ESRF	**Experiment title:** Probing the liquid-liquid transition in tellurium under pressure	**Experiment number**: SC-5298
Beamline: ID15B	**Date of experiment**: from: 20/01/2023 to: 23/01/2023	**Date of report**:
Shifts: 9	**Local contact(s)**: Michael Hanfland (hanfland@esrf.fr)	*Received at ESRF:*

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Report:

The aim of the experiment is to study the structure of supercooled liquid Te particularly approaching its liquid-liquid critical point (LLCP). In our previous work [1], we have measured the structural and thermodynamic properties of supercooled liquid Te under approximately zero (vapor) pressure, and our results have demonstrated that liquid Te and water share many similarities in their thermodynamic and structural properties. This is an interesting and scientifically important finding, because for water, there is mounting evidence for the existence of an LLCP [2] (see Figure 1), although to reach this LLCP has proven to be difficult experimentally. Our findings on the similarities between Te and water suggest that an LLCP exists in Te as well, thereby offering an alternative route to study this intriguing phenomenon, of which experimental data is currently scarce.

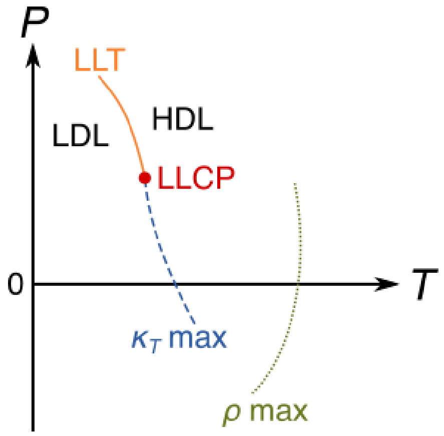

Figure 1: Schematics of a likely phase diagram of water and Te. The first-order liquid-liquid transition (LLT) separates the low-density and high-density liquid phases (LDL and HDL). The LLT ends at a LLCP, from which emanate lines of maxima in the thermodynamic response functions such as the isothermal compressibility, κ_T. Because the low-density phase lies on the low-temperature side, there exists a line of density maxima (ρ max).

In our experiment at ID15B, we have measured the temperature dependence of the structure factor at elevated pressures using a DAC setup. We have demonstrated the possibility to deeply supercool Te at pressures at least up to 0.9 GPa (9 kbar). While analysis is still ongoing, in Figure 2 we show preliminary results on the position of the first diffraction peak, Q_{m1}, as a function of the temperature, T, during three scans. The approximate pressure during each scan is shown in the legend. Although the changes in Q_{m1} are relatively small, the results are reproducible: the two scans at 0.7 GPa agree relatively well with each other, and both show somewhat lower Q_{m1} positions than the higher-pressure scan at 0.9 GPa, as expected.

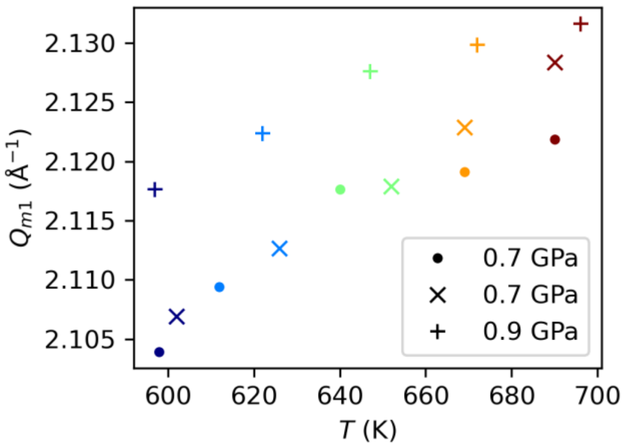

Figure 2: The extracted position of the first diffraction peak, Q_{m1}, as a function of temparture T during three scans at ID15B. Each scan is represented by a different symbol, as shown in the legend.

In comparison, Figure 3 below shows Q_{m1} as a function of T at 0.0 GPa obtained in our previous work [1]; in this study, three scans were performed to demonstrate reproducibility.

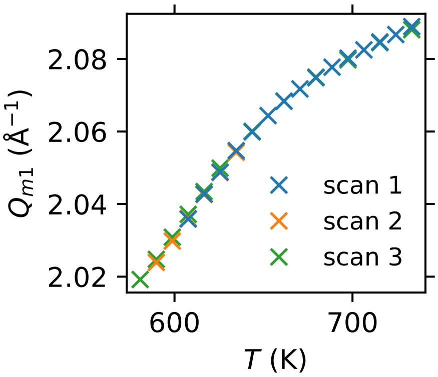

Figure 3: Q position of the center of the first diffraction peak, Q_{m1}, under $P \approx 0$, obtained in our previous work [1]. Three temperture scans were performed in this study, and the results agree with each other.

Comparing Figures 2 and 3, several observations can be made:

1. The Q_{m1} positions at elevated pressures (Figure 2) are significantly higher than those under $P \approx 0$ (Figure 3), as expected.
2. In all cases, Q_{m1} decreases with cooling. This is opposed normal liquid behavior but is consistent with the fact that liquid Te expands upon cooling [1], similar to water.
3. Upon cooling from 700 K to 600 K, the decrease in Q_{m1} at 0.7 GPa (from ~2.120 Å^{-1} to ~2.105 Å^{-1}) is to a much lesser degree than the decrease at zero pressure (from ~2.08 Å^{-1} to ~2.03 Å^{-1}). The degree of decrease is even less at 0.9 GPa (from ~2.130 Å^{-1} to ~2.120 Å^{-1}). Because a larger degree of change is expected when approaching the critical point, this observation suggests that the LLCP is likely closer to zero pressure than it is to 0.7 GPa (cf. Figure 1).

Given observation #3 above, it is important to explore the lower-pressure part of the phase diagram, ideally below 0.5 GPa. This will be the goal of future experiments.

References

[1] P. Sun et al., "Structural changes across thermodynamic maxima in supercooled liquid tellurium: A water-like scenario", *Proc. Natl. Acad. Sci.* **119**, e2202044119 (2022). doi: 10.1073/pnas.2202044119
[2] K. Kim et al., "Maxima in the thermodynamic response and correlation functions of deeply supercooled water", *Science* **358**, 1589–1593 (2017), doi: 10.1126/science.aap8269