

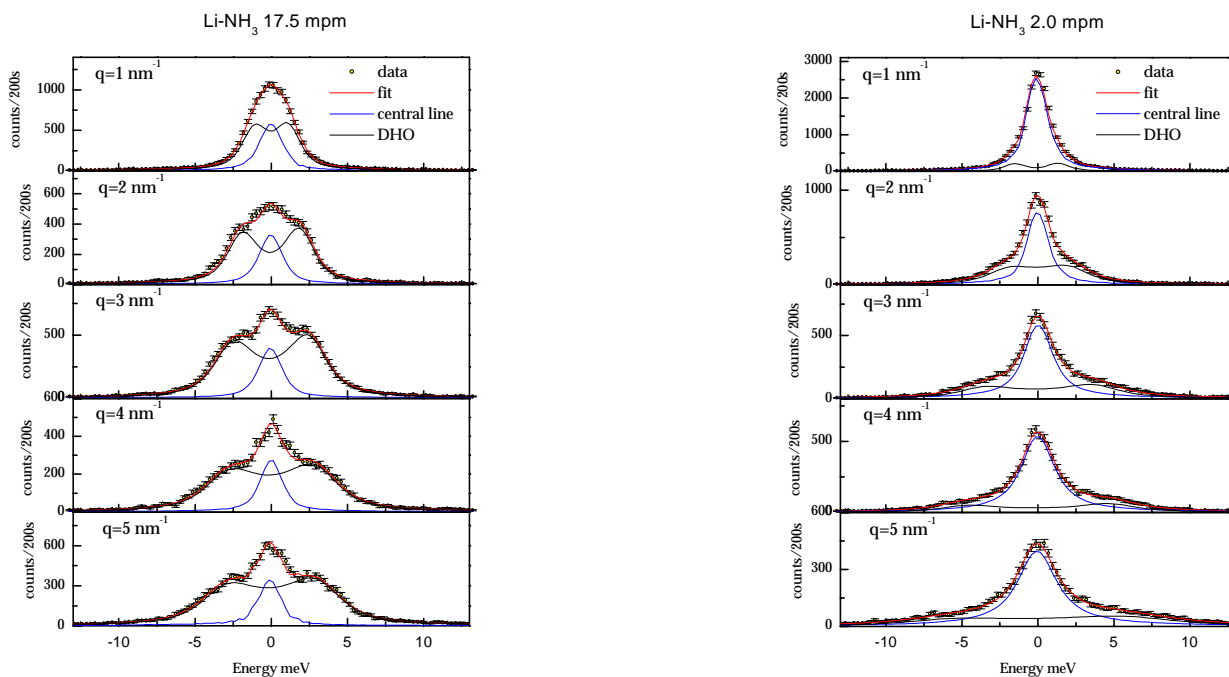


	Experiment title: IXS study of Non Metal-Metal transition in metal ammonia solutions	<b>Experiment number:</b> HS - 1601
<b>Beamline:</b>	<b>Date of experiment:</b> from: 03-10-01 (24-11-2001) to: 10-10-01 (30-11-2001)	<b>Date of report:</b> 01-03-2002
<b>Shifts:</b>	<b>Local contact(s):</b> P. Giura	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants</b> (* indicates experimentalists):  P. Giura - ESRF R. Angelini – ESRF C. Burns – Western Michigan University (USA)		

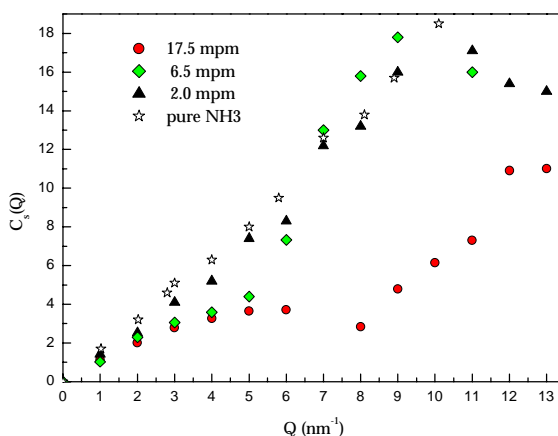
### Report:

We studied the dynamic structure factor  $S(Q, \omega)$  of three different lithium ammonia solutions ( $\text{Li-NH}_3$ ) by means of inelastic X-ray scattering (IXS). The measurements have been performed spanning the momentum transfer ( $Q$ ) range  $1\text{-}30 \text{ nm}^{-1}$ , in order to get information in the surrounding of the inverse of the molecular average distances. We used a stainless steel cell with two sapphire windows that allow the passage of the x-ray beam. The cell has been charged with the alkali metal in the glove box and then cooled down in the cryostat; after that, the right amount of ammonia has been liquefied. The  $\text{Li-NH}_3$ , as all the alkali metal ammonia solutions, shows a metal insulator transition (MIT) that occurs by increasing the number of the alkali atoms dissolved in the ammonia. For this specific system the transition appears in the concentration range  $2\div 7$  mpm (mole per cent of metal) while the limit of solubility is reached at 20 mpm. The choice of the investigated solutions has thus been done in order to follow the changes of the  $S(Q, \omega)$  passing through the MIT. We started with a highly metallic configuration (17.5 mpm) to pass then to a concentration very close to the transition and still in the metallic phase (6.5 mpm), and to finish with the insulating phase at 2 mpm. In figure 1 is reported a sample of the spectra measured for the two extreme cases at five selected  $Q$  values in the low momentum transfer region. The insulating phase is characterized by an intense central peak which is much less pronounced in the metallic phase. The intensity of this peak is strictly correlated with the structural disorder of the system. In liquid metals this disorder is generally lower than in liquid insulators. In the lithium ammonia solution, once the alkali metal starts to dissolve it loses its  $2s^1$  electrons that solvate, the  $\text{Li}^+$  ion is then surrounded by four ammonia molecules creating a stable structure in which the  $\text{Li}^+$  occupies the centre of mass. Those molecules dispose themselves forming a network with a well defined molecular average distance as it can be seen observing the static structure factor  $S(Q)$  (measured with X-rays). The dynamics of

this network fully characterises the highly metallic phase. At 17.5 mpm, indeed, the inelastic spectra shown a well-defined excitation that clearly softens in the vicinity of the first peak (Li-Li) of the  $S(Q)$ . In figure 2 the dispersion curves of the three studied solutions as well as the one of the pure ammonia are reported. It can be remarked that the dynamics behaviour of the insulating mixture (2 mpm) closely resembles the one of the pure  $\text{NH}_3$  while the two metallic solutions behave exactly in the same way for  $Q < 5 \text{ nm}^{-1}$ . The incoming metallization clearly affects the intermolecular interactions governing the collective dynamics of the system.



**Fig.1** Examples of IXS spectra taken at the indicated  $Q$  values for two different lithium ammonia solutions, one (17.5 mpm) highly metallic and the other (2.0 mpm) already insulating. The fit are the solid lines superimposed to the experimental points. They have been obtained using a fitting function composed by a damped harmonic oscillator for the inelastic signal and a lorentzian for the central line.



**Fig.2** Dispersion curves in lithium ammonia solutions as obtained from the DHO fitting model