



	<b>Experiment title:</b> Collective dynamics of liquid Te: the most non-simple liquid metal	<b>Experiment number:</b> HS2434
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### Report:

Our recent inelastic x-ray scattering (IXS) experiments on several non-simple liquid metals, such as Si [1], Sn [2], and Ga [3], have revealed characteristic common features in the collective dynamics. 1) Clear indications for propagating phonon modes were found as in simple liquid metals as liquid alkalis, whereas their lifetimes are much shorter. 2) They comprise a positive dispersion of about 5-20 % again as in liquid simple metals. 3) Very short time (sub-picosecond) retaining of the nearest-neighbour correlation is visualized by a Gaussian component in the quasielastic line shape, which may be related to short living covalent species.

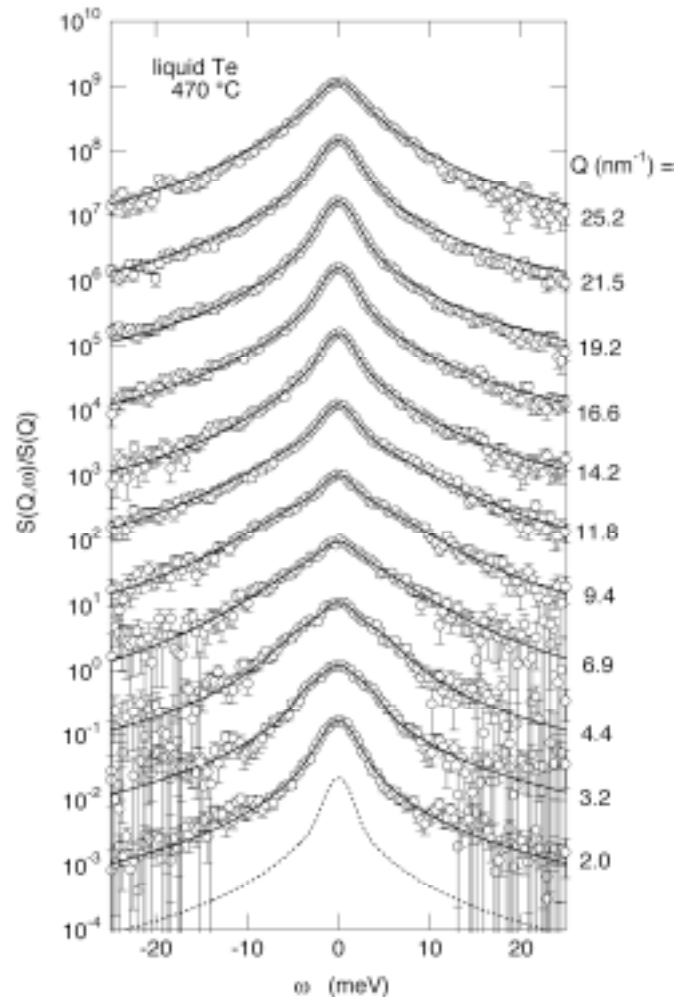
Liquid Te is a liquid metal, but comprises a strong covalent nature. Several neutron total scattering results of liquid Te [4] showed the coordination number of 2.0-3.0 near the melting point, which indicated that liquid Te is composed of short covalent chain molecules with a interchain correlation of both the metallic and van der Waals nature. Since the coordination number is extremely small for a liquid metal, liquid Te is considered to be the most non-simple liquid metal among elemental liquids.

Vibrational density of states (VDOS) of liquid Te near the melting point has been measured using inelastic neutron scattering (INS) technique by some groups. Propagating modes in  $S(Q, \omega)$  of liquid Te were, however, not yet found in these INS experiments, which may be due to the strong damping of these modes. Even a recent INS result [5] using the powerful spectrometer MARI/ISIS, could not indicate propagating modes. From this IXS

experiment, we have obtained detailed information on the collective phonon modes in  $\omega$ - $Q$  space in liquid Te.

The IXS experiment was carried out using a high energy-resolution IXS spectrometer installed at ID16/ESRF. The liquid Te sample was contained in a cell made of single-crystal sapphire. The high temperature was achieved by a resistance heating element made of Mo wire, and monitored with two W-Re thermocouples.

Figure shows logarithmic plots of the  $S(Q, \omega)$  spectra at 470 °C normalized to the corresponding energy integral. The measurements were carried out in the  $Q$  range from 2.0 to about 25 nm<sup>-1</sup>, including the first  $S(Q)$  maximum. Also given by a dashed line is the typical resolution function. In the low  $Q$  region, clear propagating modes can be visible as shoulders at both sides of the quasielastic peak. From the data fits using a damped harmonic oscillator for the inelastic signal and a Lorentzian for the quasielastic line, the obtained frequency energies of the inelastic mode deviate from the hydrodynamic value by about 40%, which is unlike other liquid metals with values of 5-20%, but similar to that in van der Waals liquid Ar. These inelastic excitations are highly damped. It should be also noted that near the  $S(Q)$  maximum, the quasielastic lineshape cannot reproduce using a Lorentzian, but a Gaussian component is necessary for it, which we have found in several non-simple liquid metals. The fraction of the Gaussian component is, however, not as large as those in the other non-simple metals, although stable, or long-living covalent bonds are suggested from the static structural experiment [4]. This may be due to the fact that the first peak in  $S(Q)$  is mainly constructed by the interchain correlation of a van der Waals-like interaction. The intrachain correlation with a covalent nature forms the second maximum in  $S(Q)$ , where the previous INS experiment [5] obtained a strong Gaussian-like feature in the quasielastic line.



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