Local structure of solid Rb at megabar pressures

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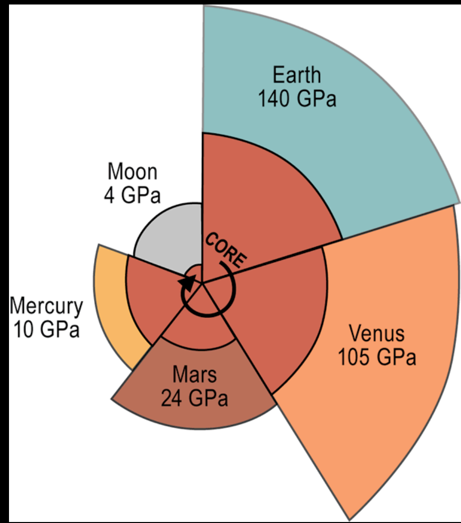
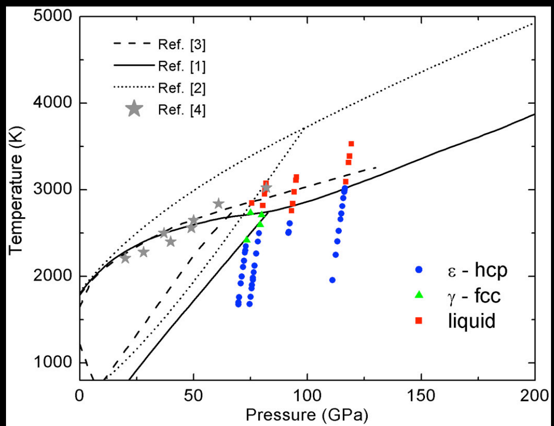
High pressure above 100 GPa + XAS ➔ electronic and local structure properties

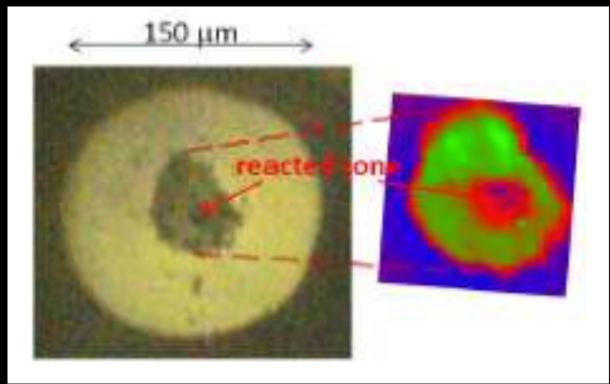
- Access to local order in melts ➔ planetary interiors
- speciation and oxidation state ➔ geophysical interests
- synthesis on new materials ➔ material science
- magnetism and structure correlation ➔ fundamental properties of matter





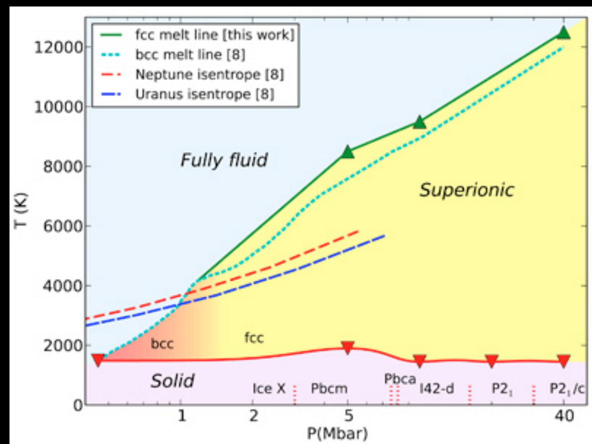
Melting of Fe

Aquilanti et al., PNAS (2015)



Synthesis of Xe oxide

Zhu *et al.,* Nat. Chem. **5**, 61 (2013)

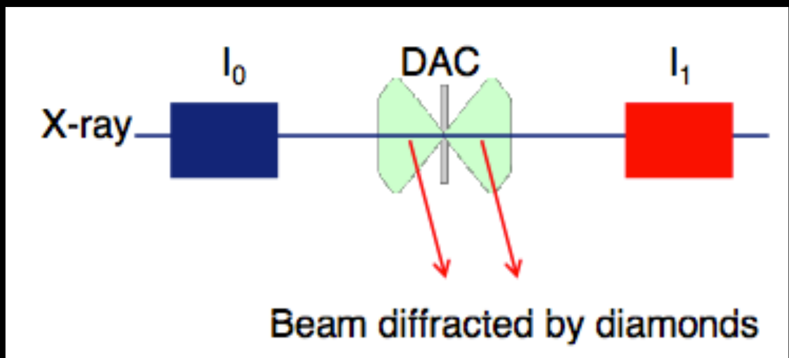


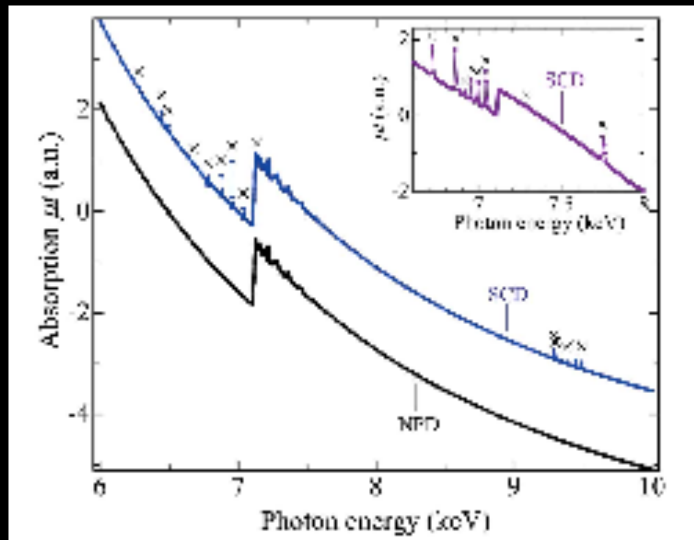
Superionic phase of water

Wilson et al., PRL 110, 151102 (2013).

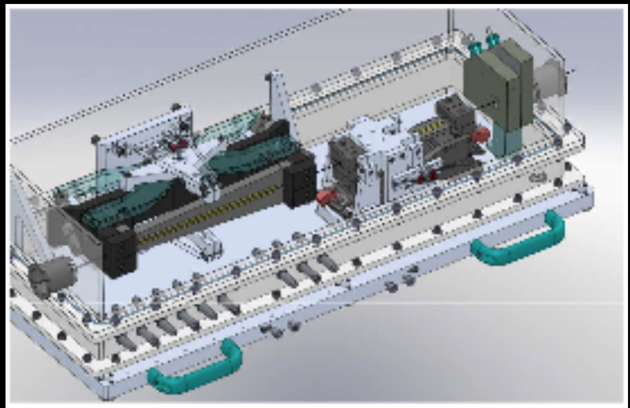
X-ray absorption spectroscopy experiments at extreme high pressures are hindered by two major limitations:

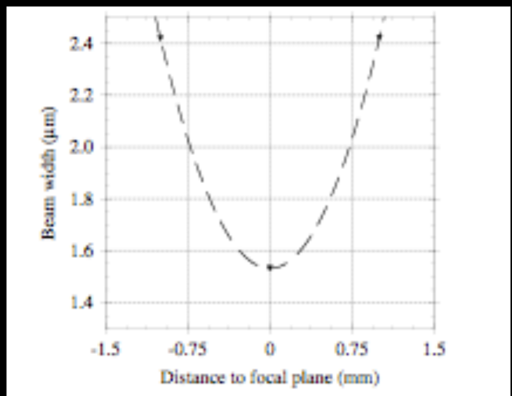
- Small sample transversal dimensions (< 10 x 10 μm^2)
- artificial modulation of the absorption signal due to diffraction by the diamonds





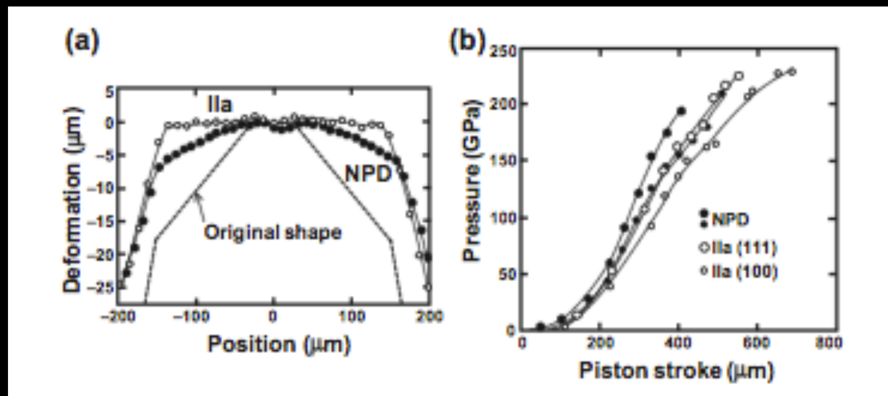
Micro-focusing K-B multilayer mirror device



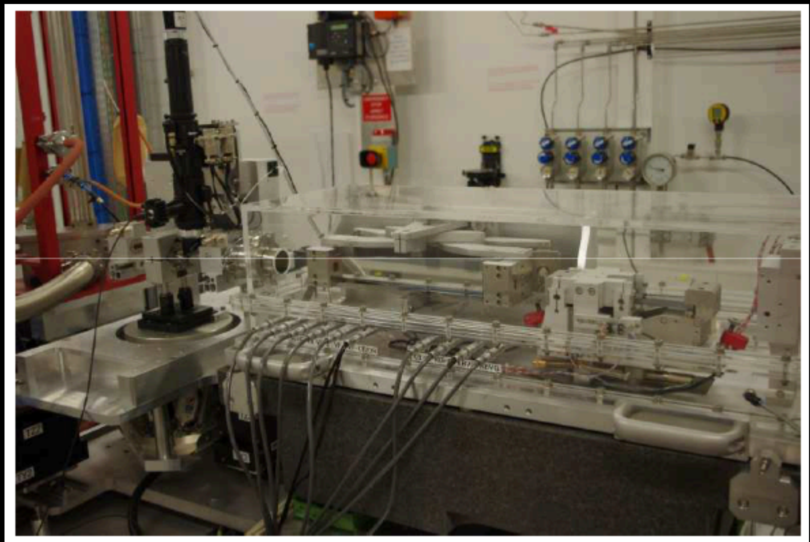


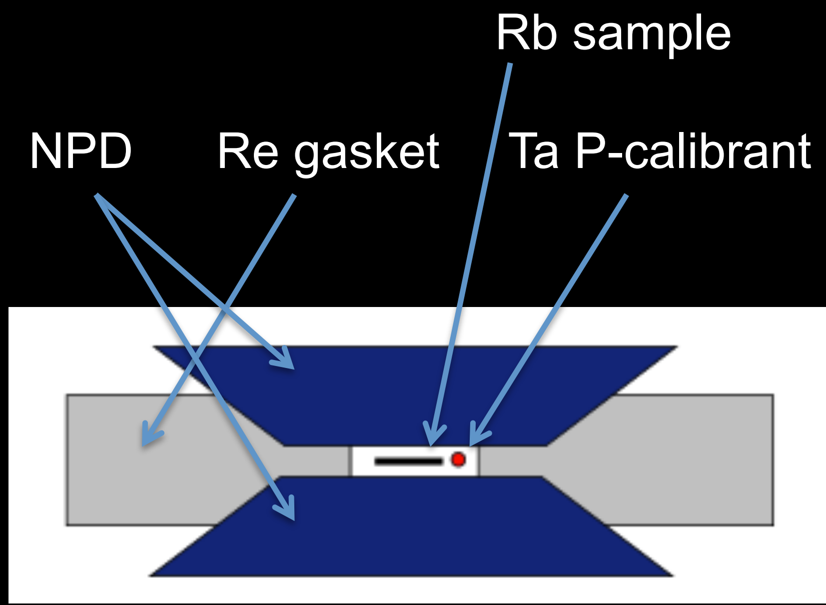
E. Ziegler, S. De Panfilis et al., *X-ray Spectr.* (2009) 38, 250

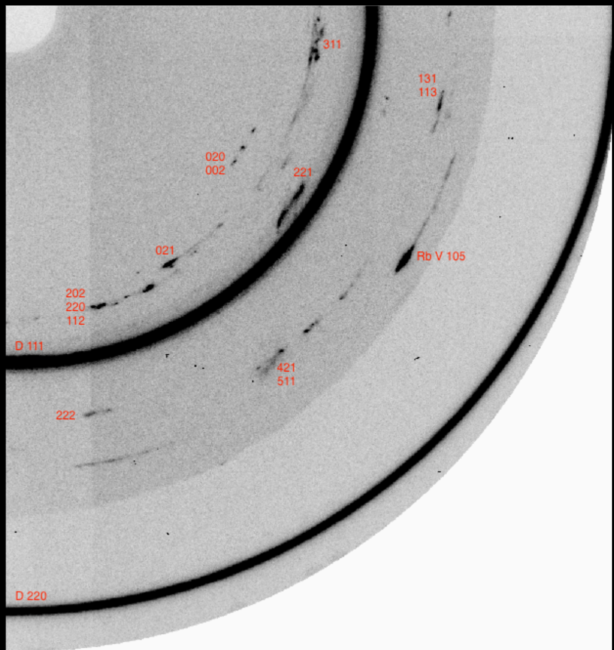
Nanopolycristalline diamonds without binder



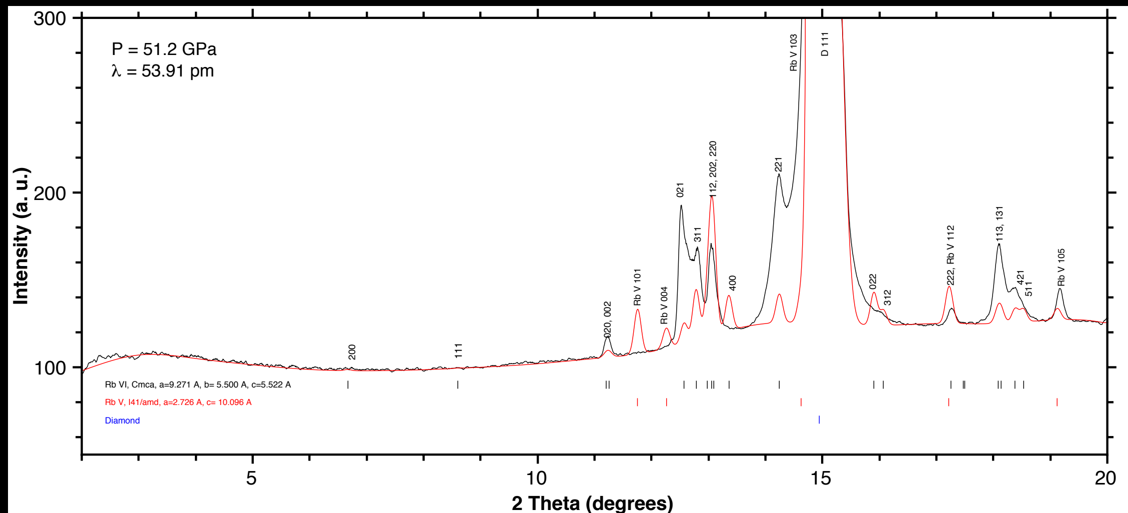
T. Irifune et al., *Nature* 421, 599 (2003).





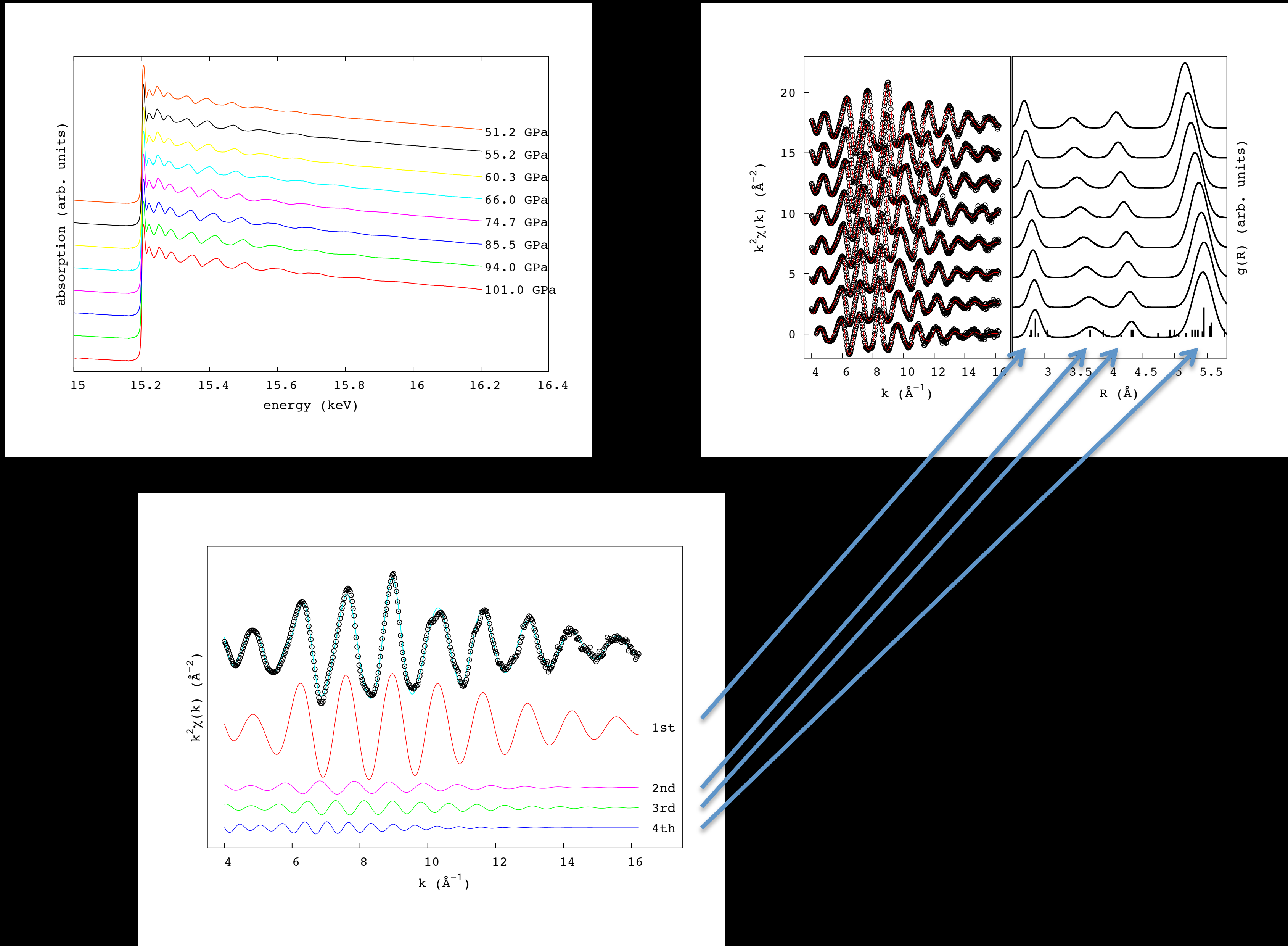


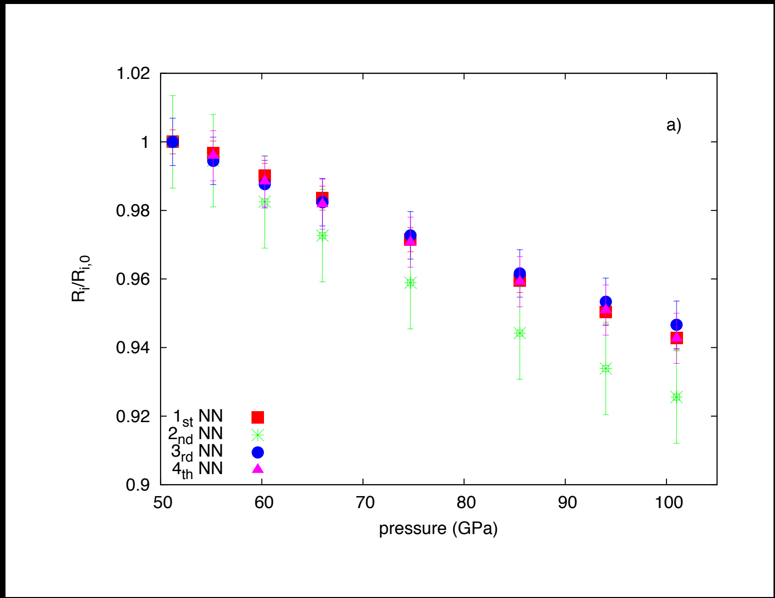
Rb-VI at 50 GPa + residual 3% of Rb-V



$\mu(E)=\log(I_0/I_1)$

$X(k)=(\mu-\mu_0)/\Delta\mu$





Homogenous compression of the volume with no further phase transitions which are expected above 230 GPa.

$$\sigma^2(P,T) = \frac{\hbar}{2\mu\omega_E(V)} \frac{1+\exp[-\hbar\beta\omega_E(V)]}{1-\exp[-\hbar\beta\omega_E(V)]}$$

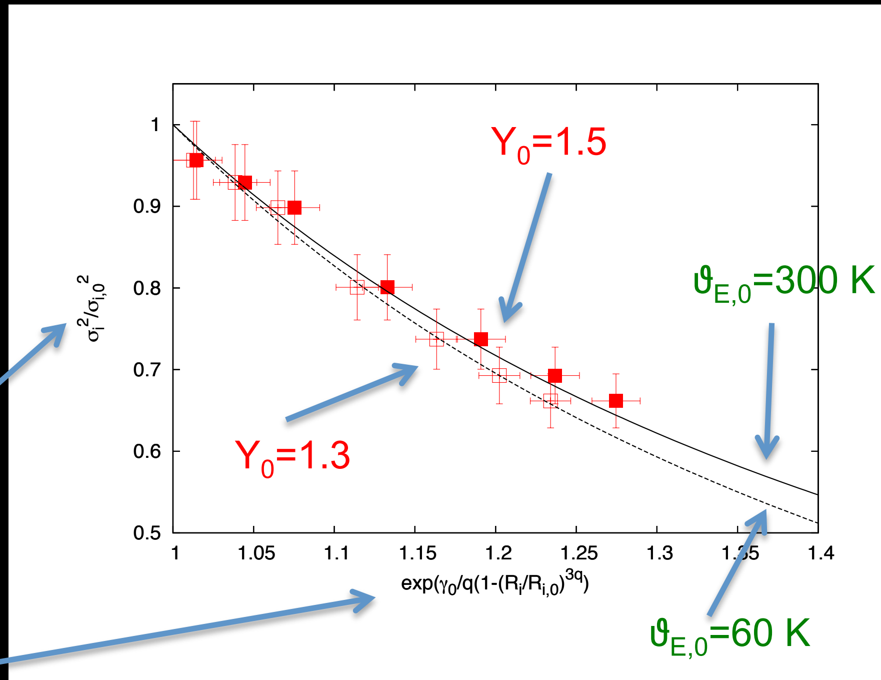
$$= \frac{\hbar}{2\mu\omega_E(V)} \coth\left[\frac{\theta_E(V)}{2T}\right],$$

$$\gamma = \gamma_0 \left(\frac{V}{V_0}\right)^q,$$

$$\omega_E[V(P)] = \omega_{E,0} \exp\left\{\frac{\gamma_0}{q}\left[1-\left(\frac{V}{V_0}\right)^q\right]\right\}$$

$$\frac{\sigma^2(P,T)}{\sigma^2(0,T)} = \frac{1}{x} \tanh\left(\frac{\theta_{E,0}}{2T}\right) \coth\left(\frac{x\theta_{E,0}}{2T}\right)$$

$$x = \frac{\omega_E[V(P)]}{\omega_{E,0}}$$



Smaller values of γ_0 would imply a null $\vartheta_{E,0}$, whereas larger γ_0 unphysically large Einstein temperature.

S. De Panfilis et al., J. Chem. Phys. 142, 214503 (2015)

P. Fornasini et al., J. Synchr. Rad. 22, (2015).

Conclusions

- We demonstrated the possibility to perform high quality XAS experiments on a scanning energy synchrotron beamline above the megabar pressure range by exploiting the performances of two pivotal experimental solutions: a micro-focusing device and the use of nano-polycrystalline diamonds.

- We collected XAS and XRD data of the Rb-VI phase from 50 to 101 GPa and we observed a continuous homogeneous volume compression with no evidence of further phase transitions.

- Via a simple Einstein model of the crystalline vibration, we estimated the Rb-VI Grüneisen bond parameter to be within 1.3 and 1.5.