ESRF	**Experiment title:** High frequency dynamics in liquid tellurium at high pressure	**Experiment number**: HD 241
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Report:

Liquid tellurium was studied by IXS at high pressure (P) and high temperature (T). The aim of this experiment was to investigate the evolution of the high frequency dynamics of this system while the interatomic interaction changes as pressure increases.

Liquid Te is reported to be a metallic liquid already at room pressure, despite the semiconductive character of the solid phase, and the metallicity increases smoothly with temperature, the metal to non-metal transition being localized in the supercooled liquid [1]. At high pressure another transition has been identified: it is a first order transition, located at 800 K and 4.7 GPa, which is due to the collapse of the atomic chains length.
At low pressure, P < 6 GPa, liquid Te undergoes an anisotropic compression: the chains get closer while the intra-chain interatomic distance increases because of the increasing inter-chain interaction. After 6 GPa this mechanism cannot be used anymore for further volume reduction and a uniform compression regime starts, with the chain collapse. At very high pressure, liquid Te closely resembles a simple liquid [2,3].
The study of liquid Te at high pressure thus allows for the investigation of the link between the high frequency dynamics and the interatomic interaction, which is continuously changing.

For this experiment Te powder was loaded in a diamond anvil cell, separated form the metallic gasket by a thin NaCl ring in order to avoid any chemical reaction. The cell was contained in a vacuum chamber expressively designed for high pressure high temperature experiments, which is equipped with a resistive heater able to produce temperatures as high as 1000K.
The IXS spectra were collected using the (999) reflection of the Silicon monochromator, with an energy resolution of 3~meV.
We could collect data at only one pressure and temperature point, mainly because of the technical difficulties met during the experiment. Indeed, the heater broke during temperature stabilization and an important amount of time was needed in order to cool down the cell and replace the heater with a new one. Furthermore, a long time was needed to reach the aimed (P,T) conditions and the low counting rate made it necessary to count up to 1000s per energy point.
Eventually, while we were increasing pressure and temperature to reach a (P,T) point beyond the liquid liquid transition, the hole in the gasket became unstable and we lost the sample.

We collected data at 750K and 2.5 GPa. At this pressure, the inelastic features in the IXS spectra are much more visible than at room pressure and at the same temperature [4]. We have made a first analysis using the same fitting function used in previous published work on liquid Te at room pressure [4,5], i.e. a lorentzian function for the elastic line and a damped harmonic oscillator for the inelastic peaks, in order to compare our results with the literature.

At room pressure it was found that the high frequency acoustic velocity is enhanced with respect to the adiabatic one (positive dispersion) of as much as 65% [4, 5]. We find here that the acoustic velocity increases strongly with pressure, but if we estimate the adiabatic velocity using published diffraction data at similar (P,T) conditions [3], we find that the positive dispersion is basically the same as at room pressure (Fig.1).

At room pressure it was found that the positive dispersion decreases with decreasing density, down to 25% when the density is reduced of only 3-4% [5]. Here we estimate to have a compression of the order of 13%, without any effect on the positive dispersion.

A more detailed analysis of the high pressure data is currently underway.

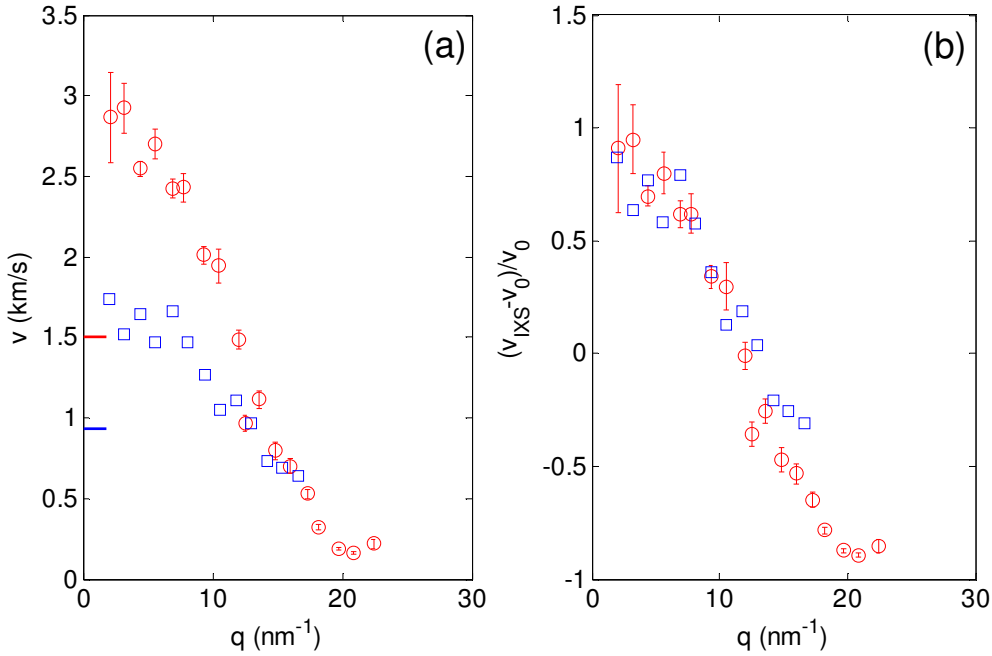

Fig.1: **(a): Acoustic velocity data from the present work (red circles) and from the IXS experiment of Ref.[4] (blue squares). The two horizontal lines are the adiabatic sound velocity at room pressure and 750 K the lower and 3 GPa and 850 K the upper one. (b): positive dispersion as percentage difference between high frequency acoustic velocity and adiabatic sound velocity, same meaning of symbols. It is clear that at low q the same amount of positive dispersion is found at low and high pressure.**

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