

Inelastic X-ray scattering from Phonons at the ESRF



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Outline

Introduction

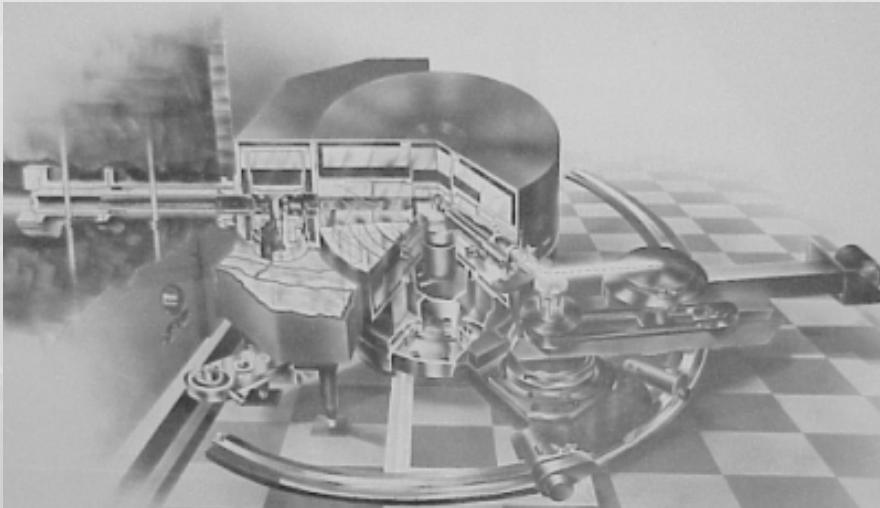
Highlights from “standard” experiments

Recent developments

- Phonon density-of-states
- Phonons at surfaces
- Polycrystalline materials -> single crystal properties
- IXS and (thermal) diffuse scattering

Outlook

Inelastic Scattering from Phonons



Brockhouse (1955)

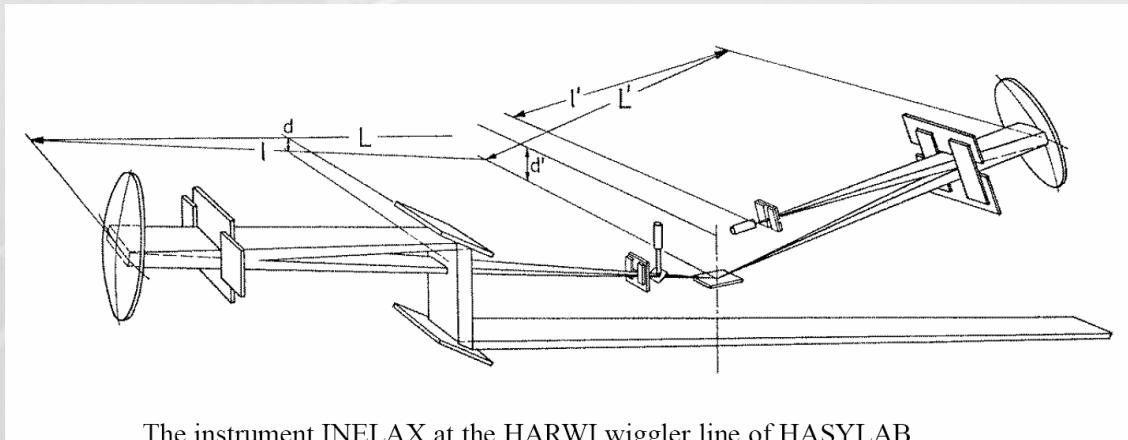
Thermal neutrons:

$$E_i = 25 \text{ meV}$$

$$k_i = 38.5 \text{ nm}^{-1}$$

$$\Delta E/E = 0.01 - 0.1$$

large beam



The instrument INELAX at the HARWI wiggler line of HASYLAB.

Burkel, Dorner and Peisl (1987)

Hard X-rays:

$$E_i = 18 \text{ keV}$$

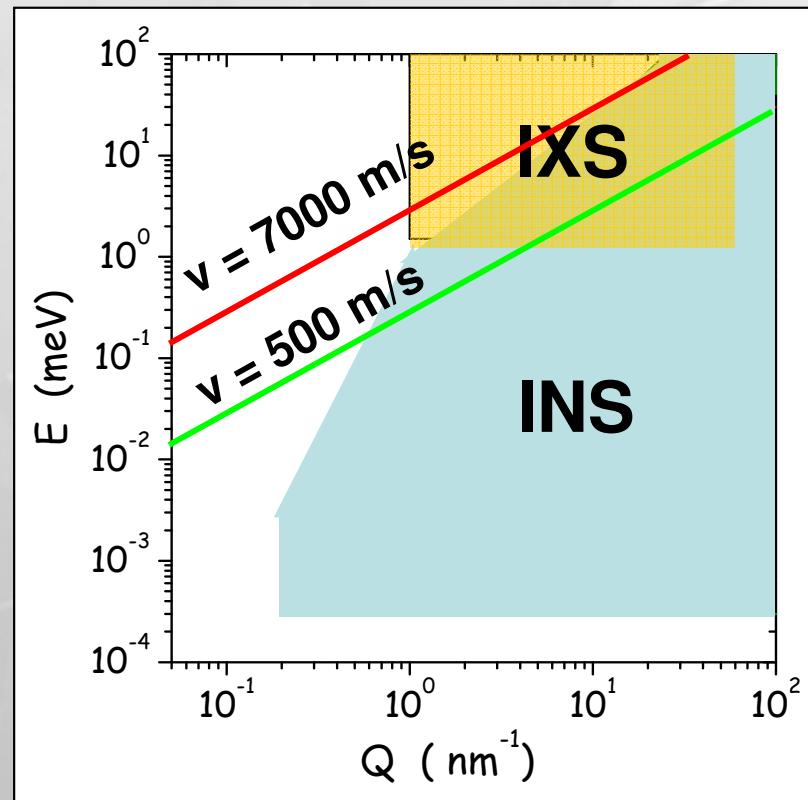
$$k_i = 91.2 \text{ nm}^{-1}$$

$$\Delta E/E \leq 1 \times 10^{-7}$$

small beam

Scientific themes (I)

Disordered systems: Explore new Q-E range



- Interplay between structure and dynamics
- Structural and other relaxations
- Excess of the VDOS (Boson peak)
- Nature of sound propagation and attenuation

Scientific themes (II)

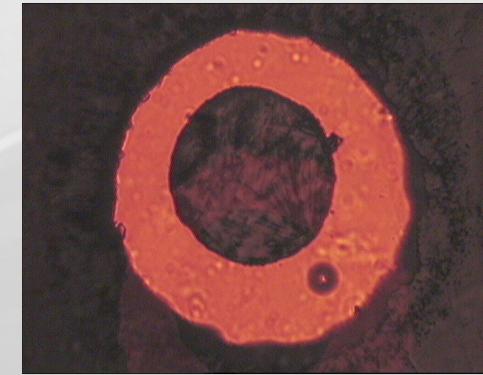
Crystalline systems: small samples, high pressure



$V = 10^{-4} - 10^{-5} \text{ mm}^3$

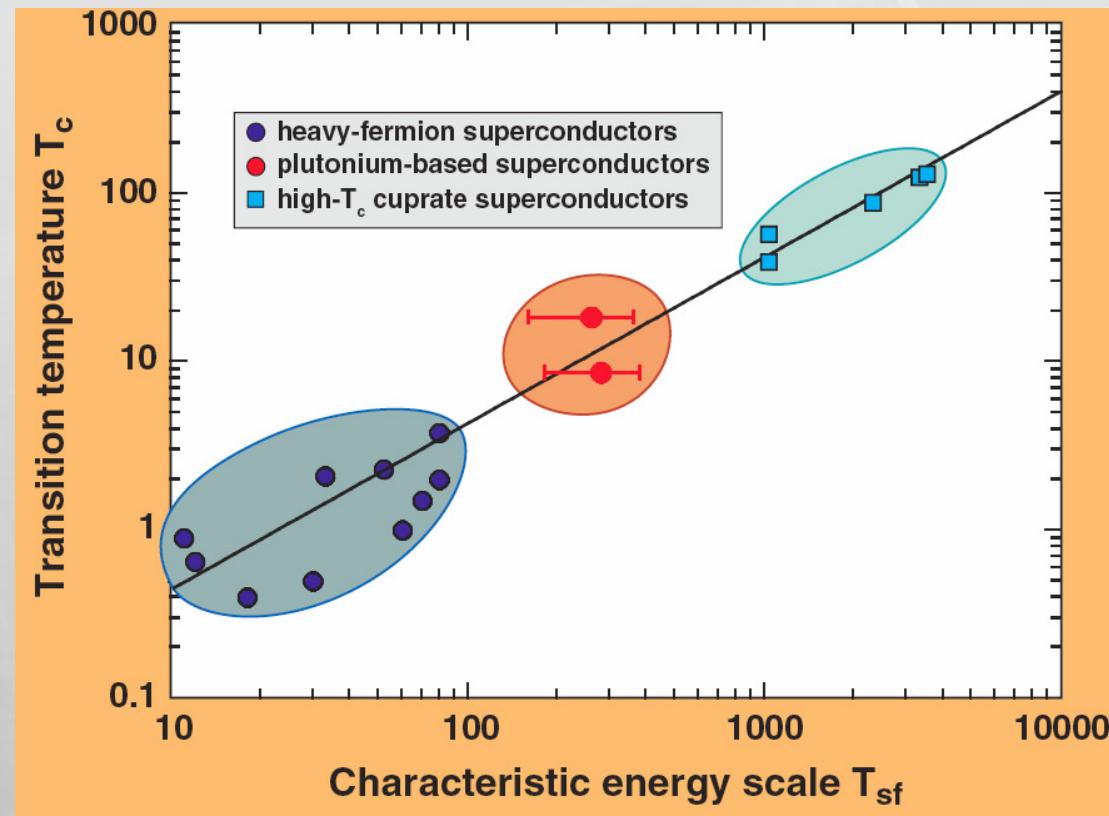
Diamond anvil cells

Thin films and surfaces

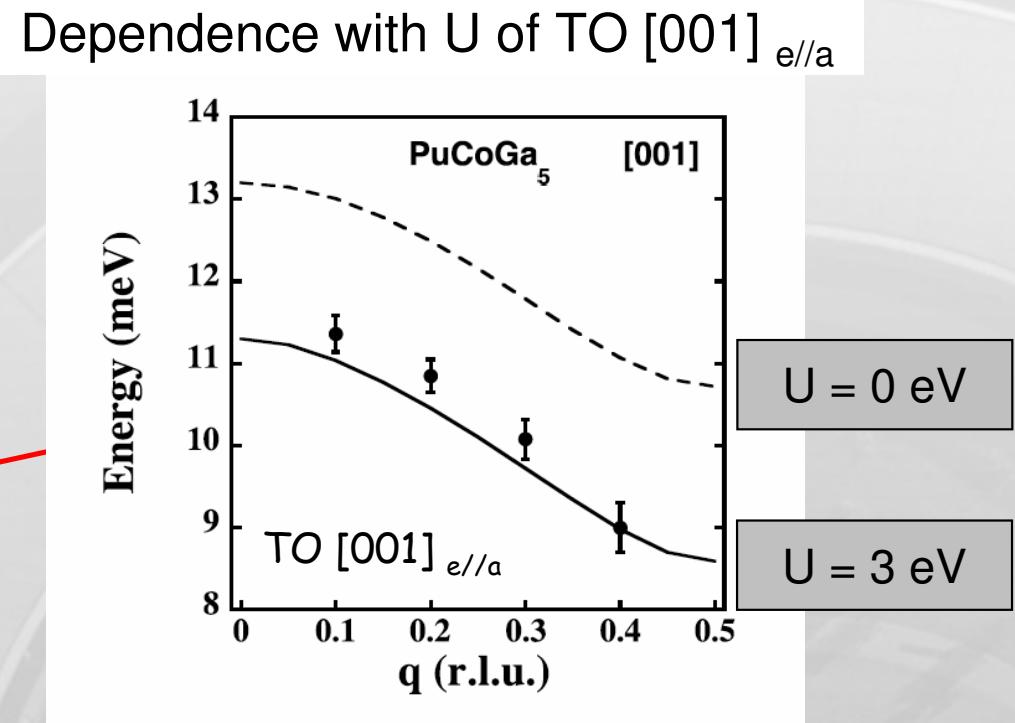
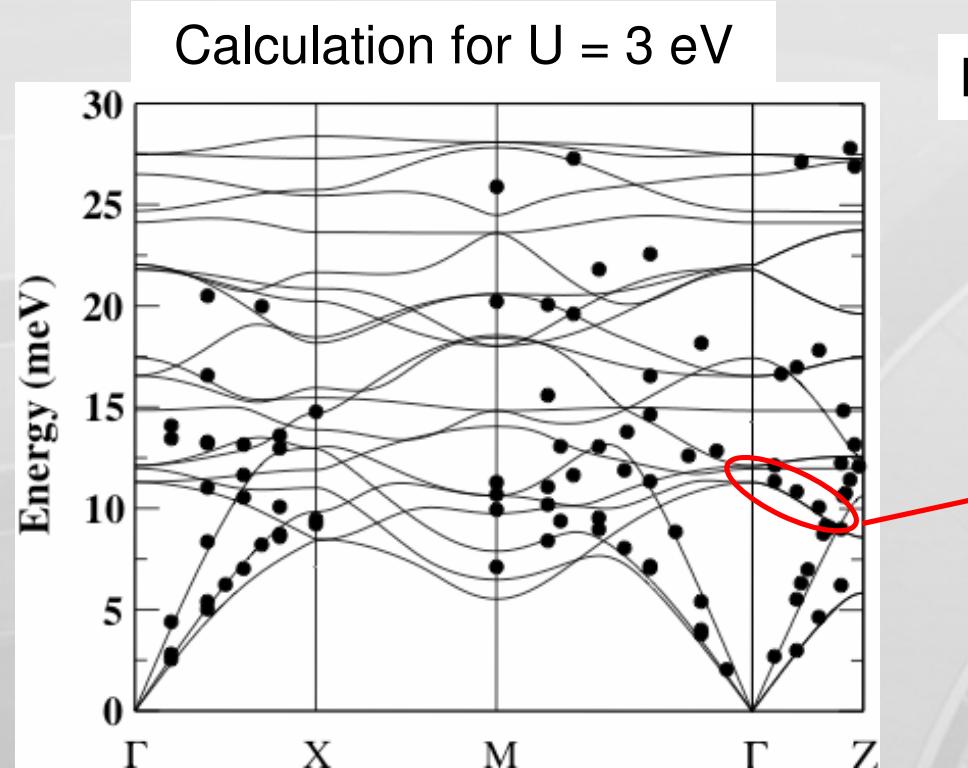


- correlated electron systems
 - actinides, superconductors, CDW systems
- novel materials
- “old” materials at very high pressures
- minerals relevant in Earth science

Phonon dispersion of PuCoGa₅

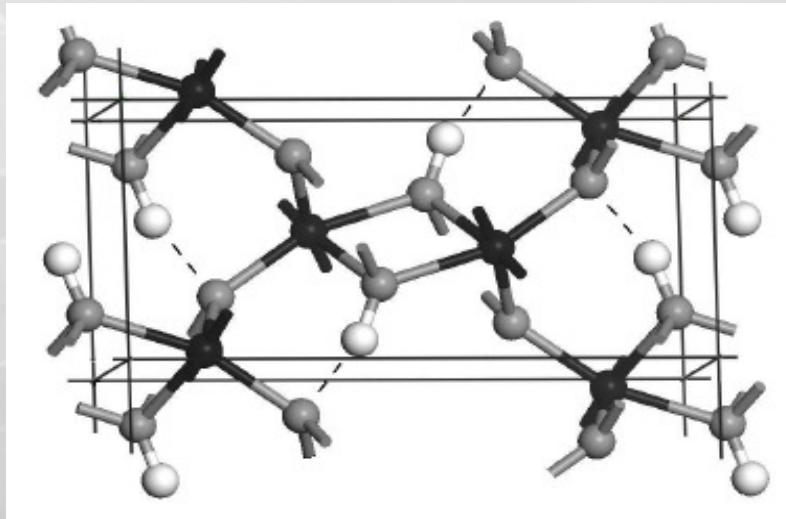


- Sample : ²⁴²Pu from Ga flux method (ITU Karlsruhe)
- Ab-initio calculation : GGA + U; (P. Piekarz et al., Phys. Rev. B 72, 01452 (2005))

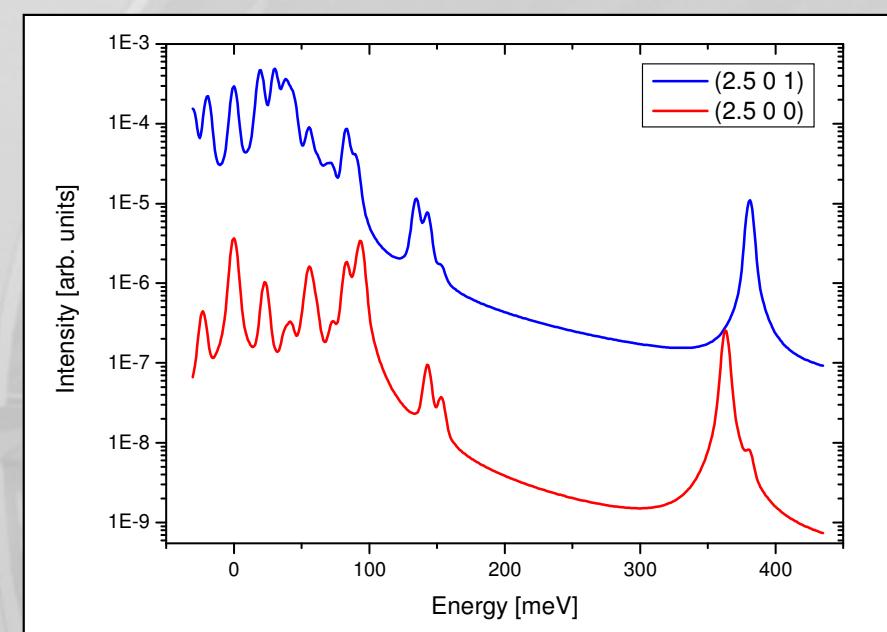
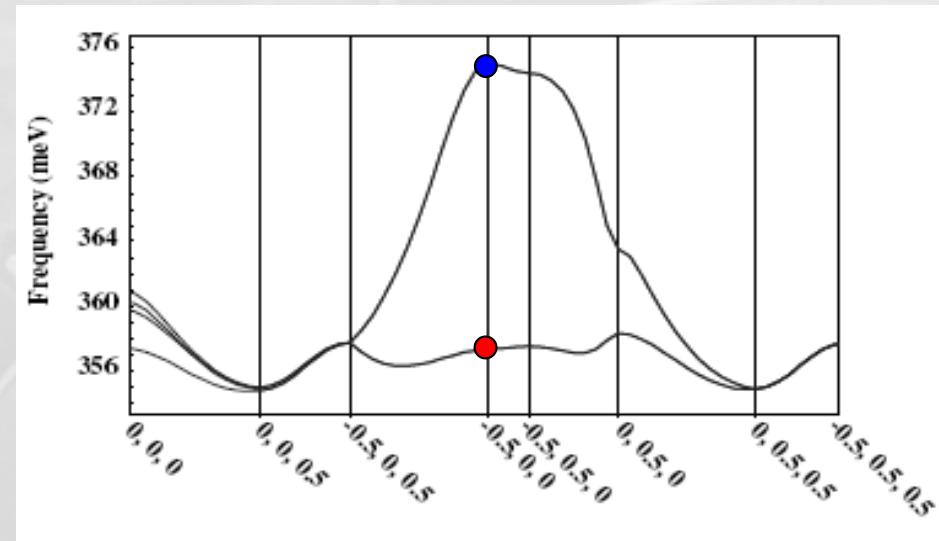


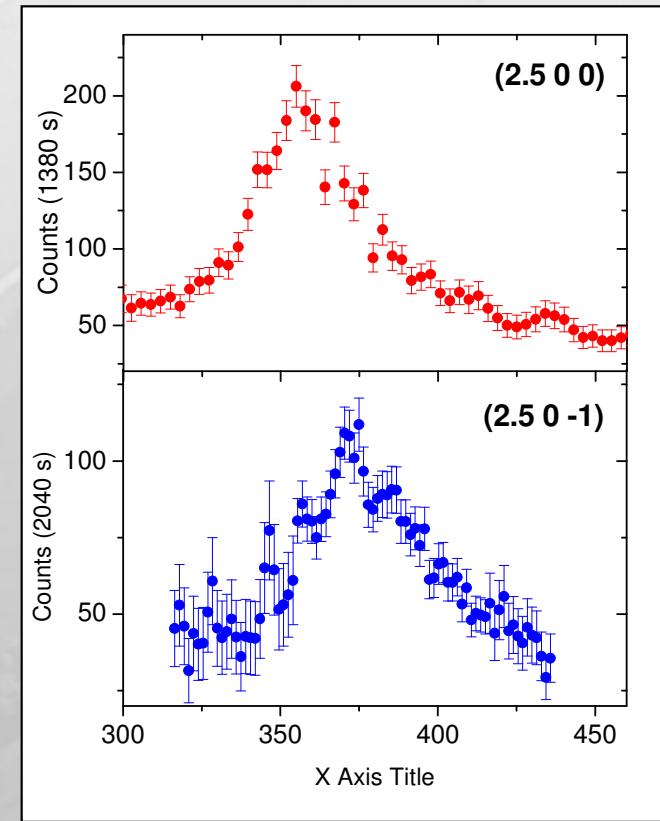
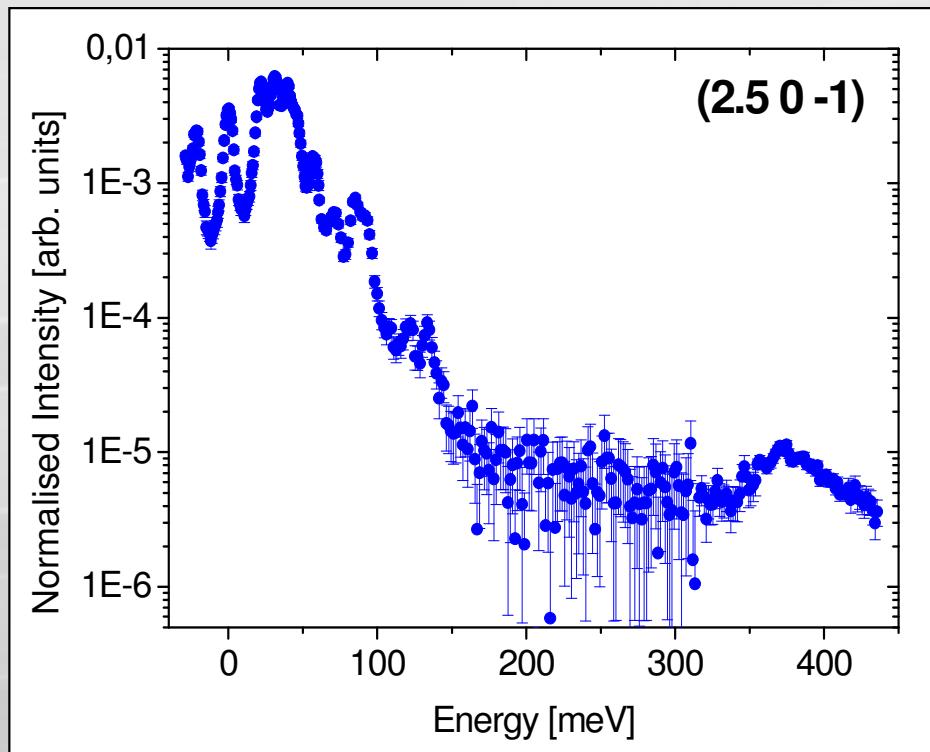
- Main effect : softening of some phonon frequencies in relation with $U > 0$
- => Sensitivity of phonon spectrum to 5f charge distribution

OH-stretching vibrations in diaspore



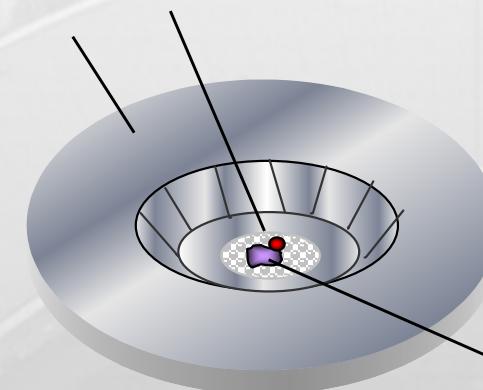
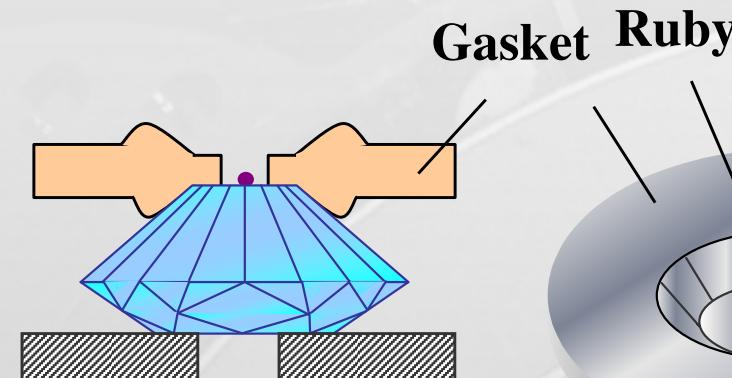
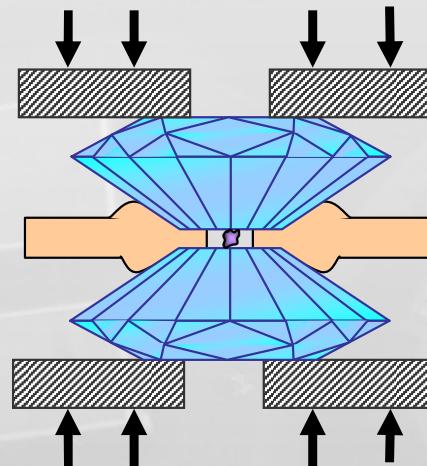
AIOOH, orthorhombic
H-bond of intermediate strength





	E_{exp} [meV]	E_{theo} [meV]
(2.5 0 -1)	374	375
(2.5 0 0)	357	357

IXS at very high pressures



Pressure measurement by frequency shift of ruby fluorescence

