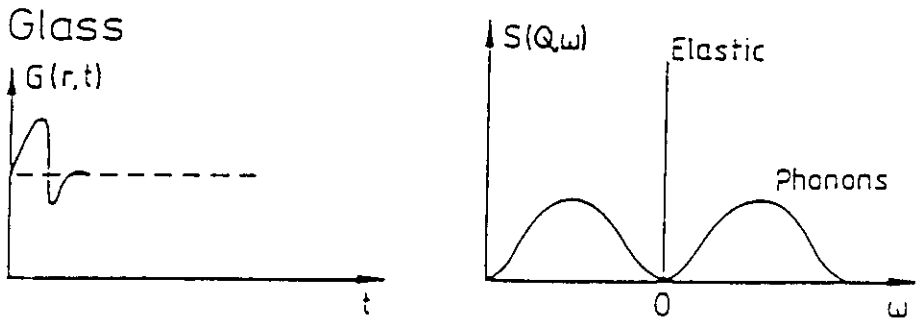
C) Glasses

- static disorder yields an average $G(\vec{r},t)$.
- strongly damped oscillations around quasi-equilibrium sites.

=> Damped oscillations of $G(\vec{r},t)$.

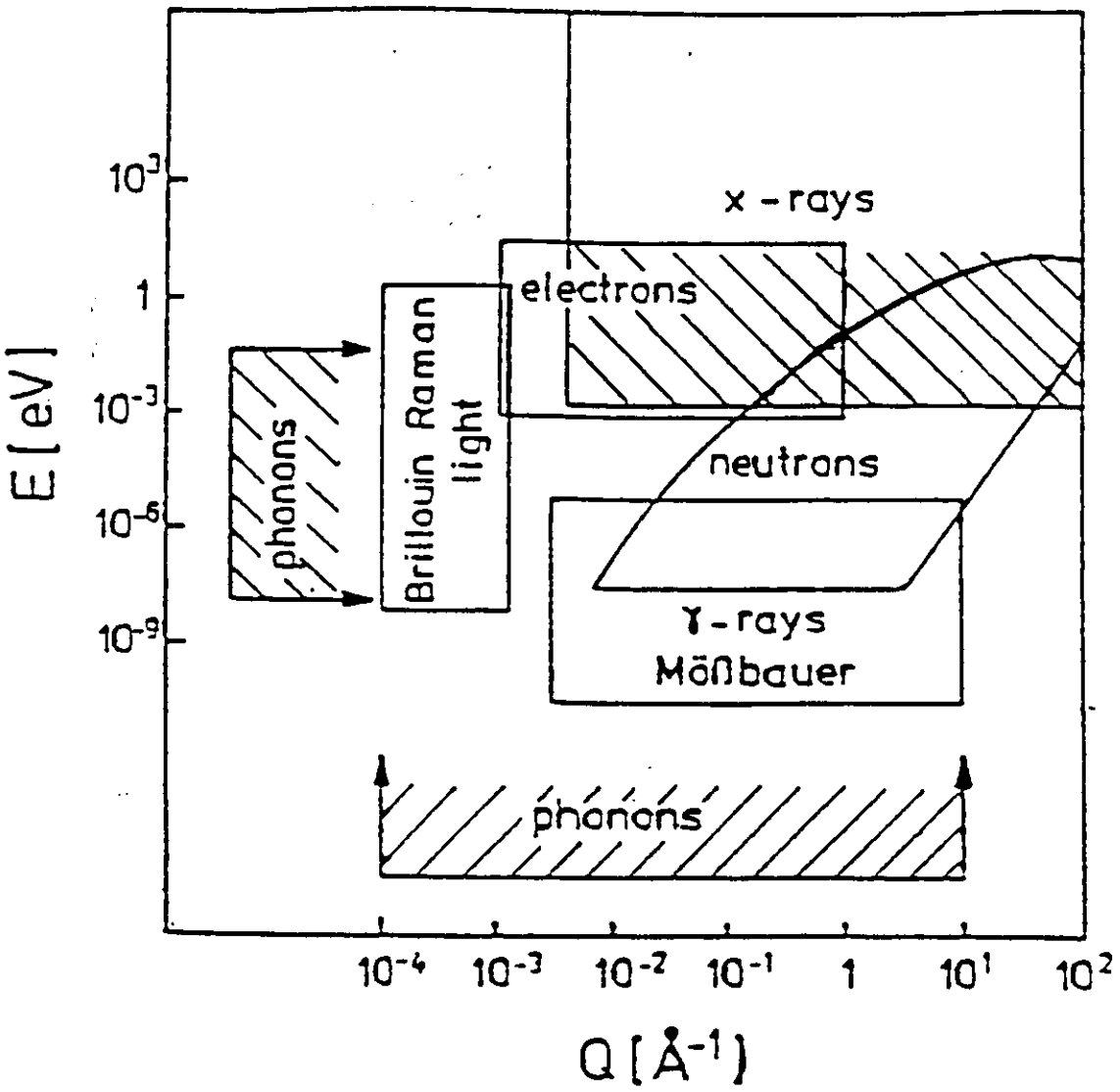
$S(\vec{Q},\omega)$:

- Elastic intensity with quasi zero ω-width.
- phonon-like excitations



There is a distinction between a liquid and a glass!

Probes for Phonons



Advantages using X-rays

- Complementary to the neutrons in an important region of $\vec{q}$ - ω space.
- Dynamics of disordered system as liquids, amorphous materials and biological systems can be measured.

Scattering from Particle Density Fluctuations: Neutrons versus X-rays

Neutrons: $\lambda = 1$ A => $E_1 = 82$ meV ΔE = some meV $E_1 = E_2$

$$q = \sqrt{k_1^2 + k_2^2 - 2k_1k_2\cos\theta_s}$$

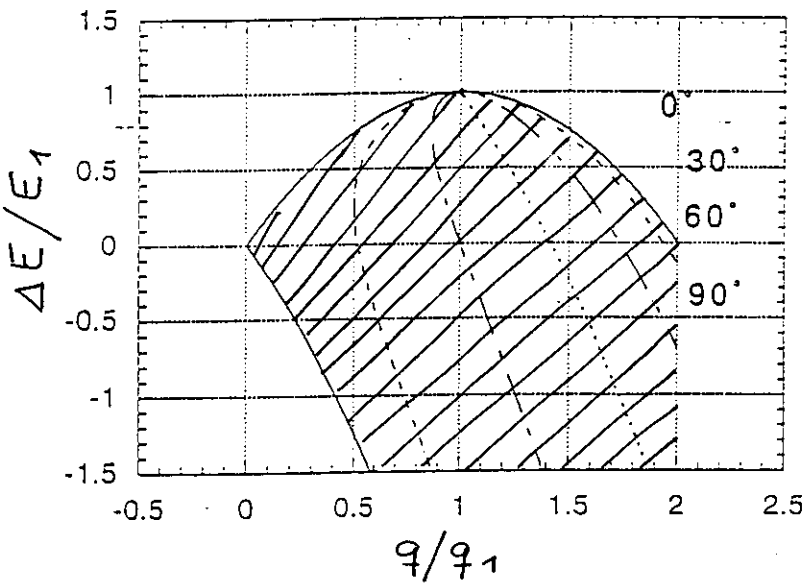
=> ΔE_{max} for a given q-transfer

X-rays: $\lambda = 1$ A => $E_1 = 12.398$ keV ΔE = some meV $E_1 \approx E_2$

$$q = 2k_1 \sin(\theta_s / 2)$$

=> q-transfer controlled only by scattering angle Θ.

Energy-Momentum Transfer Region for a Neutron of Energy E_1 and Momentum k_1



Where do have X-rays an advantage with respect to neutrons?

Disordered systems with a high speed of sound: $v_g = \frac{\partial\omega}{\partial q}$

Incoherent Scattering

Small samples, extreme thermodynamic conditions

X-rays versus Neutrons

• X-rays, For small Q: fQ ~Z, and:

$$\frac{d^2\sigma}{d\omega_2 d\Omega} = r_o^2 \frac{\omega_2}{\omega_1}\left(\vec{e}_1 \vec{e}_2\right) Z^2 \, S\left(\vec{Q},\omega\right)$$

with r_o: classical electron radius, ~ $2.8 \cdot 10^{-15}$ m.

$$\text{Count rate} \sim \frac{Z^2 r_o^2}{\sigma_t}$$

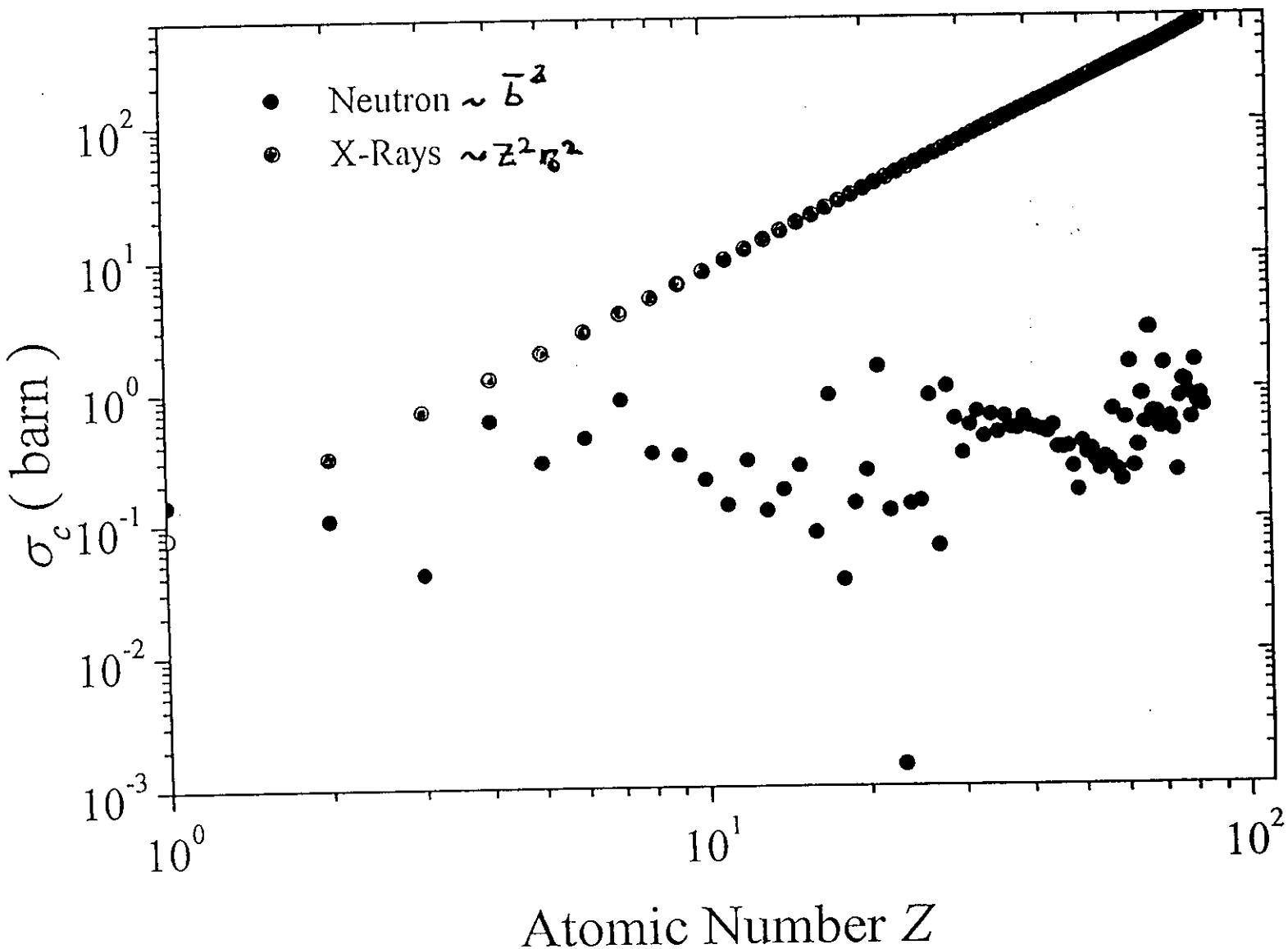
- x-ray cross section σ_t dominated by photoelectric absorption: $\sim \lambda^3 \cdot Z^4$
- f(Q) decreases exponentially at large Q
- small beams (100μm x 300 μm)
- $\Delta E/E = 10^{-7} - 10^{-8}$

• Neutrons:

$$\frac{d^2\sigma}{d\omega_2 d\Omega} = b^2 \frac{k_2}{k_1} \, S\left(\vec{Q},\omega\right)$$

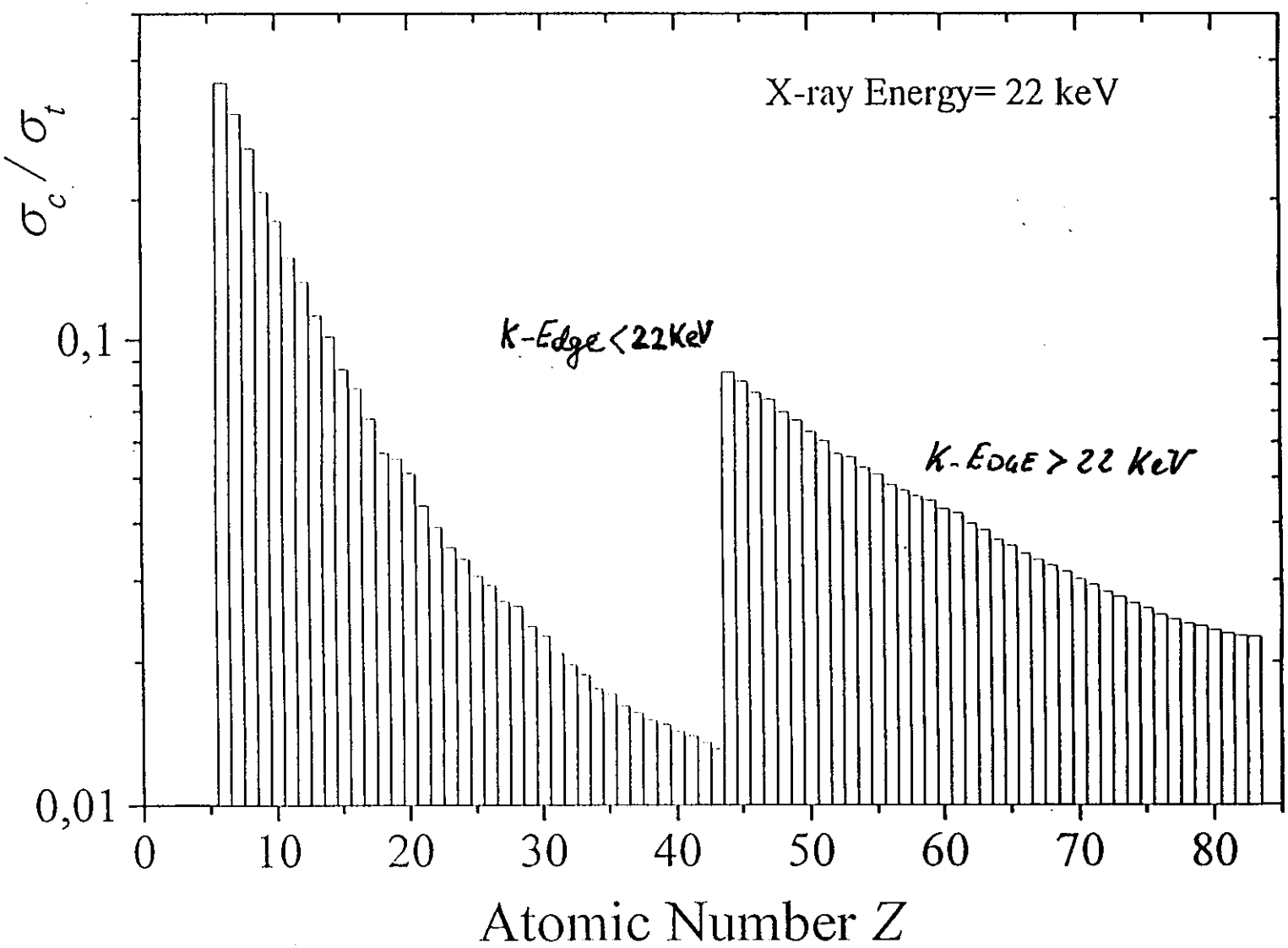
with b: neutron scattering length, ~ 10^{-15} m.

- absorption cross section weak, => multiple scattering
- incoherent scattering contribution
- large beams
- $\Delta E/E = 10^{-1} - 10^{-2}$


Neutron ~ $\bar{b}^2$
X-Rays ~ $Z^2 r_0^2$
σ_c (barn)
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^0
10^1
10^2
Atomic Number Z

$$\text{COUNT RATE} = N_0 \frac{\partial^2\sigma}{\partial\Omega\,\partial E}\,\Delta\Omega\,\Delta E\,\rho L e^{-\mu L} \propto \frac{Z^2 n_0^2}{\sigma_t}$$

σ_t = TOTAL CROSS-SECTION PER ATOM



Inelastic x-ray scattering from collective ion excitations

$\Delta E/E = 10^{-7}$ to 10^{-8} and match the source divergence?

- High order reflections from perfect crystals (silicon).
- Bragg angles very close to 90 degrees.

- Intrinsic Energy Resolution:

$$\frac{\Delta E}{E} = \frac{d}{\pi \Lambda_{ext}}$$

- Extinction Depth Λ_{ext} ($\alpha = 0$):

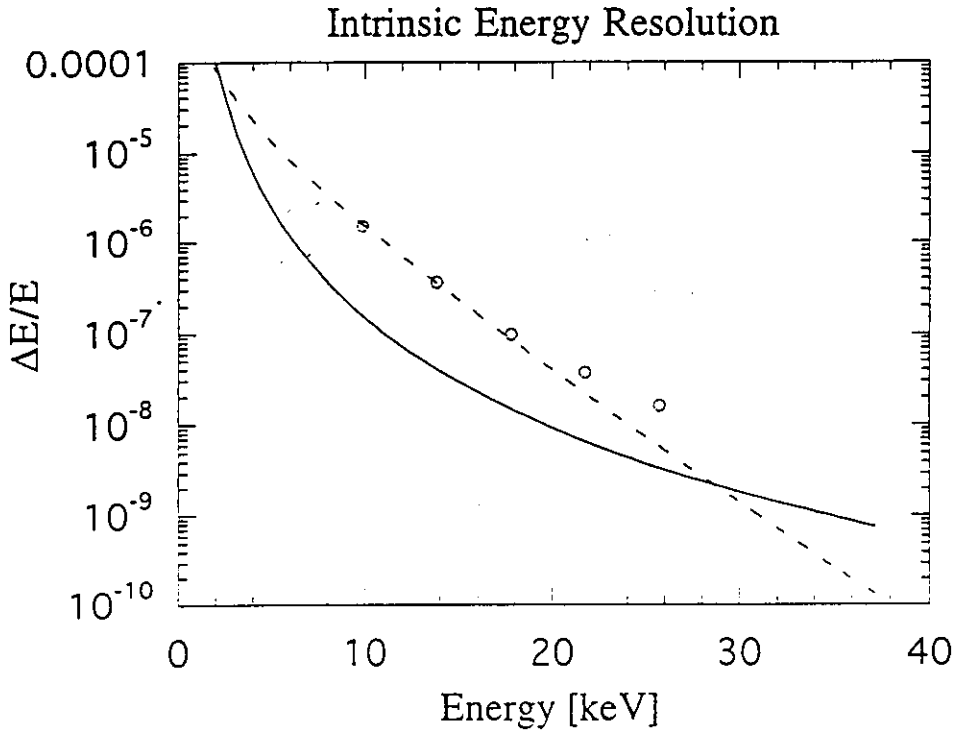
$$\Lambda_{ext} = \frac{V}{4 r_e d\left(f_0 + f\right) F_{hkl} C\, e^{-DWF}}$$

- Angular Acceptance (Darwin width) ω_D ($\alpha = 0$) :

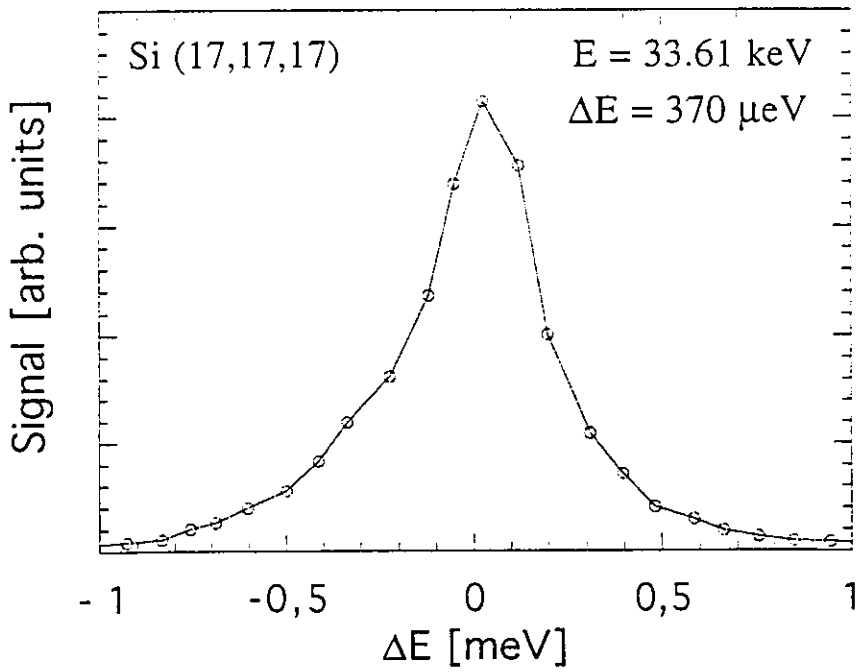
$$\omega_D = \frac{\lambda}{2\pi \Lambda_{ext} \cos\theta_B} = \frac{\Delta E}{E} \tan\theta_B$$

V: unit cell volume, r_e: classical electron radius, f_0: atomic form factor, f': real part of the dispersion correction, C: polarisation factor, F_{hkl}: structure factor, DWF: Debye-Waller factor

Ultimately, the energy resolution becomes absorption limited !!!



Best energy resolution so far obtained with perfect crystal optics



Perfection of silicon crystals: $\frac{\Delta E}{E} = -\frac{\Delta d}{d} \sim 10^{-8}$

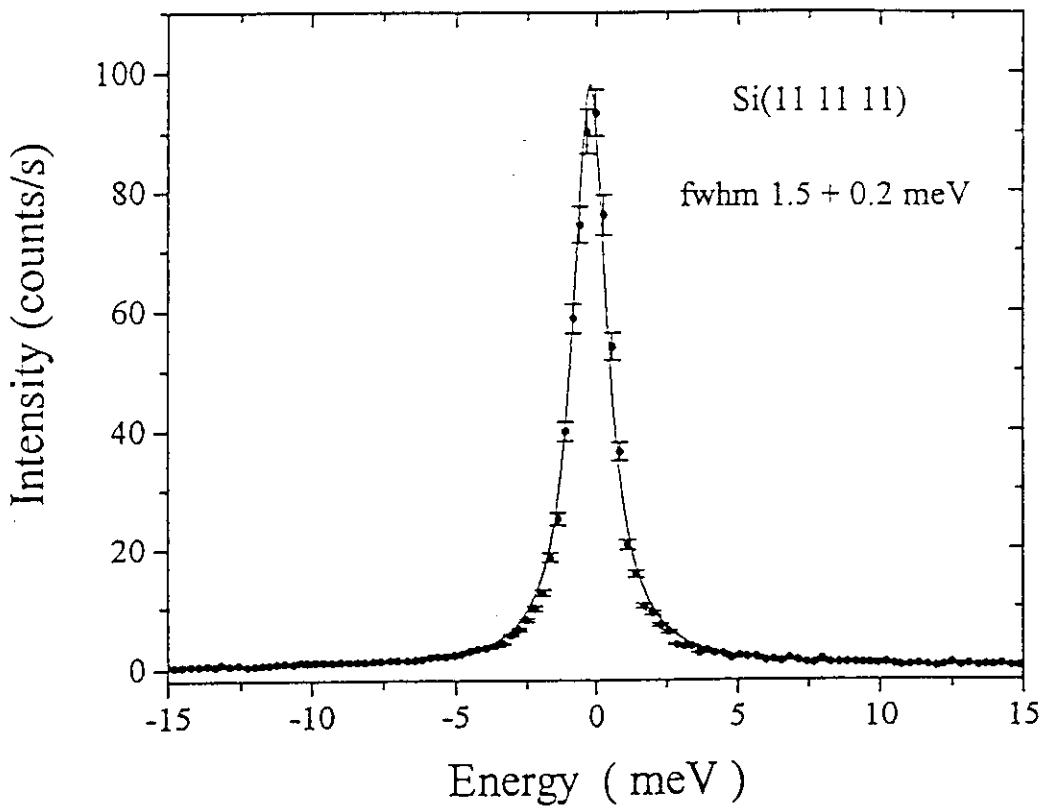
Inelastic Scattering by phonon excitations:

$\Delta E/E = 10^{-7} - 10^{-8}$ and some solid angle?

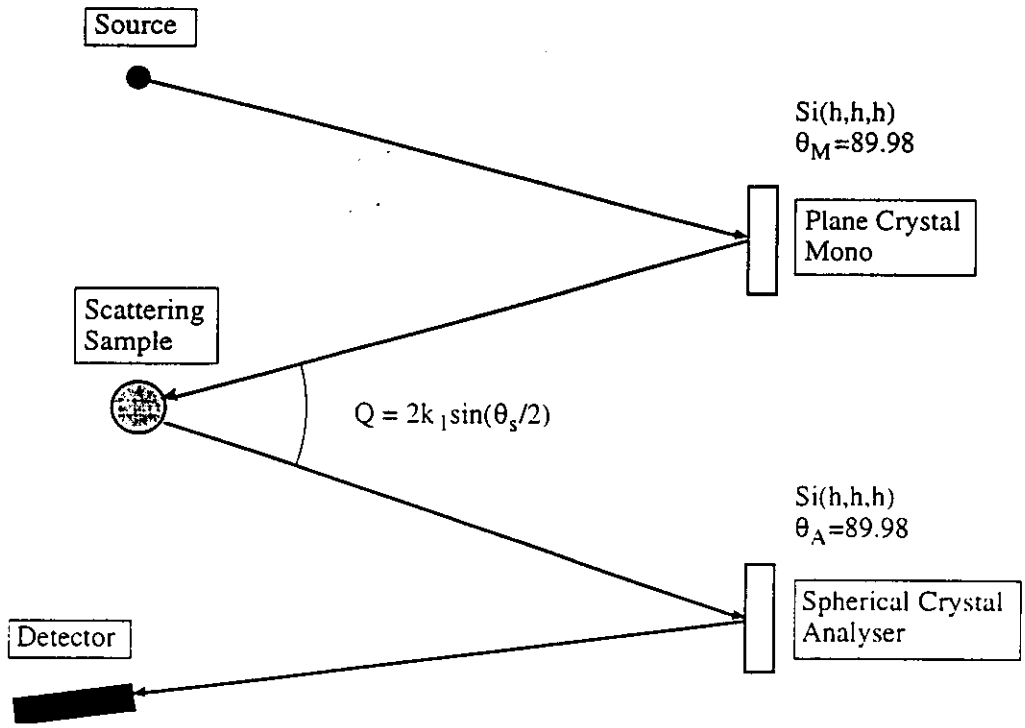
High order reflections and Bragg angle larger than 89.92 degrees

Rowland circle geometry

Glue ≈ 7500 0.6x0.6x3 mm^3 silicon cubes on a spherical substrate, with ≈ 10 arcsecs tolerance in the relative alignment among cubes.



Experimental Principle for X-ray scattering with meV Energy Resolution

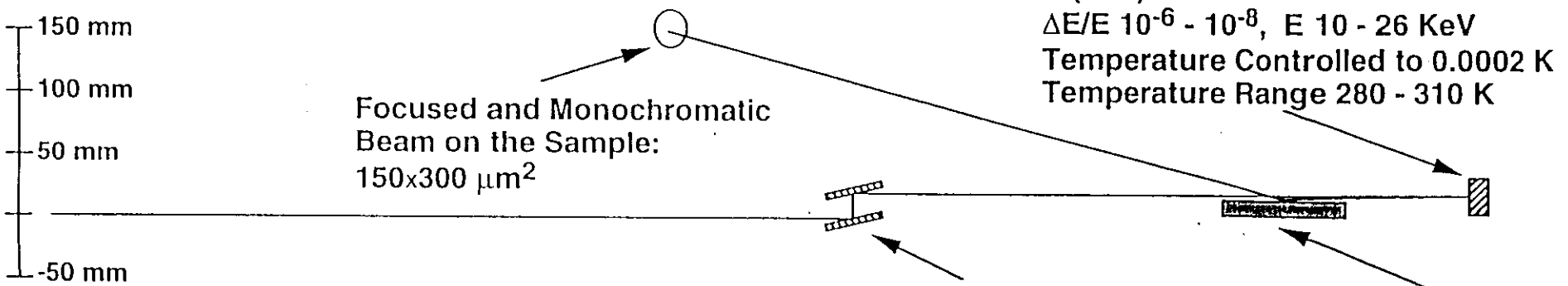


Energy Transfer Change: $\frac{\Delta E}{E} = -\frac{\Delta d}{d} = \alpha \Delta T$

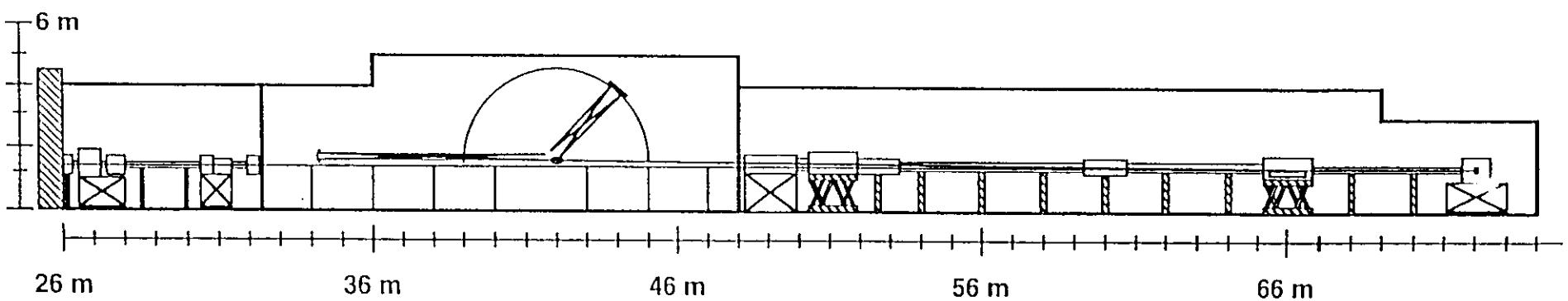
Changing the energy transfer by varying the temperature of the Mono.

Inelastic X-ray Scattering Beamline at the ESRF: BL21-ID16

Monochromatization Beam Path



Schematic Beamline Lay-out: Side view



White Beam Hutch:
Selects Undulator Central Cone Radiation

Sample Hutch:
Inelastic X-ray Scattering with Spherical Analyser Crystals in Backscattering and Rowland geometry.
3m Radius Analyser on Vertical Arm, θ_s 0-160
7m Radius Analyser on Horizontal Arm, θ_s 0-13

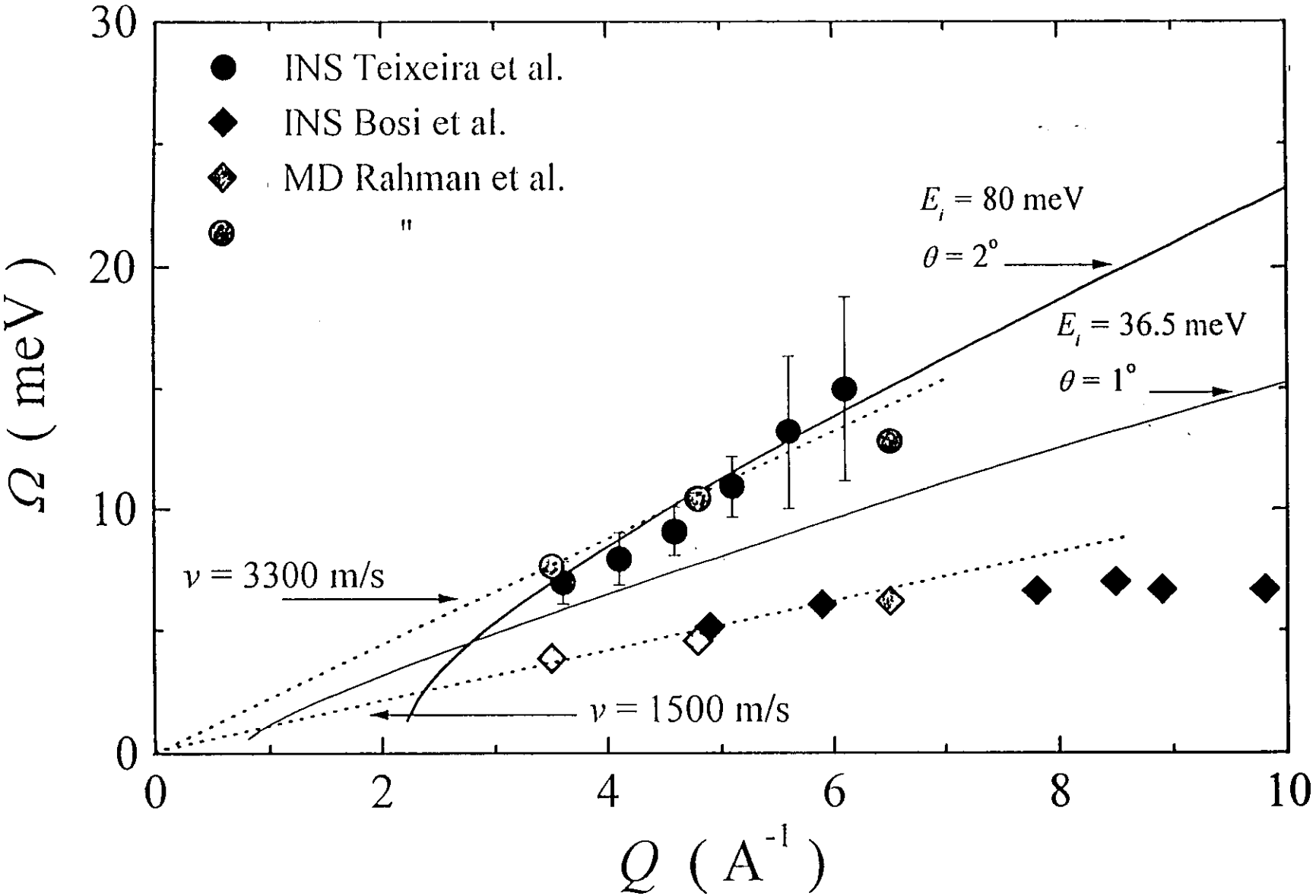
Monochromator Hutch:
Si(111) DC Pre-monochromator
HR Si(hhh) Backscattering Monochromator
Focusing Toroidal Mirror

High Frequency Collective Dynamics in Water

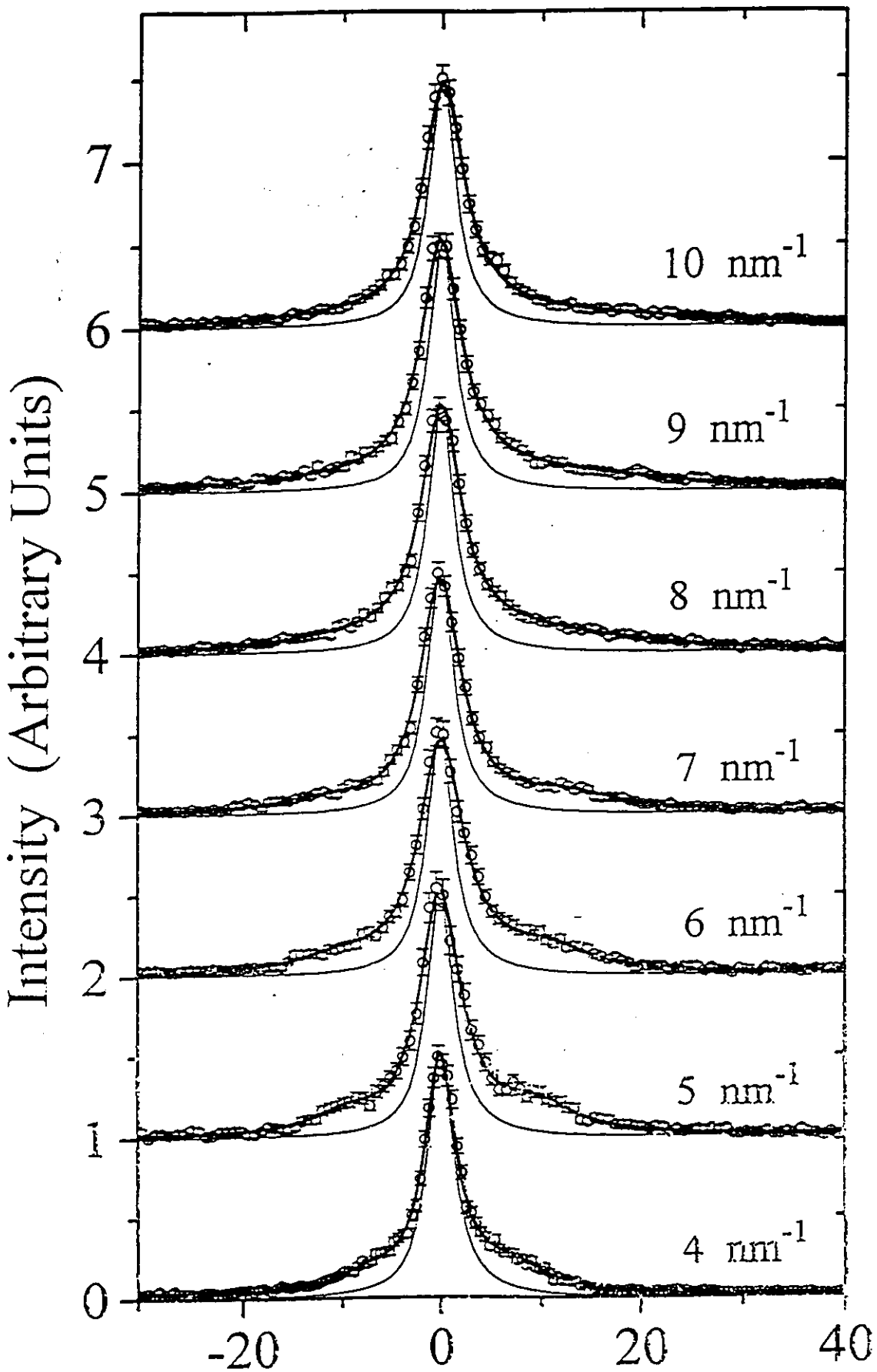
Motivation

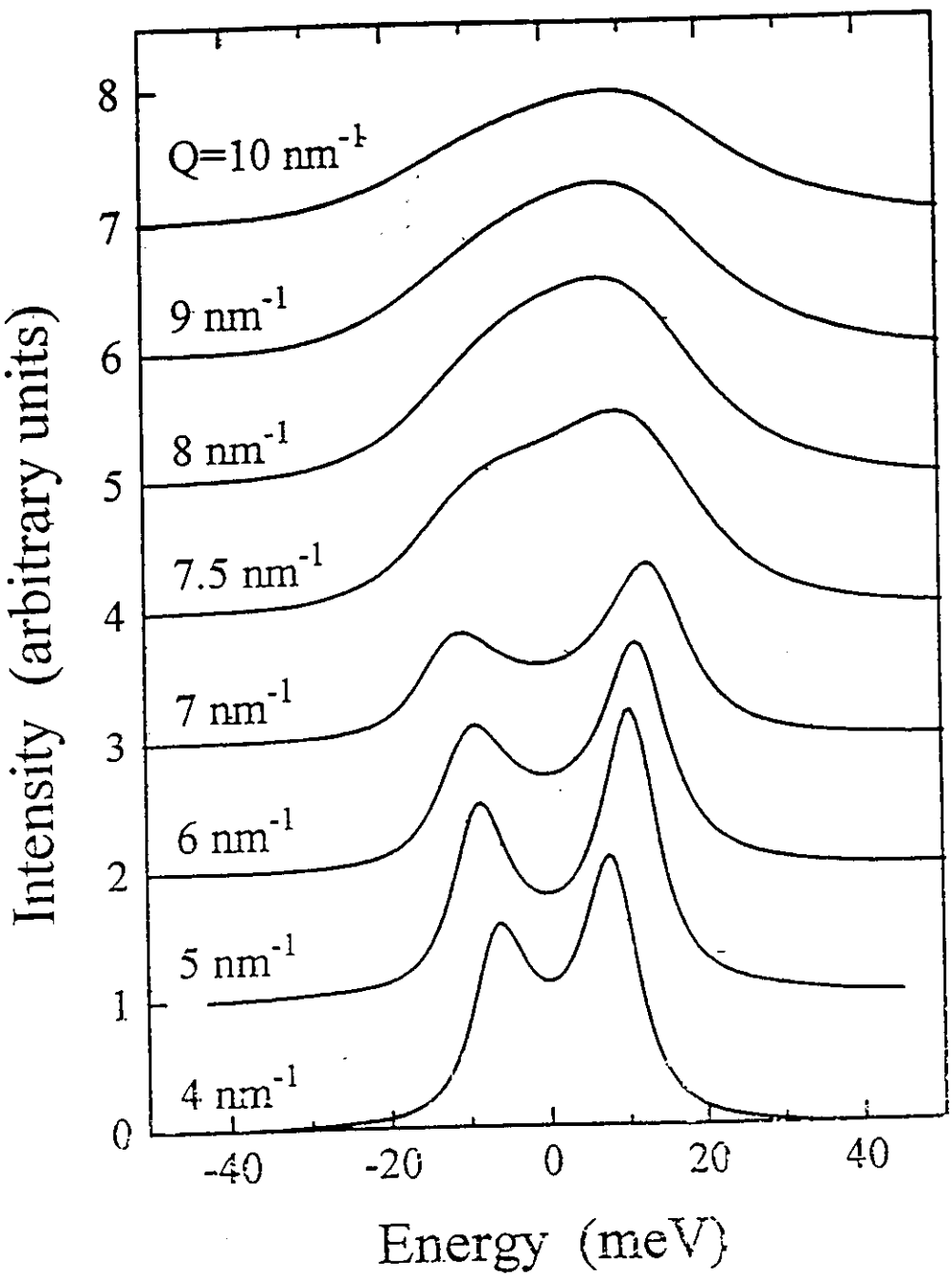
General: Are there propagating collective excitations in disordered systems, when $Q \sim 2\pi/d$?

- Controversial neutron experiments
- Molecular Dynamics (MD) studies
  - 2 different speeds of sound?
  - Existence of fast sound in water?
  - Nature of excitations: hydrogen bonds vs. whole molecule
  - Water versus Ice


INS Teixeira et al.
INS Bosi et al.
MD Rahman et al.
"
E_i = 80 meV
θ = 2°
E_i = 36.5 meV
θ = 1°
v = 3300 m/s
v = 1500 m/s
Ω (meV)
Q (A^{-1})
0
10
20
30
0
2
4
6
8
10

Liquid H_2O at +4°C

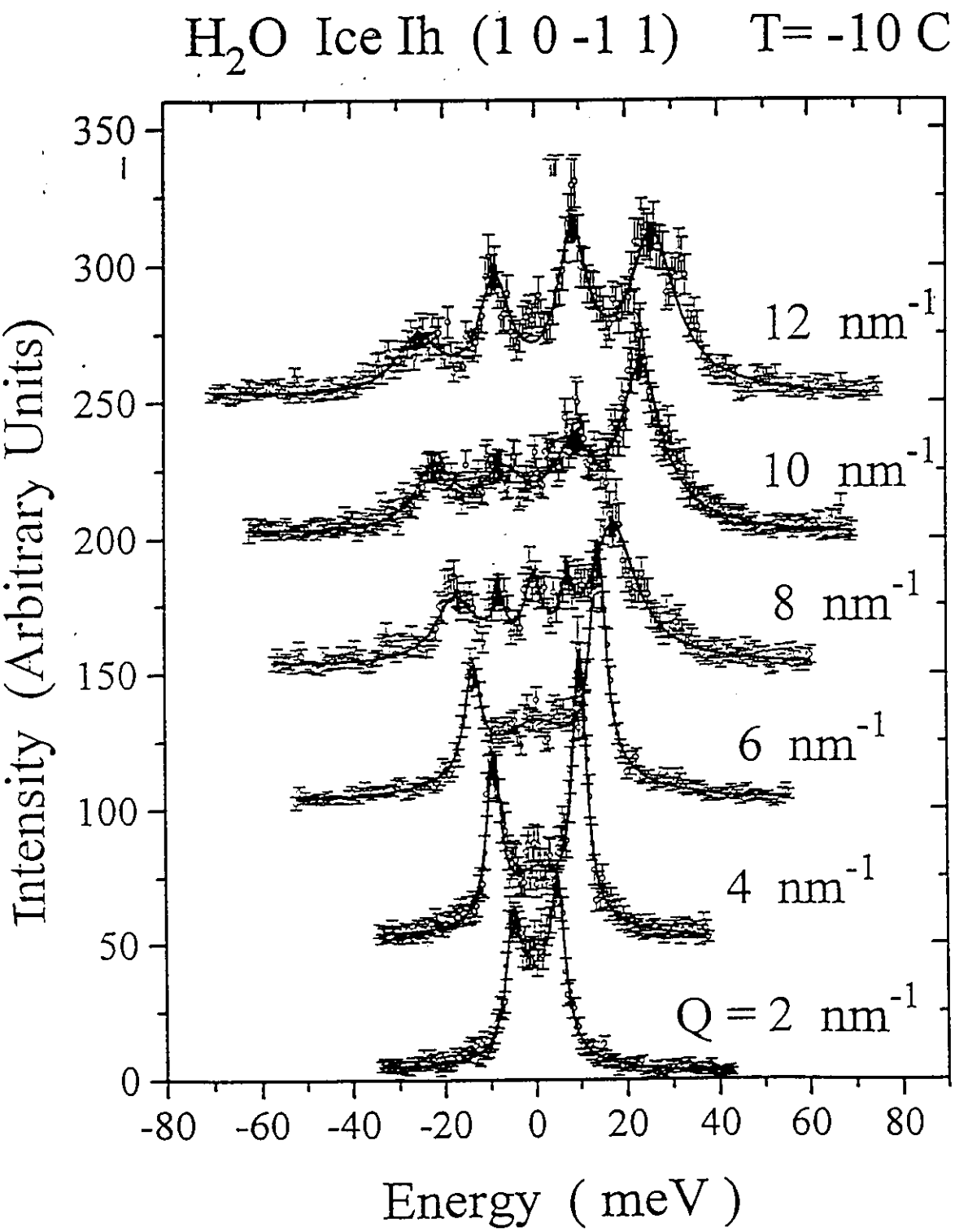


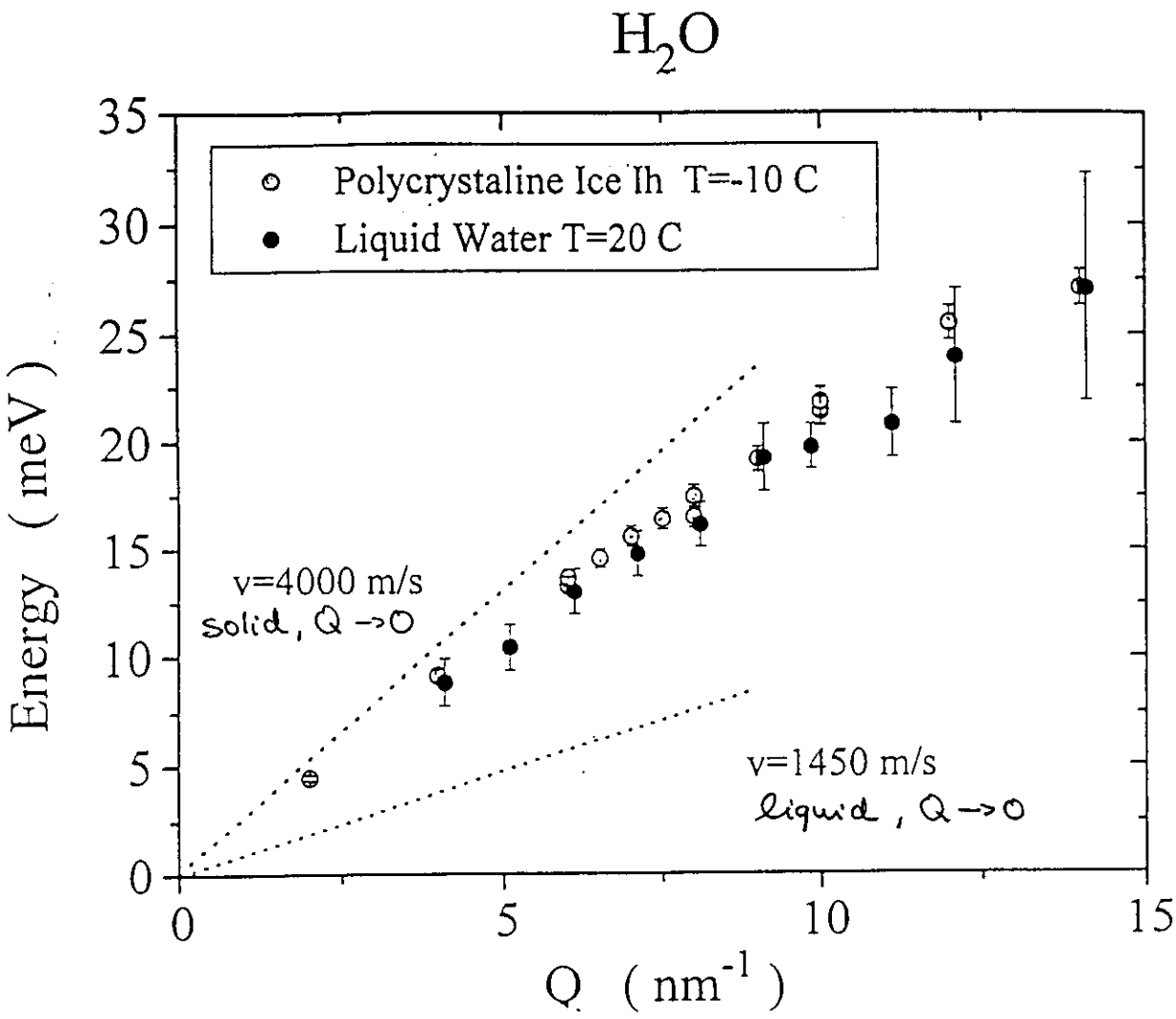


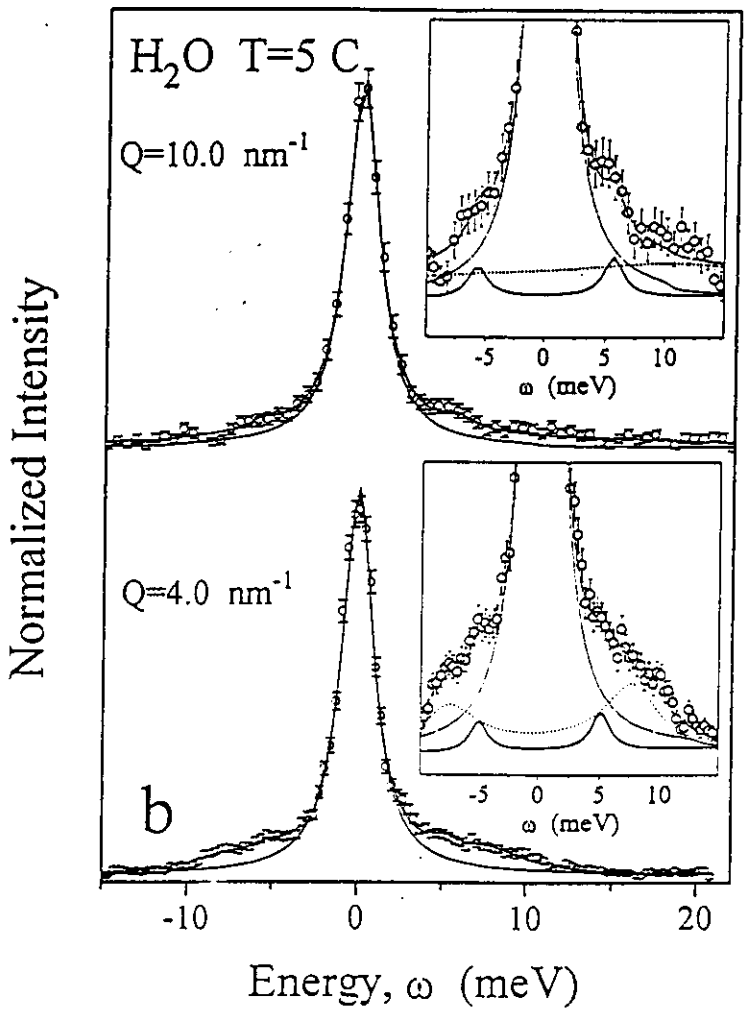
Fitting Function DHO:

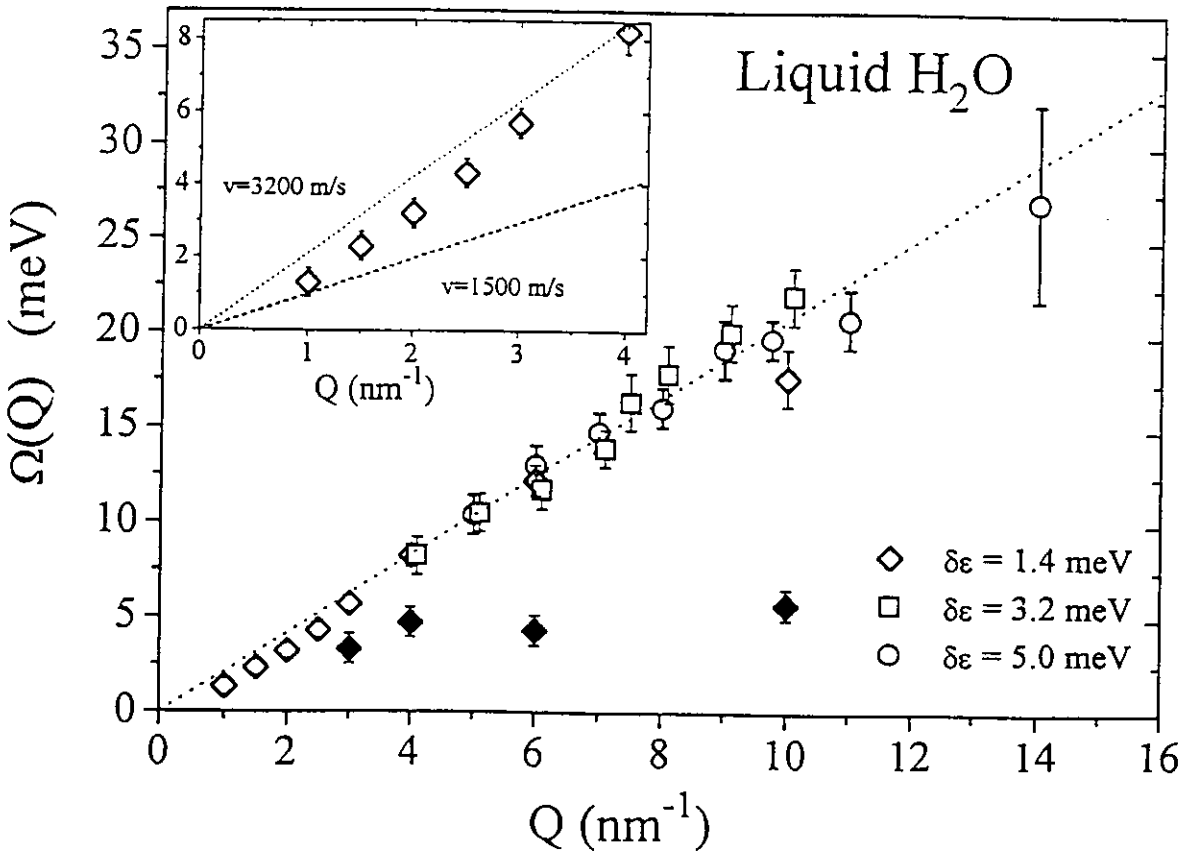
$$I_0(q) \cdot \frac{\Gamma_0(q)^2}{\Gamma_0(q)^2 + \omega^2} +$$

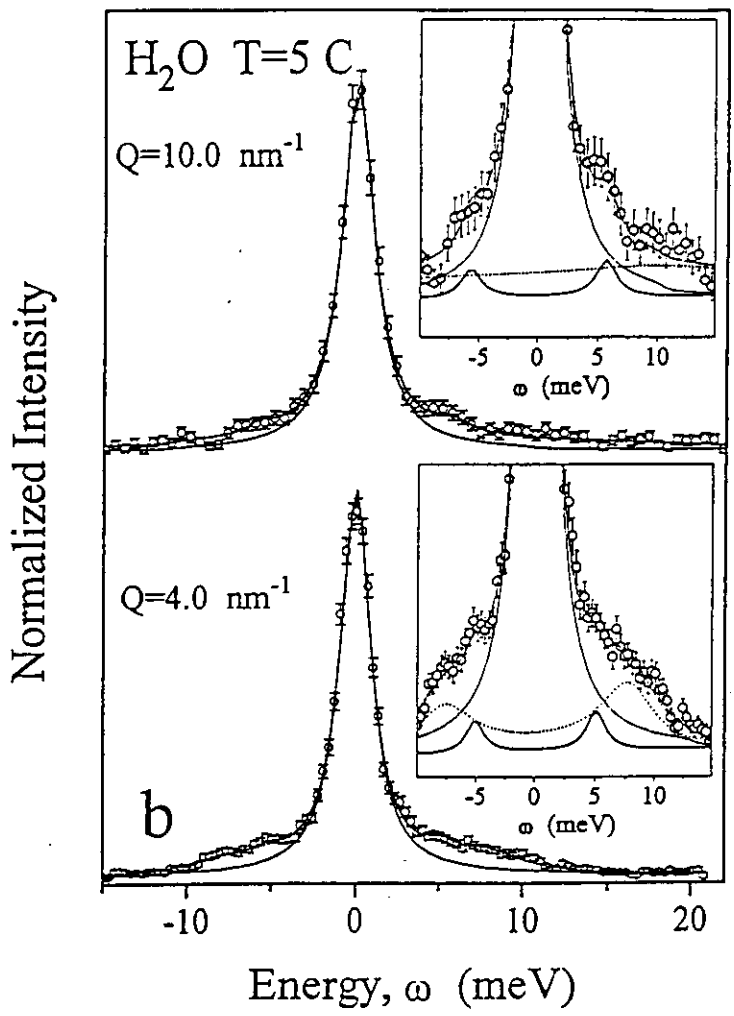
$$[n(\omega)+1] \cdot I(q) \frac{\omega \Gamma(q)^2 \Omega(q)}{[\Omega(q)^2 - \omega^2]^2 + \Gamma(q)^2 \omega^2}$$

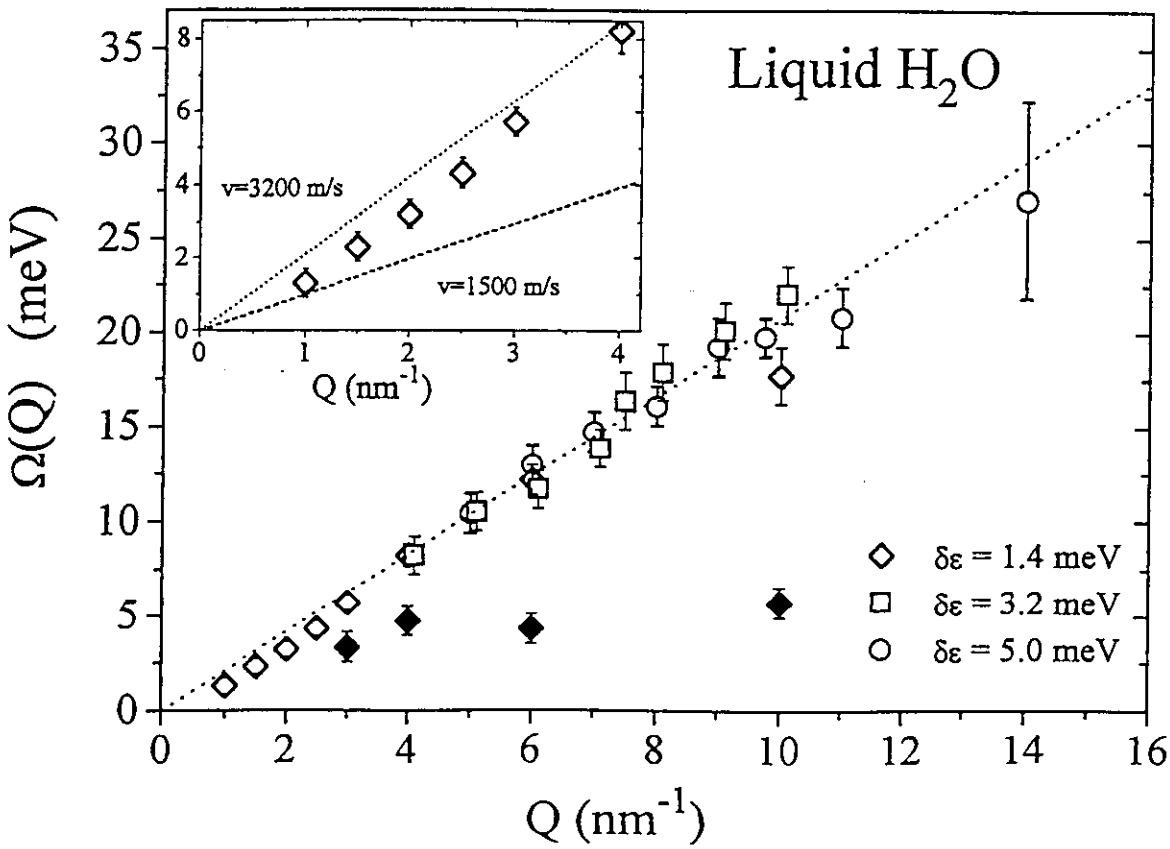

H2O Ice Ih (1 0 -1 1) T= -10 C
Intensity (Arbitrary Units)
Energy (meV)
12 nm-1
10 nm-1
8 nm-1
6 nm-1
4 nm-1
Q = 2 nm-1
350
300
250
200
150
100
50
0
-80
-60
-40
-20
0
20
40
60
80


H_2O
Polycrystaline Ice Ih T=-10 C
Liquid Water T=20 C
v=4000 m/s
solid, Q ->0
v=1450 m/s
liquid, Q->0
Energy (meV)
Q (nm^{-1})
0
5
10
15
20
25
30
35


H2O T=5 C
Q=10.0 nm-1
Q=4.0 nm-1
b
Normalized Intensity
ω (meV)
Energy, ω (meV)


Liquid H2O
v=3200 m/s
v=1500 m/s
Q (nm-1)
Ω(Q) (meV)
δε = 1.4 meV
δε = 3.2 meV
δε = 5.0 meV


H2O T=5 C
Q=10.0 nm-1
Q=4.0 nm-1
b
ω (meV)
Normalized Intensity
Energy, ω (meV)


Liquid H2O
v=3200 m/s
v=1500 m/s
Q (nm-1)
Ω(Q) (meV)
δε = 1.4 meV
δε = 3.2 meV
δε = 5.0 meV

Conclusions

• Confirm the existence of fast sound in water.

• Absence of large isotope shift.

=> collective motion of whole molecule

• Equivalence of the speed of sound in solid and liquid water.

=> Fast sound corresponds to the infinite frequency sound velocity, i.e. the solid-like dynamics well above any relaxation process.

• Transition from fast sound towards normal sound between Q = 1 and $4nm^{-1}$.

=> Relaxation process with a typical relaxation time $\tau \sim 0.6$ ps.

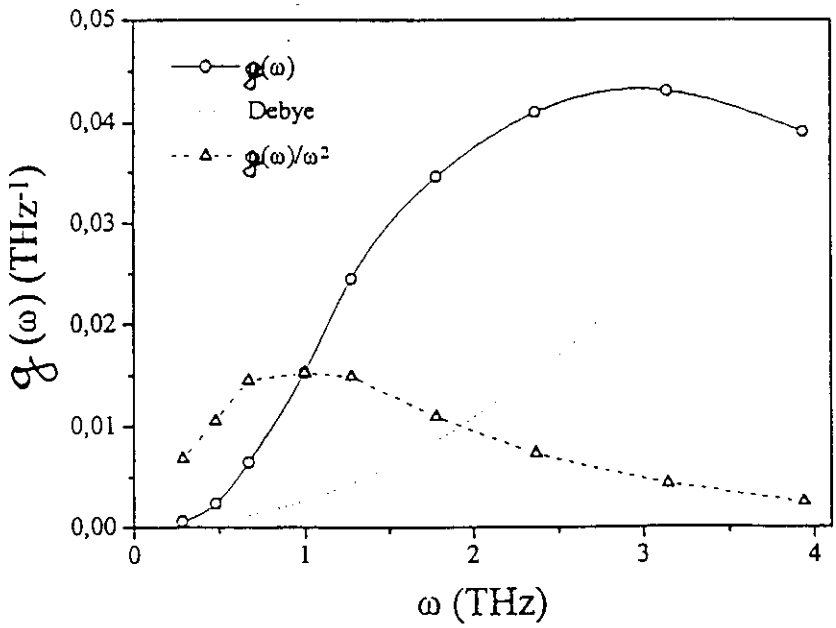
High frequency collective dynamics in glasses

Questions to address:

- Origin of the anomaly in the temperature dependence of the specific heat

$$C_v(T) = 3Nk_B \int g(\omega) \left(\frac{\omega}{k_B T}\right)^2 \frac{\exp(\omega/k_B T)}{\left(\exp(\omega/k_B T) - 1\right)^2} d\omega$$

- Incoherent light-and neutron measurements indicate that the anomaly is due to an excess in the vibrational density of states (Boson peak).

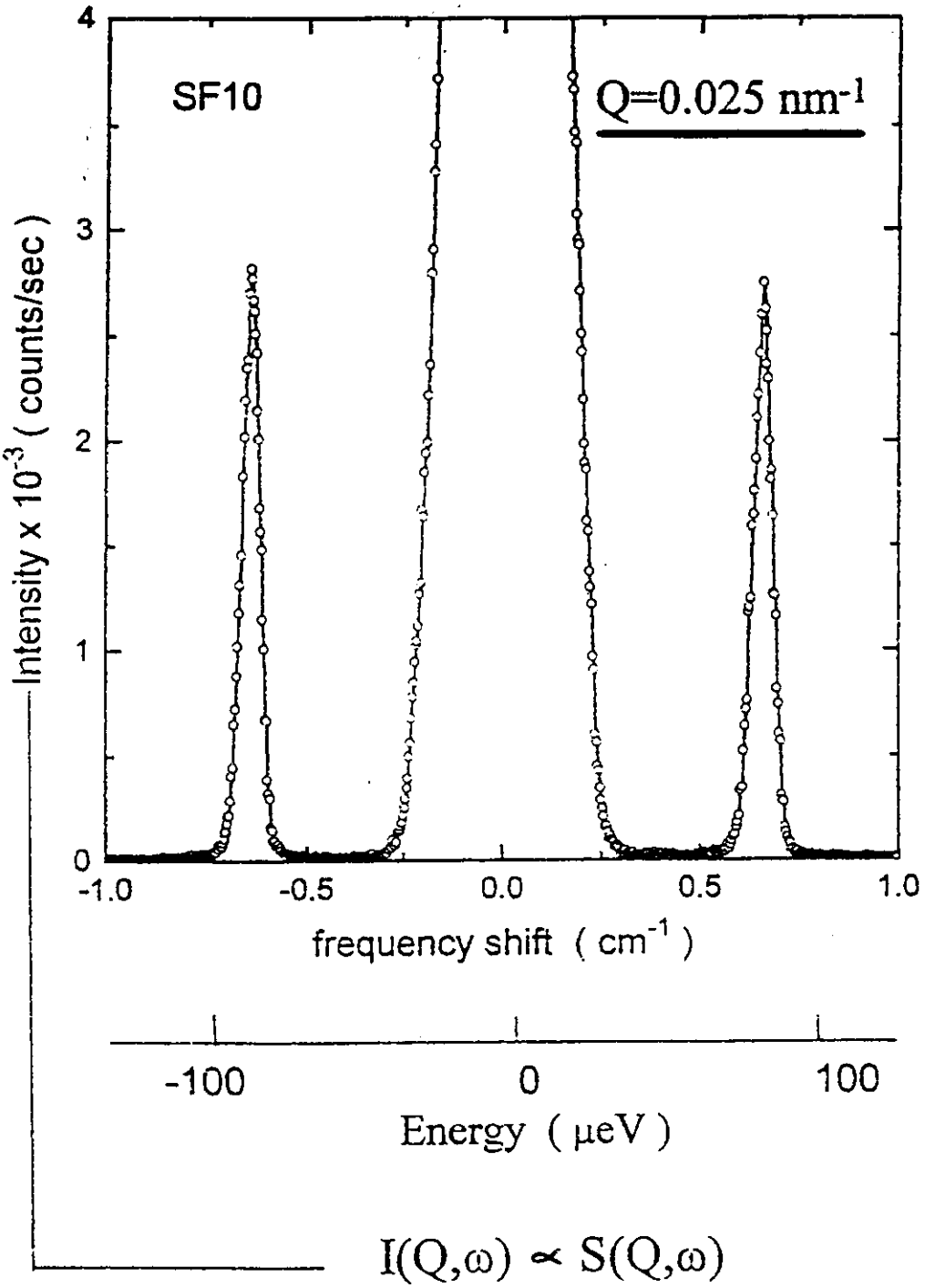


- Nature of these excitations

- Dynamics of the liquid-to-glass transition, definition of the glass transition temperature Tg.

Brillouin Light Scattering (BLS)

SiO_2 : Pb



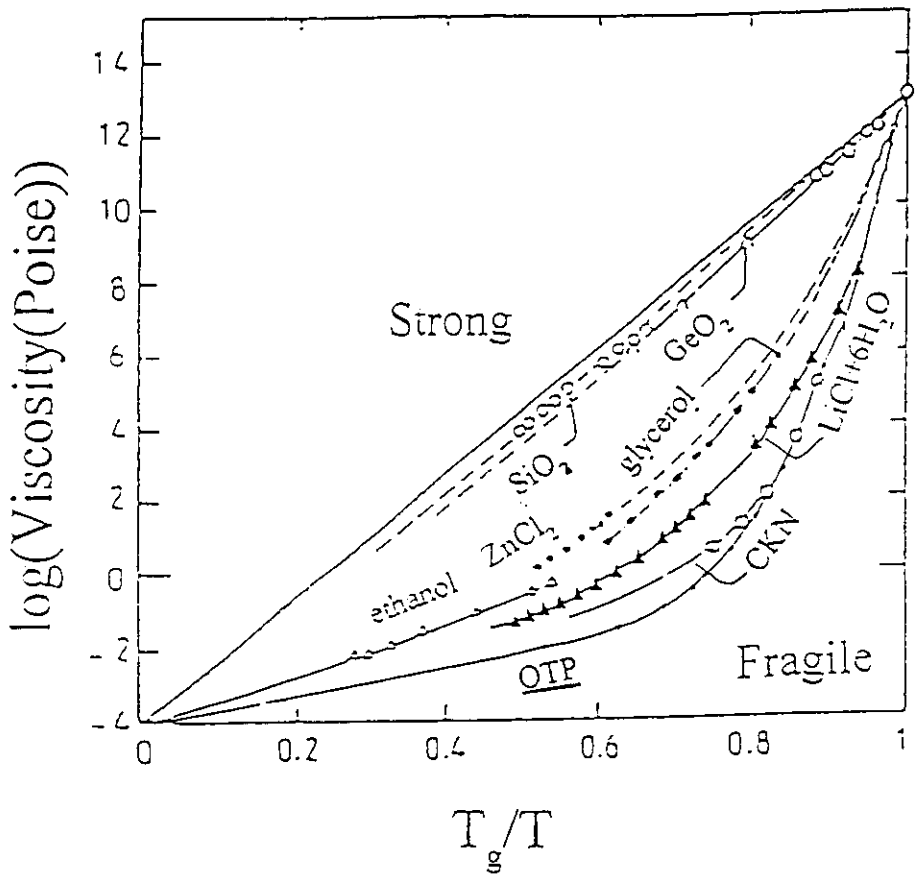
$$I(Q,\omega) \propto S(Q,\omega)$$

Introduction

Cooling down quickly a liquid the crystallization can be avoied and the system becomes a glass (glass-former).

Classification:

C. A. ANGELL 1985



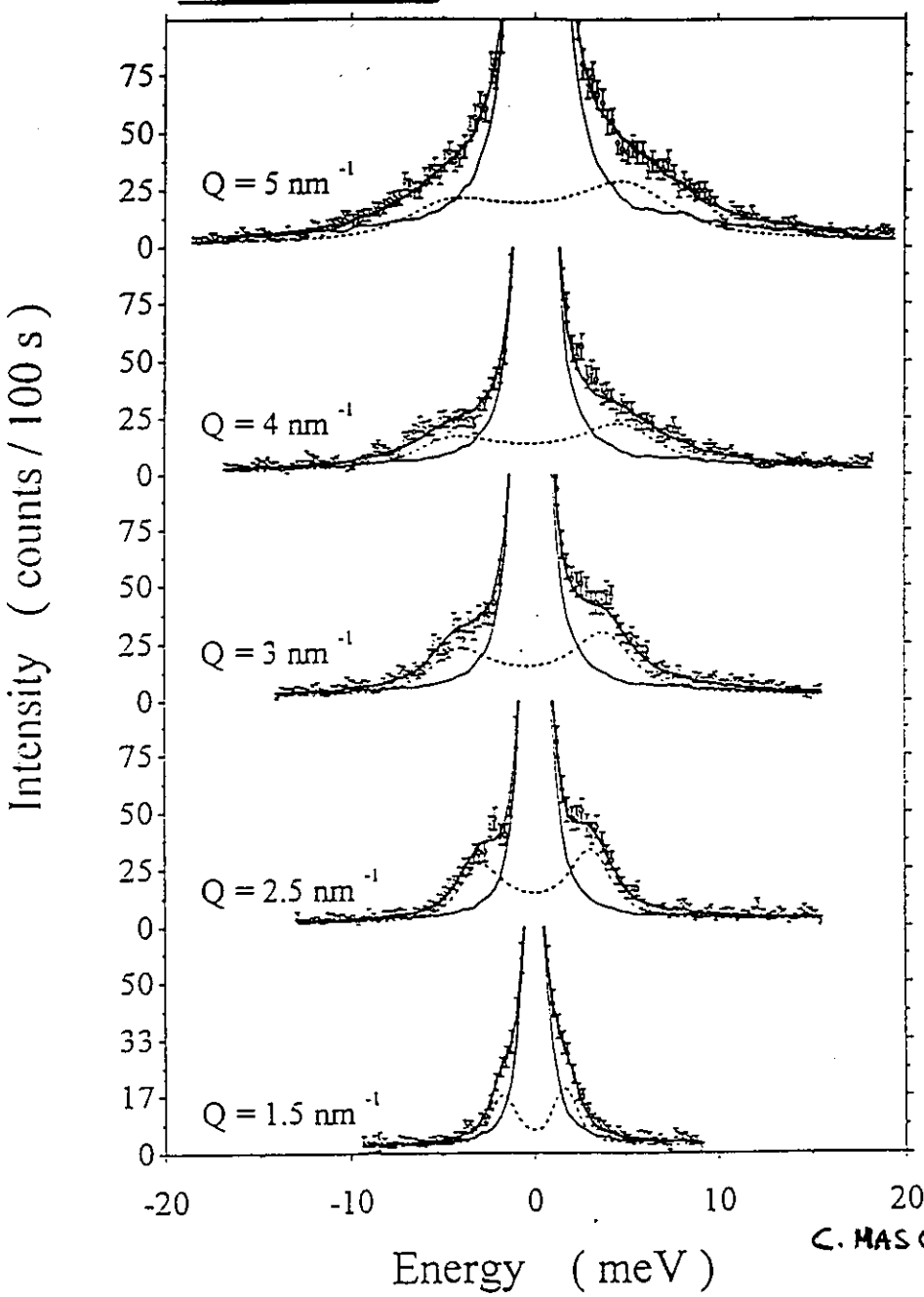
The dynamics of glass-forming systems is not well established , especially at the microscopic scale, because of the lack of experimental investigations.

The Mode Coupling Theory (MCT) describes from a microscopic point of view the liquid to glass transition.

IXS Spectra

Si(11 11 11) ΔE=1.5 meV ΔQ=0.3 nm^{-1}

o-Terphenyl T=156 K (glass)

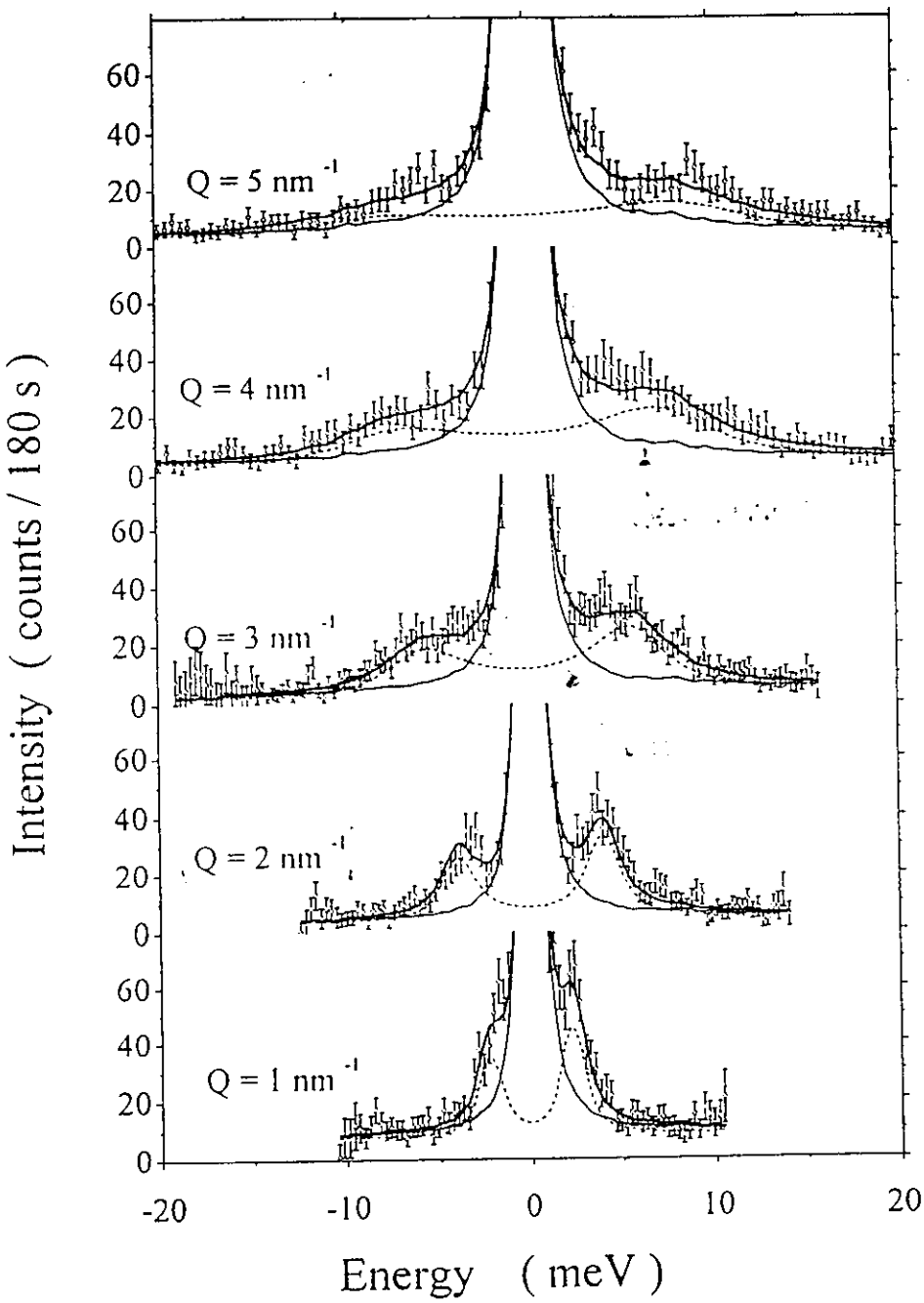


C. MASCIOVECCHIO ET AL 1997

IXS Spectra

Si (11 11 11) ΔE=1.5 meV ΔQ=0.3 nm^{-1}

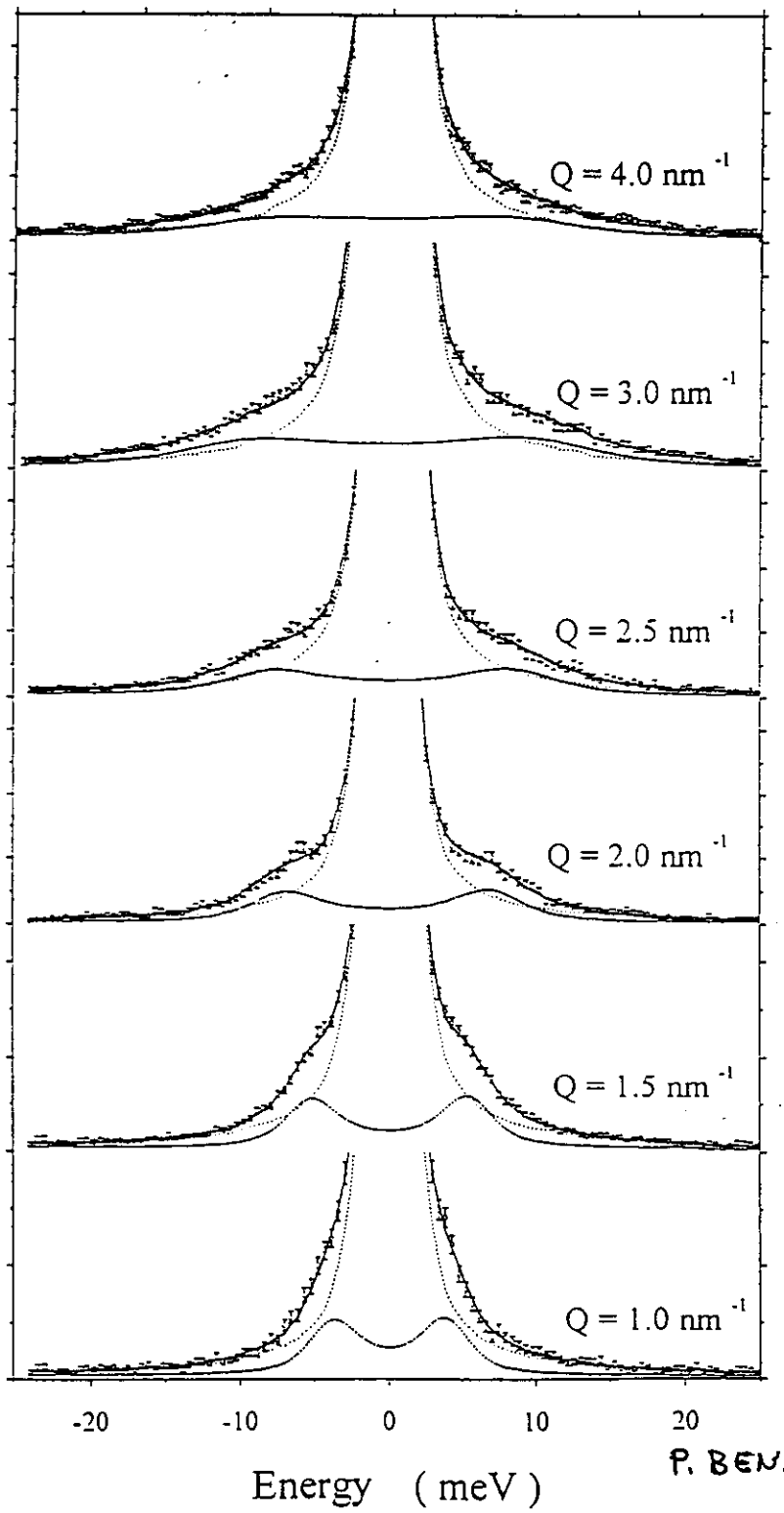
Glycerol T=175 K (glass)



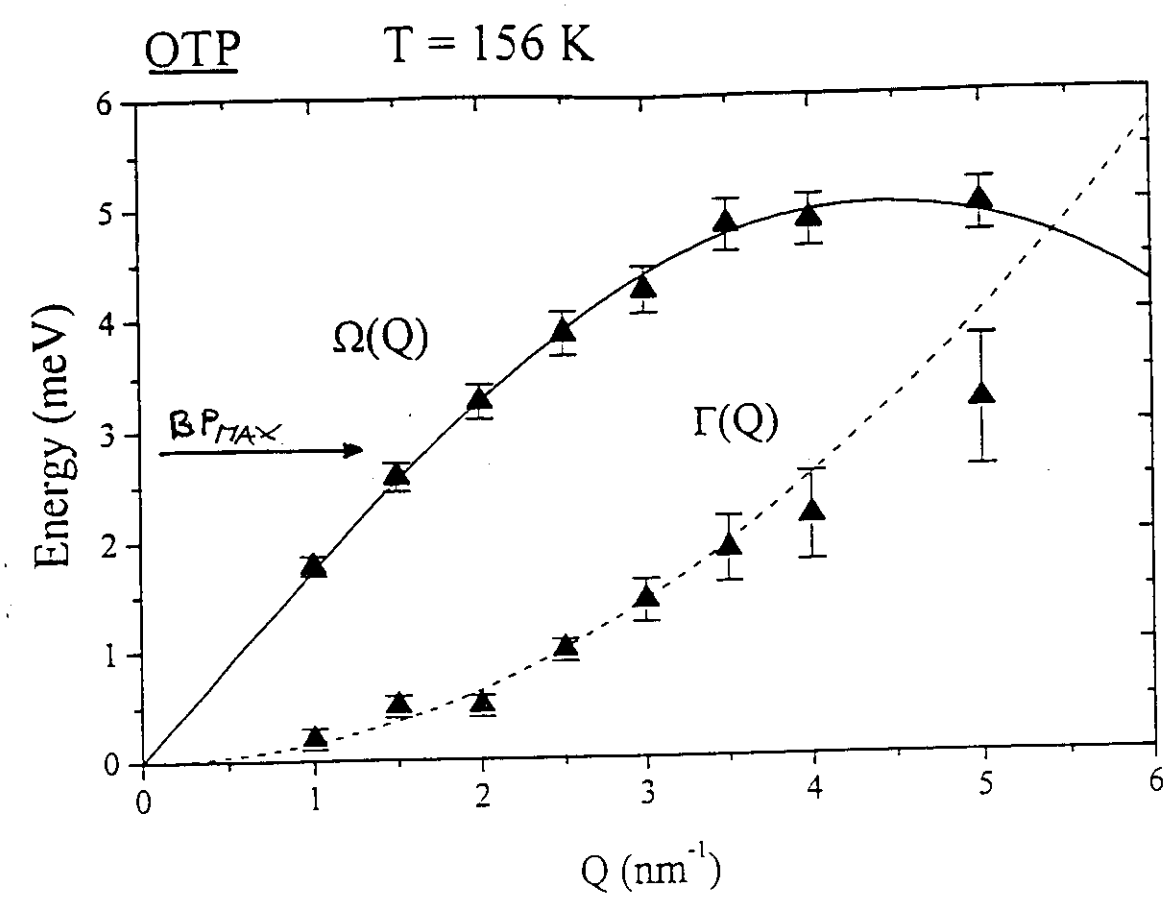
IXS Spectra

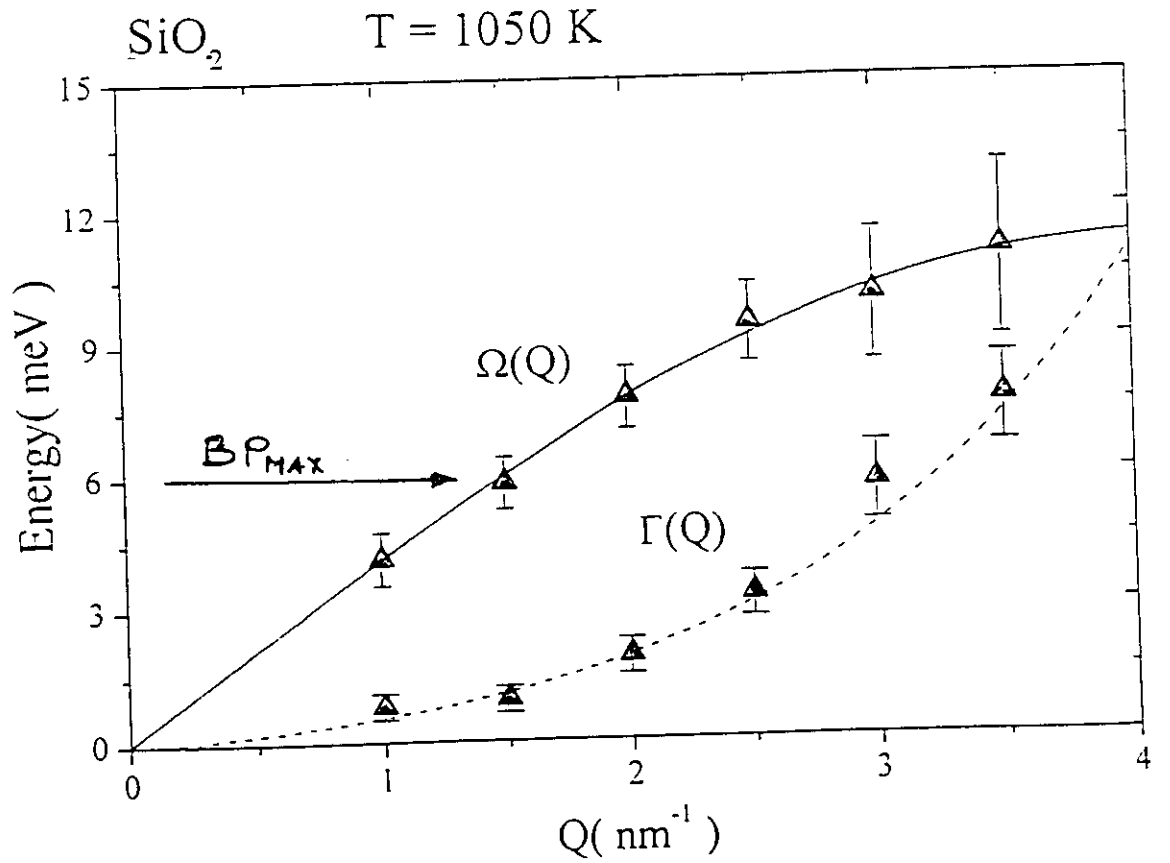
Si(9 9 9) ΔE=3.2 meV ΔQ=0.3 nm^{-1}

$V\text{-}SiO_2$ T=1050 K (glass)



P. BENASSI ET AL 1996



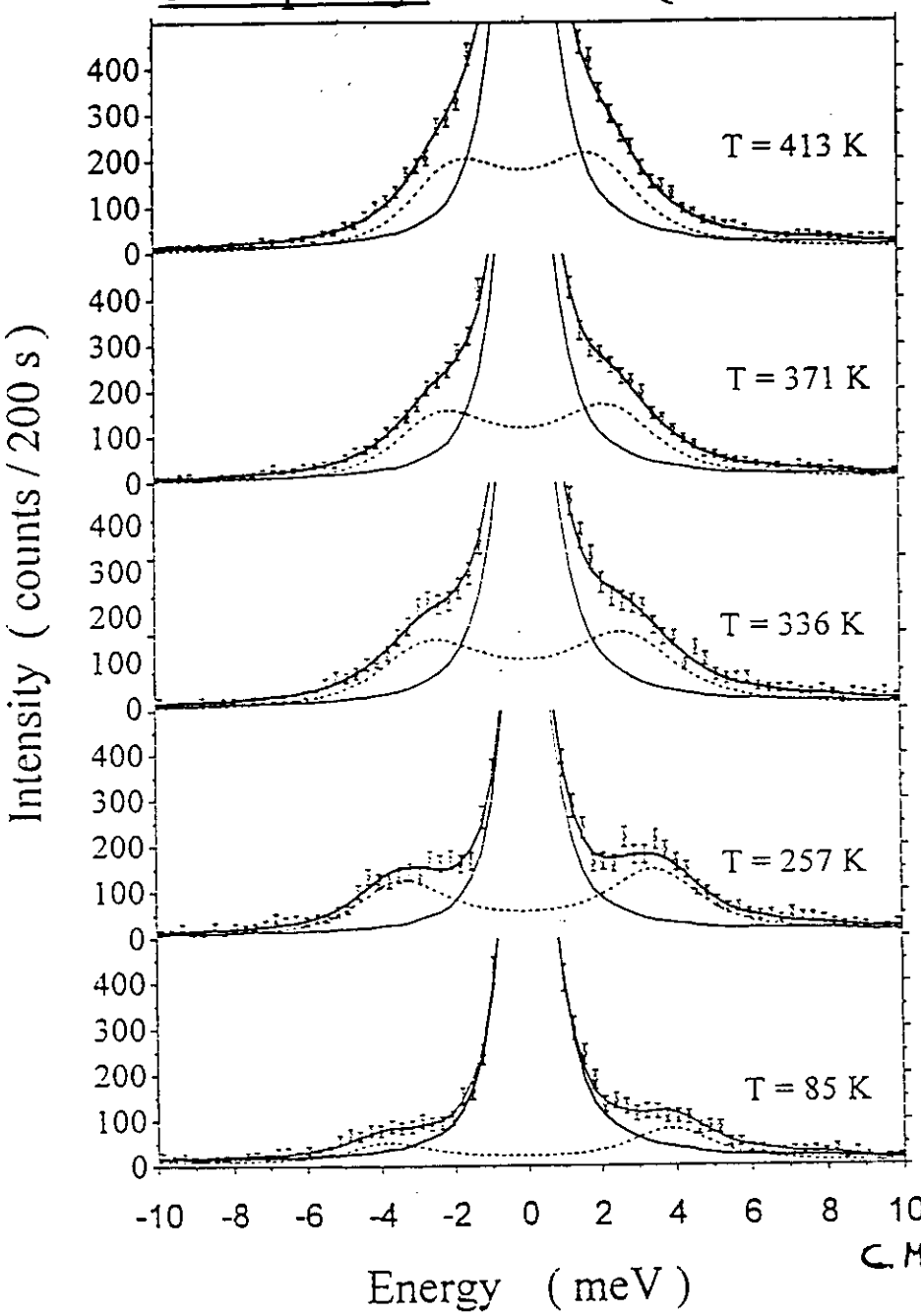


EXISTENCE OF PROPAGATING COLLECTIVE EXCITATIONS IN THE SAME ENERGY RANGE OF THE "BOSON PEAK" ▽ ○

IXS Spectra

Si (11 11 11) ΔE=1.5 meV ΔQ=0.3 nm^{-1}

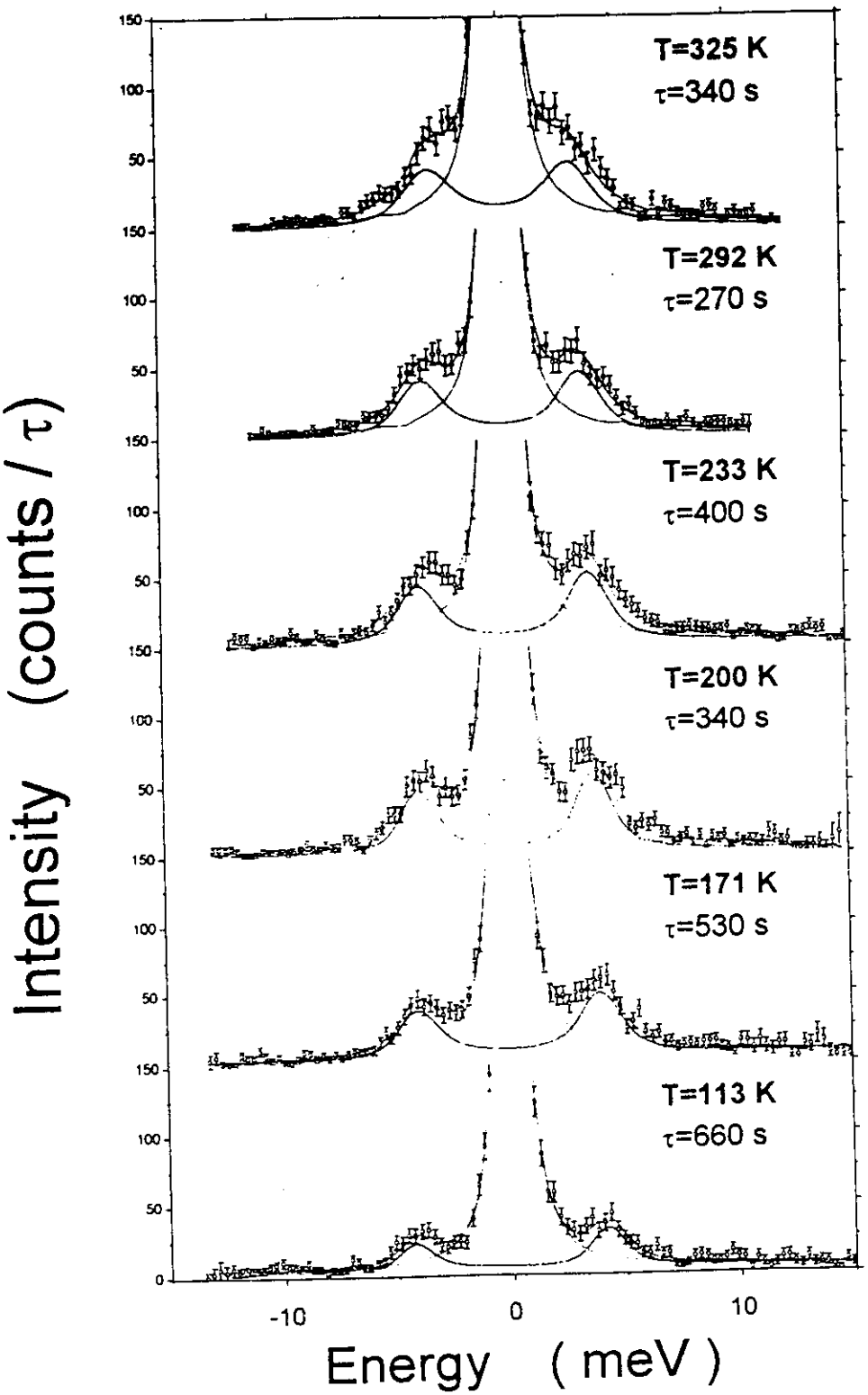
o-Terphenyl $Q = 2.5$ nm^{-1}



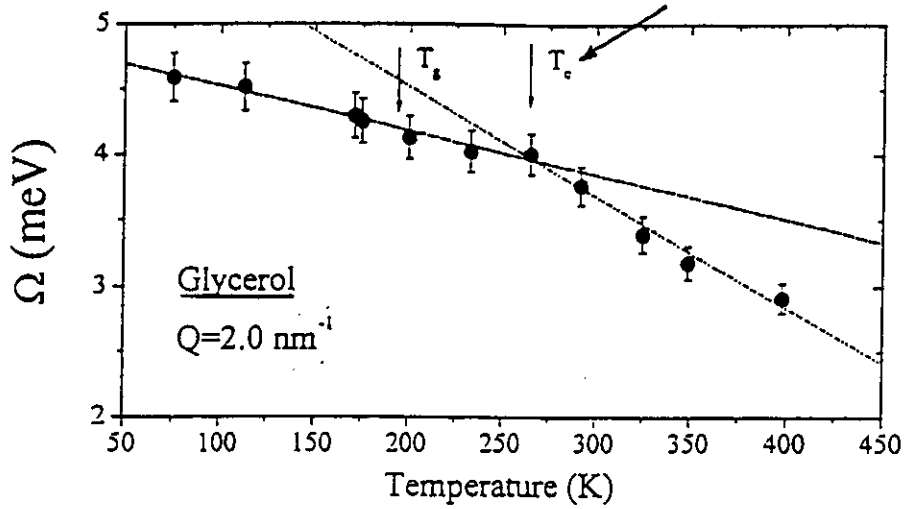
C. MASCIOVECCHIO ETAL. 1997

Glycerol

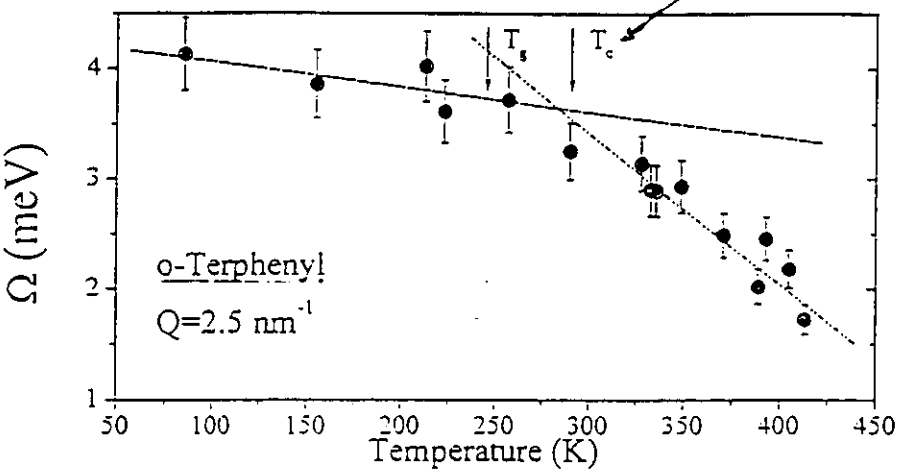
Q = 2 nm^{-1}

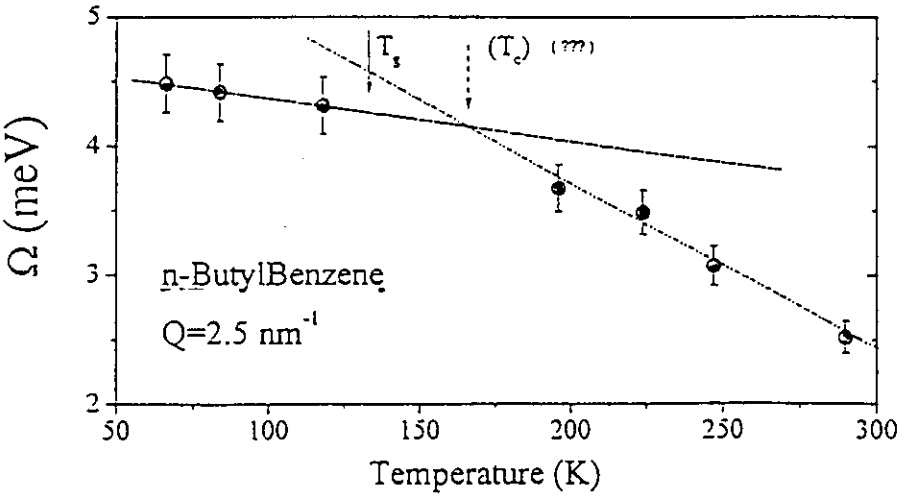


(ε" , Lunkenheimer et al. 1996)



(Raman depol , Steffen et al. 1994)





$\frac{T_c}{T_g} \approx 1.2$

BREAK AT T_c, THE MCT CROSSOVER TEMPERATURE.

Conclusions

• Existence of collective propagating dynamics spanning the energy region of the Boson peak.

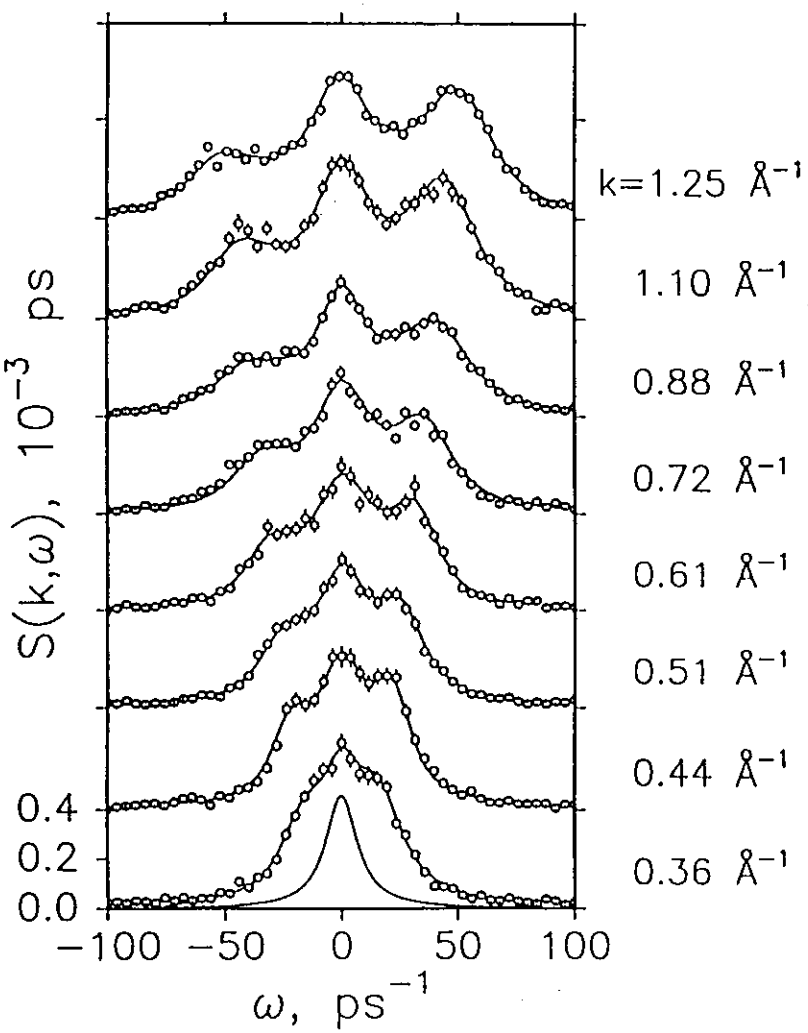
=> Boson peak must have contributions from these excitations.

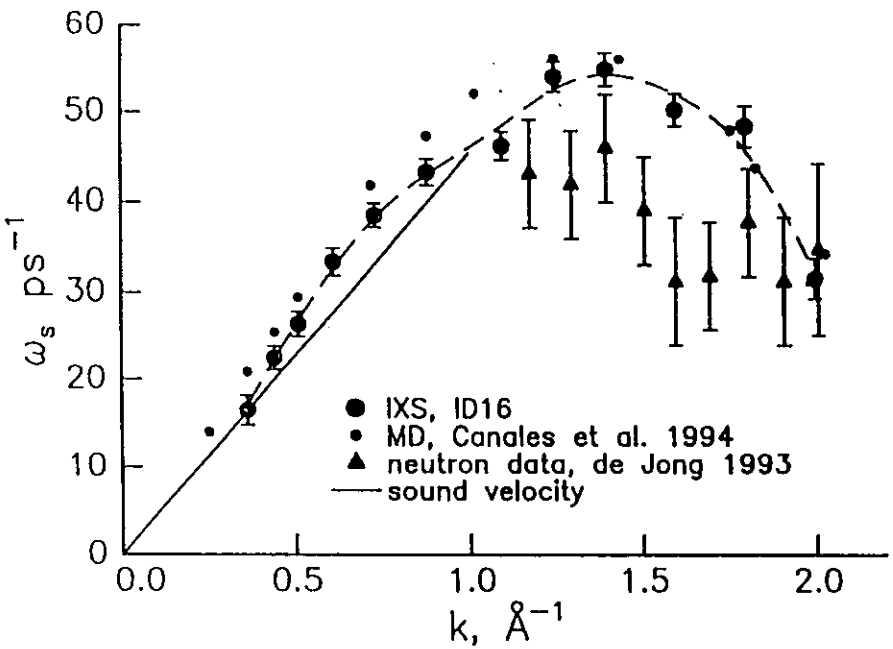
• Break in the sound velocity at a temperature $T > T_C$.

=> Microscopically, clusters of particles already "freeze" their motion at higher temperatures. Size of clusters approximately $2\pi/Q$.

Collective Dynamics in Liquid Lithium

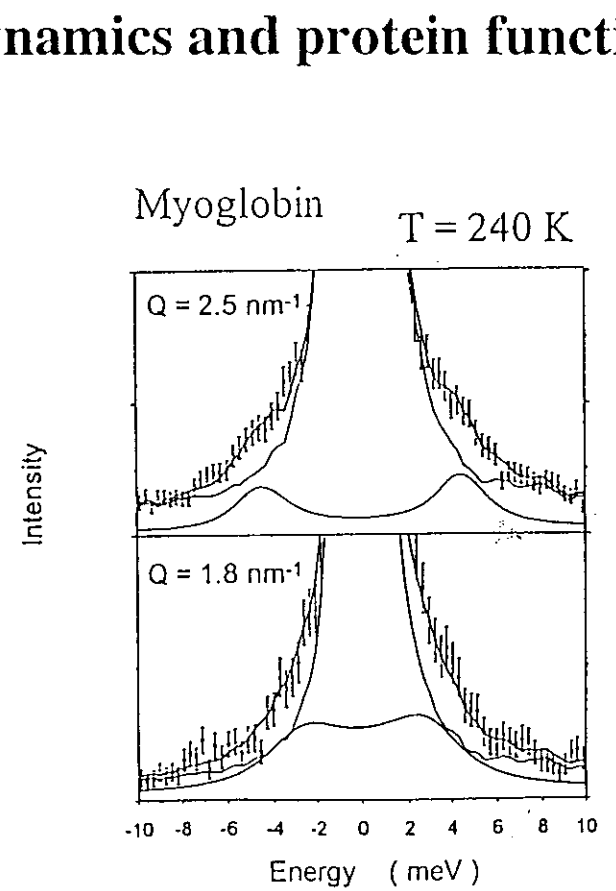
- Velocity of Sound ~ 5000 m/s

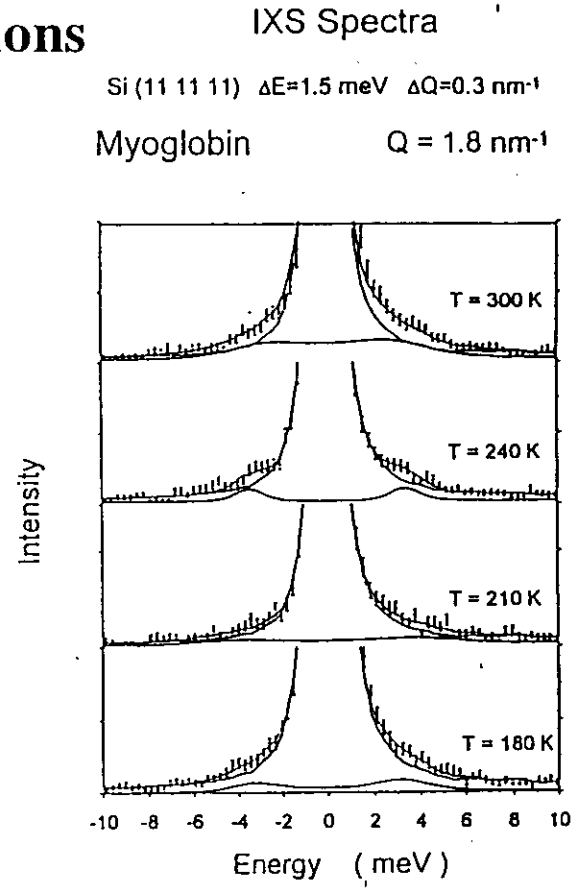




Collective Dynamics in Hydrated Proteins: Myoglobin

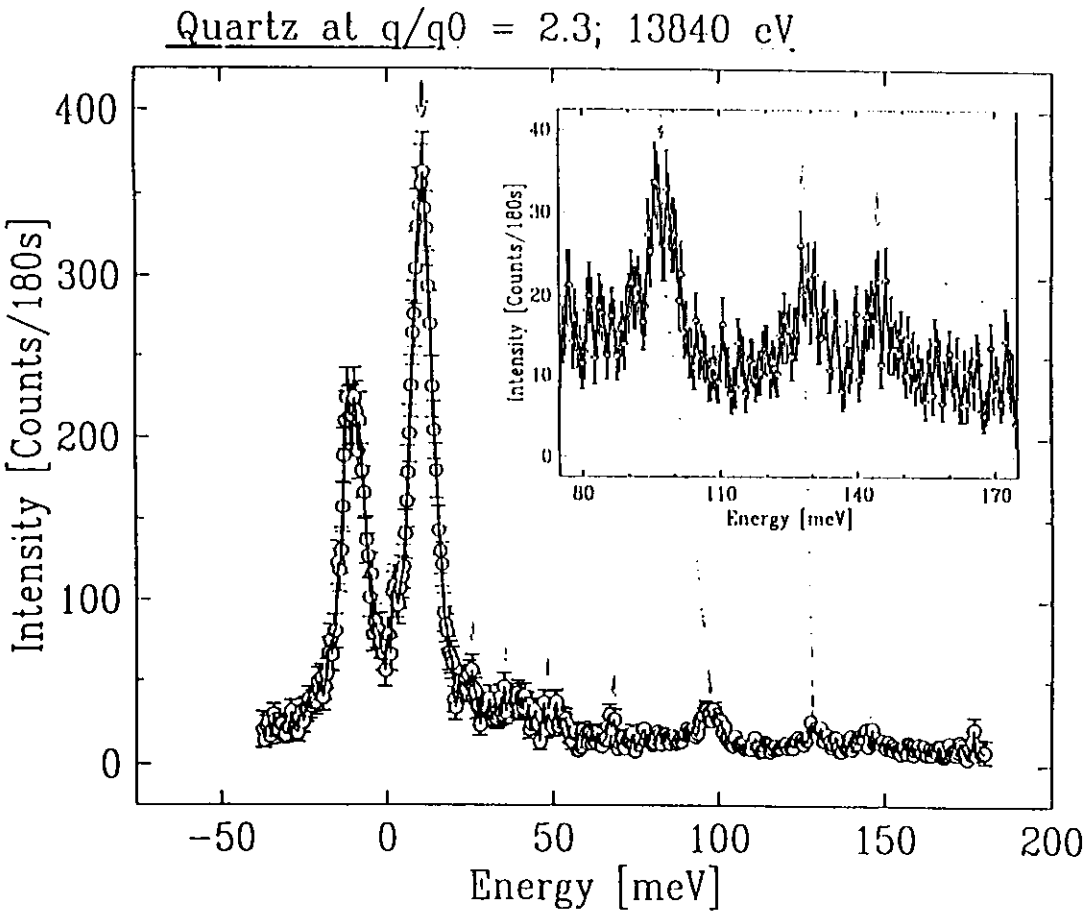
- **Existence of collective excitations**
- **Relation between dynamics and protein functions**

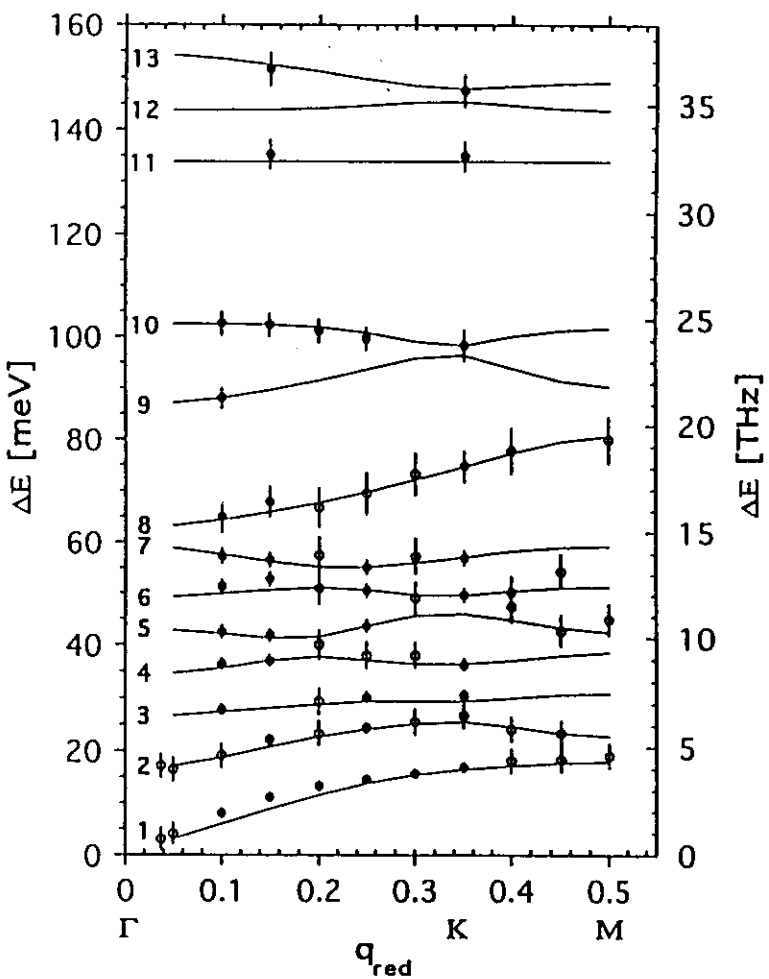




Phonon Dispersion Curves in Quartz

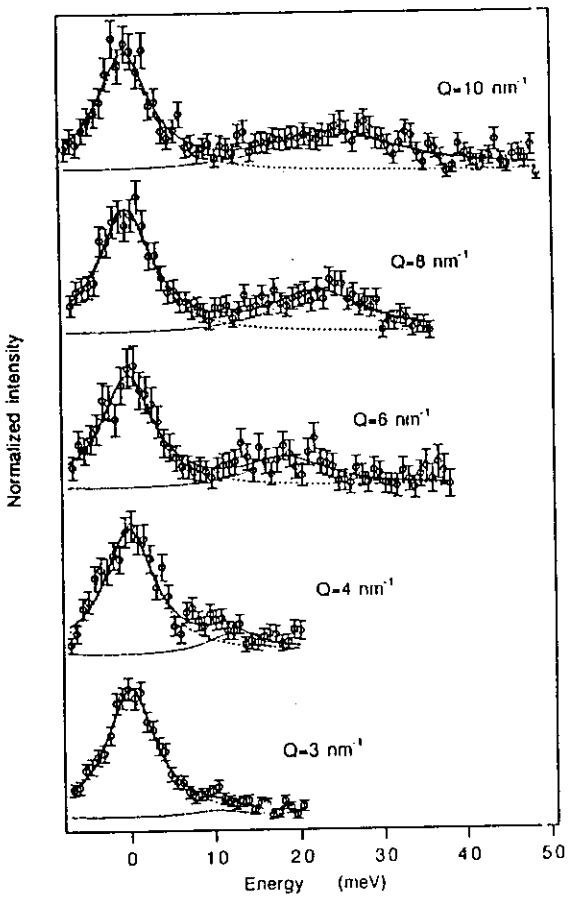
- **Basically unlimited energy transfer**

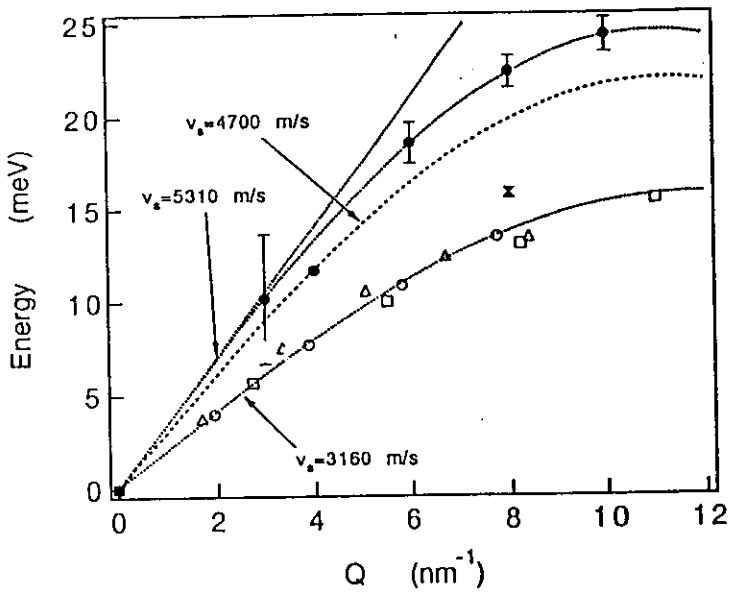




Collective dynamics of high Z materials in an Anvil cell

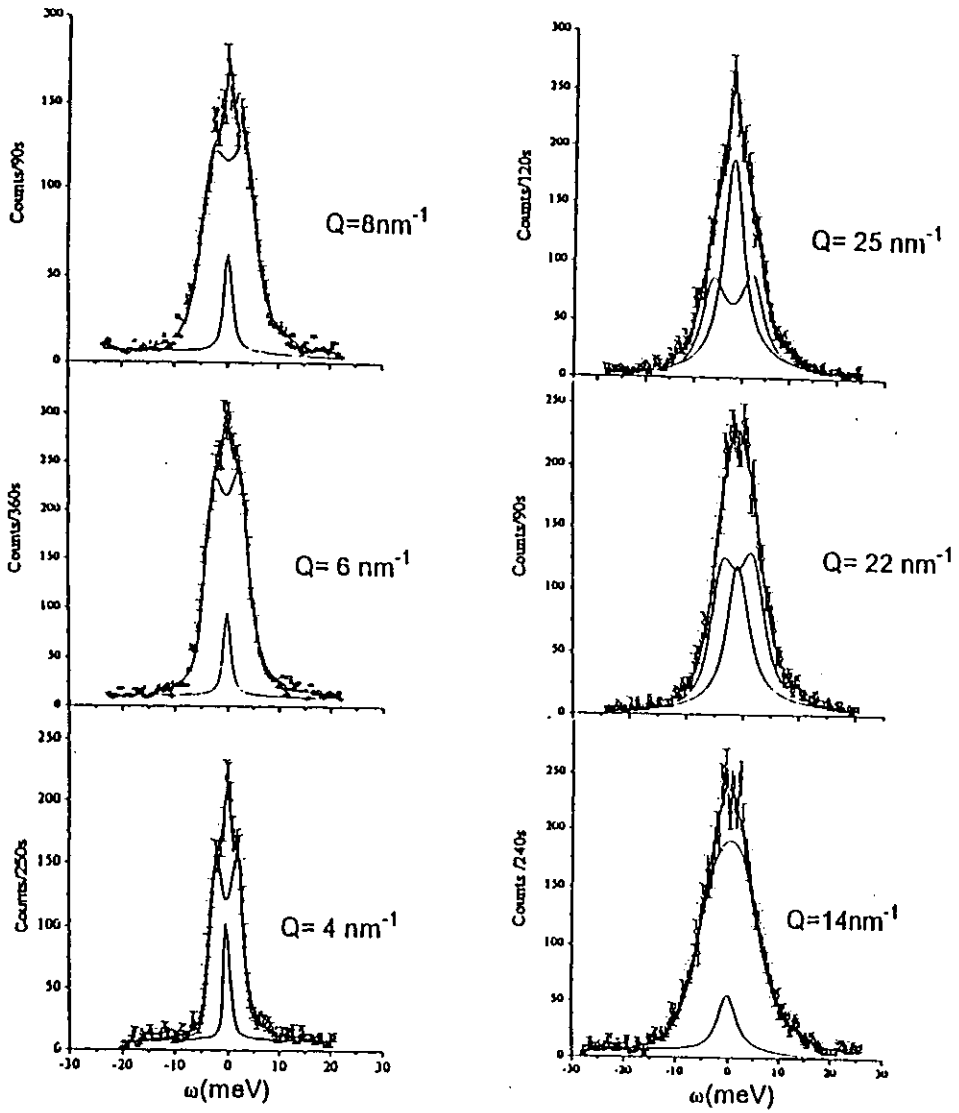
- CdTe at 11GPa
- Phase transition from the Zinc Blende to the Rock Salt structure
- Sample size in the cell: 150 μm diameter - 25 μm thick

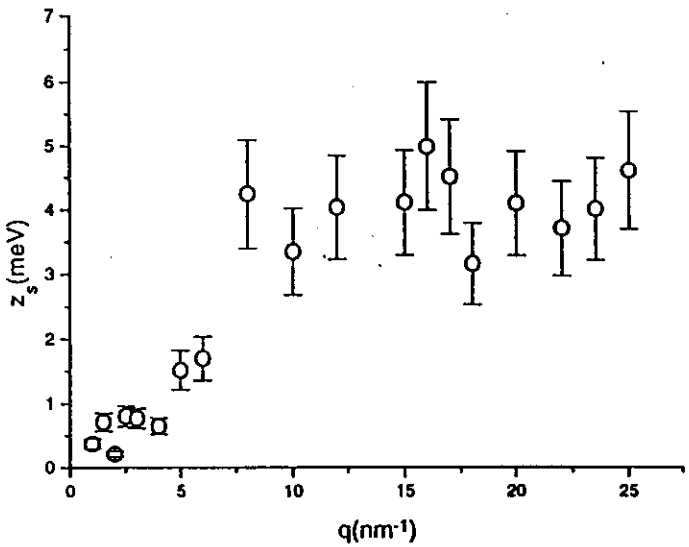


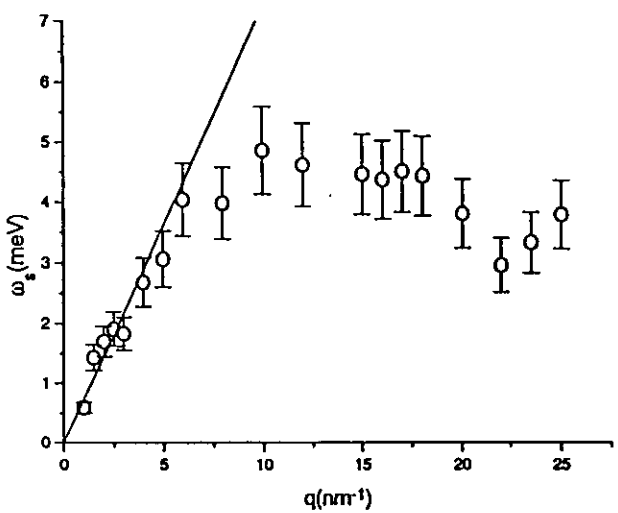


Collective dynamics of noble gases at high pressure

- Neon at 3 kbar







Summary

• IXS from collective ion excitations is a powerful complementary technique to the well established inelastic neutron spectroscopies.

- Study of liquids, glasses and gases in Q-ω space, not accessible with neutrons.

- Study of matter in extreme thermodynamical conditions. (high pressure, high/low temperature)

- Study of crystals which are only available in small sizes.

- Study of biological samples (no need for deuteration).