



Experiment title: The dynamic structure factor of Liquid Lithium	Experiment number: HS-853	
Beamline: ID 16	Date of experiment: from: 15-02-99 to: 22-02-99	Date of report: 16-06-99
Shifts: 21	Local contact(s): R. Verbeni	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Prof. G. Ruocco* – University of L’Aquila – I Dr. Tullio Scopigno* – University of Trento – I Dr. Umberto Balucani – CNR Firenze – I		

Report:

We used IXS to measure the dynamic structure factor of liquid Lithium at two different temperatures: $T=475$ and 600K . Thanks to the high resolution achievable we have been able to perform the first detailed lineshape analysis on this system: we collected fixed- Q scan at more than twenty values with an energy resolution of 3meV .

The obtained results allowed to investigate about merits and drawbacks of the simple viscoelastic approach, commonly used to analyze neutron scattering experiment and molecular dynamic simulations on alkali metals. In this respect IXS plays in fact a privileged role: there are no kinematic restrictions limiting the accessible (E, Q) space neither incoherent contribution to the cross-section as in the case of neutrons, and the results are not affected by the necessary a priori guess about suitable interatomic potential.

From the raw data is clearly evident the presence of a double timescale i.e. of a double slope in the quasi-elastic part of the collected spectra. The inescapable conclusion we reached is that it's *necessary* to postulate the presence of a secondary relaxation mechanism beside the single “shear relaxation” described by the viscoelastic model. The nature of this secondary mechanism is still open task and further investigations, in particular devoted to the temperature behaviour of the spectra in a wider range around the melting point are required.

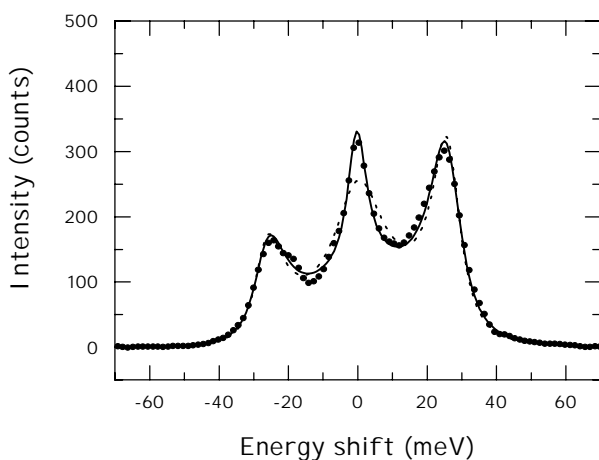
We report below one example of collected spectrum with the relative fit based on our two relaxation times model at $Q=7.0 \text{ nm}^{-1}$.

From the fit it has been possible to extract significant physical parameters such as the two relaxation times, the strength of the relaxations and the sound velocity.

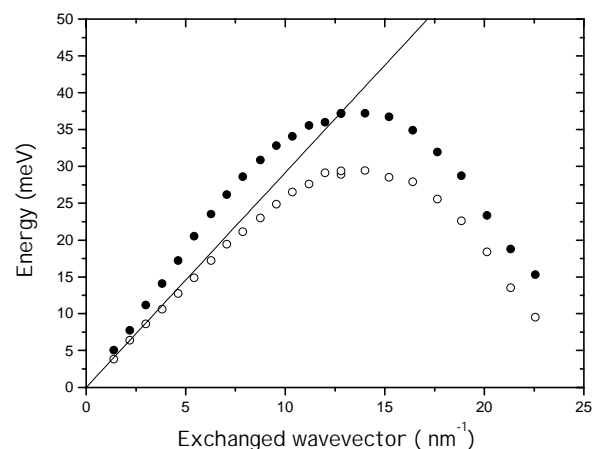
Positive dispersion of the latter quantity has been observed confirming the results of several molecular dynamics simulations and “pioneeristic” low resolution inelastic scattering experiment. Anyway it seems that the origin of such dispersion has to be ascribed to the fast relaxation mechanism rather than to the shear mechanism as the viscoelastic model would predict.

As mentioned above the nature of such secondary mechanism is still debated and important indications could be inferred by its temperature behavior. Further experiment in this direction could be determinant and experimental efforts are required in order to solve the experimental problem related to the handling of a so reactive sample when heated several hundreds degrees above the melting point.

We enclose below the sound velocity dispersion curve as measured in the experiment here reported. The evidence of positive dispersion: the energy position of the excitation deviates from the isothermal value undergoing the transition to the infinite frequency value of sound speed.



Dots: Experimental data. Dotted line: simple viscoelastic model. Full line: two relaxations model



Full line: thermodynamic isothermal sound speed. Open dots: same quantity as from the fit. Full dots: longitudinal current maxima.