MICROSCOPIC DYNAMICS OF NON-SIMPLE LIQUIDS

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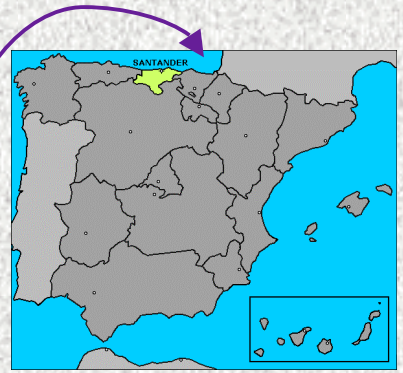


Study of microscopic dynamics of liquid metals

- Study of the collective dynamics of molten metals by inelastic neutron scattering and its dependence with temperature in a microscopic scale.
  - Beyond the hydrodynamic limit (Q,ω-->0) the measured spectra may show peaks at finite frequency which cannot be identified with the hydrodynamic sound.
  - They are understood as density oscillations with a given frequency ω_Q.
- Study of the stochastic dynamics of these metals by means of quasielastic neutron scattering

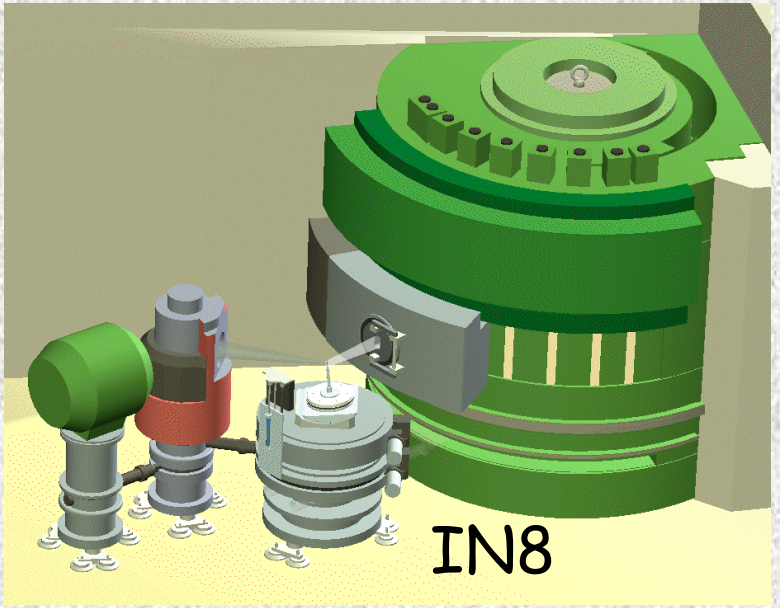
STUDY OF COLLECTIVE MODES IN LIQUID TELLURIUM

Why tellurium?

It displays an anomalous behaviour of the sound velocity with increasing T.

Contrary to other chalcogenide elements, the sound velocity increases with T, from 890 m/s at melting (723K) up to ~1140 m/s at 850K

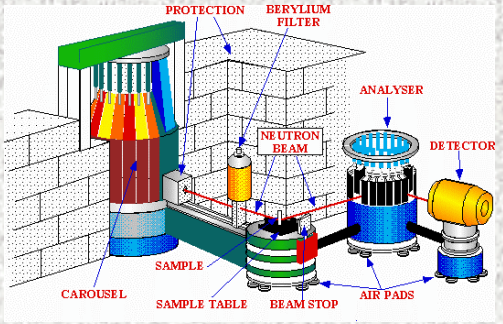
Is not a density effect, since it decreases with increasing Temperature



Configuration: k_f=4.1 $Å^{-1}$ as the sound velocity ~1140 m/s
30'-Cu200-20' --Te-- 20'-Cu111-30'

Experiment cancelled because of a problem associated to the furnace.

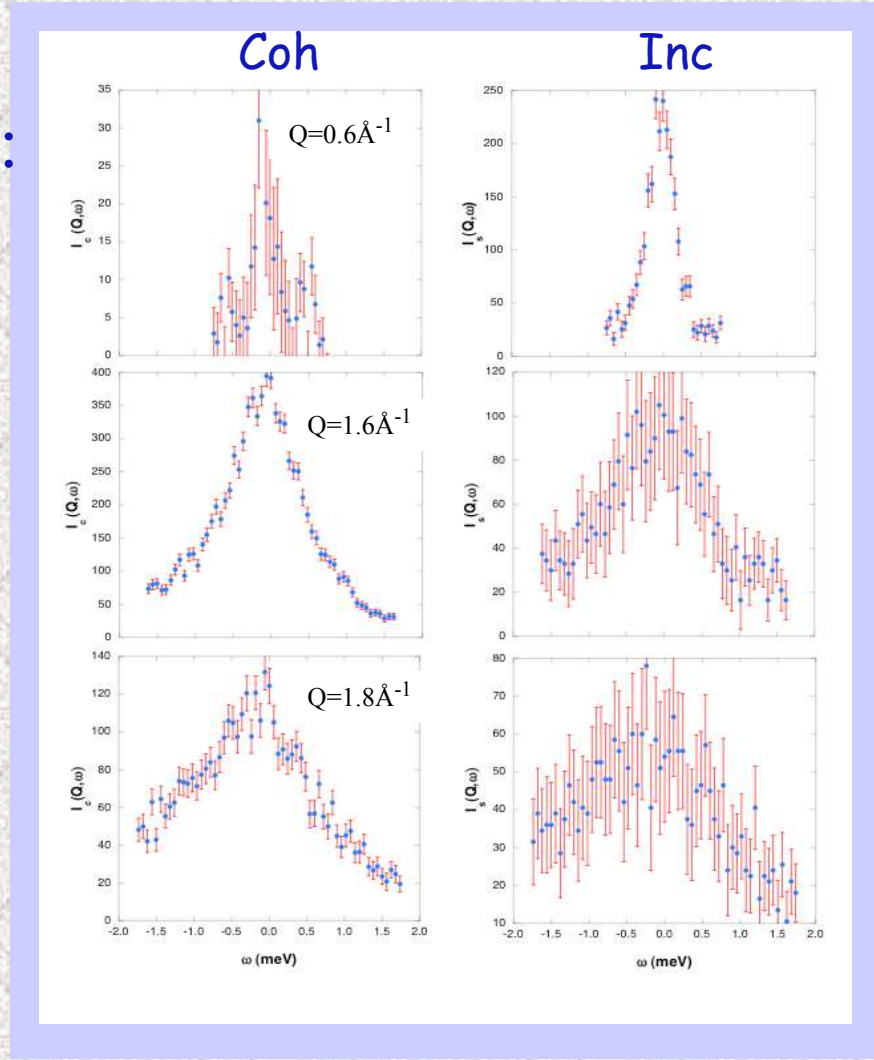
Stochastic dynamics in liquid potassium



Carried out on IN14 :

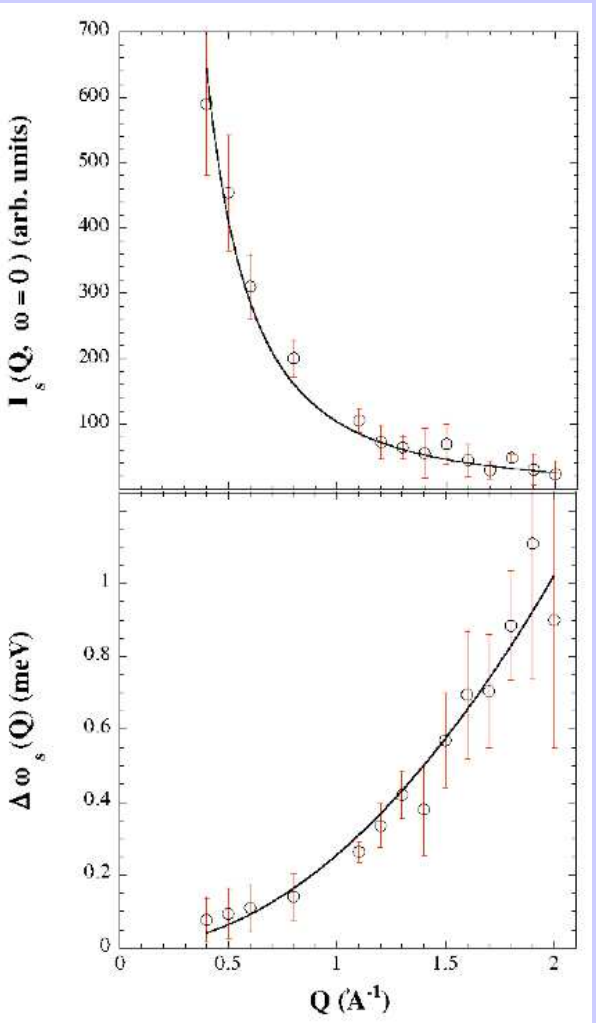
- Polarization analysis options
- Separation of the two components:
  - Coherent $\left.\frac{d^2\sigma}{d\Omega dE}\right|_{coh} = \frac{1}{4K}\left[\frac{3(N^+ - N^-)}{P_0} + (N^+ + N^-)\right]$
  - Incoherent $\left.\frac{d^2\sigma}{d\Omega dE}\right|_{inc} = \frac{3}{4K}\left[(N^+ + N^-) - \frac{(N^+ - N^-)}{P_0}\right]$
- Study of the linewidth of the two components: $I(Q,\omega) \propto L(Q,\omega) \otimes \Re(Q,\omega)$
- k_i-constant scan = 1.97 Å^{-1}

  ΔE = 0.11 meV



Results

Incoherent



$\Delta\omega_S(Q)=D_{eff}Q^2$, D_{eff}=0.25meVÅ^2

D_{eff}<D=0.327

$\Rightarrow$ retardation due to a strong coupling with long. collective modes

I_c follows S(Q) $\Rightarrow$ max at Q_p

$\Delta\omega_c(Q)$: minimum at Q_p and follows the $D_{eff}Q^2$ curve

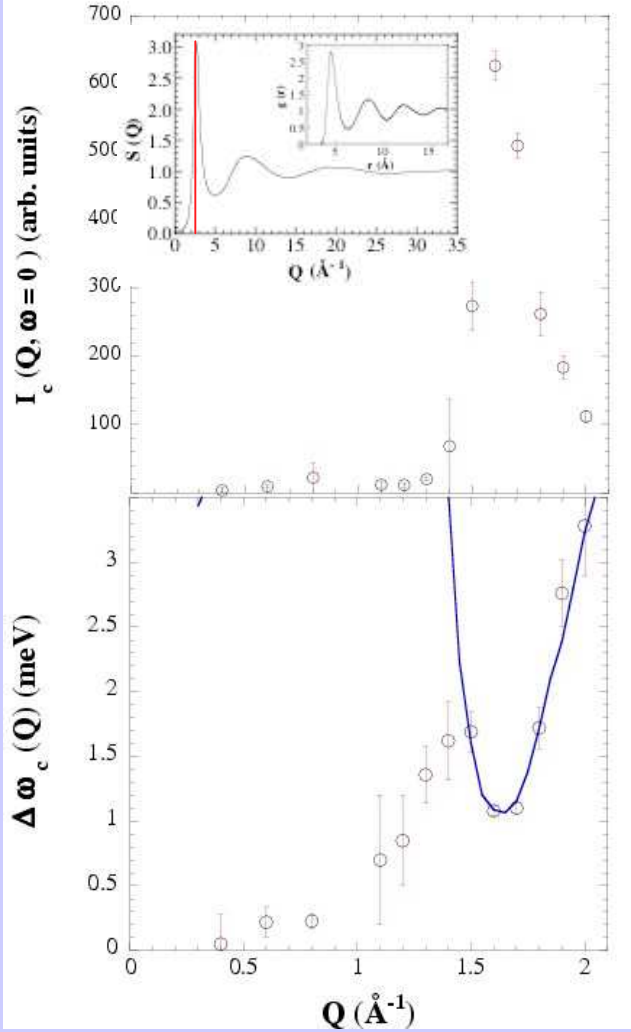
Within the region close to Q_p:

$$\Delta\omega_c = \frac{D_E Q^2}{S(Q)[1 - j_0(Q\sigma) + 2j_2(Q\sigma)]}$$

D_E, the hard-sphere diffusion coefficient and j_x, the spherical Bessel functions

Motions cannot be explained in terms of a single time scale.

Coherent



F.J.Bermejo *et al.* LAM12 Conference Proceedings (to be published in Journal of non-cryst. Solids)

Future experiments

Ni and K

- Study of diffusive dynamics close to melting
- Compare characteristics of packed liquid metals (Ni) to alkali ones (K)
- See the possible effects of packing and its influence in the self-diffusion

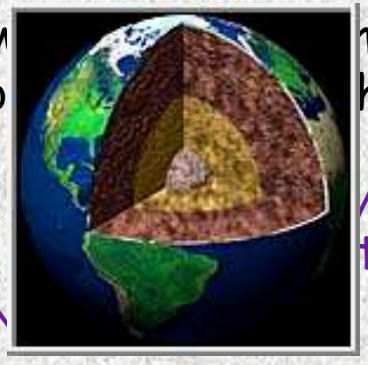
Ni --> quasielastic exp. on IN4 & IN5

K --> quasielastic exp. for higher Q values with polarization analysis

Fe-Ni-S and Te

Fe-Ni-S:

- Study of alloys of geophysical interest, components of the planetary cores
- Contrary to other molten transition metals, the acoustic velocity increases with the temperature
- Compare to a reference sample Fe-Ni --> see effects of the interaction alloy - sulphur atoms
- Te show maly in the sound velocity when co her lements



Fe-Ni-S /s, lity t, I

Te --> I cycle

Thanks for your attention!

Acknowledgments

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