Structure of Liquid Chalcogen under Pressure

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Crystalline tellurium is a semi-conductor: the lone-pair states form top of the valence band and anti-bonding states form empty conduction band, while liquid tellurium is metallic. In crystalline tellurium, pressure-induced phase transitions occur at high pressures to phases with larger coordination numbers. To study the structural change of liquid tellurium under pressure we have performed energy-dispersive x-ray diffraction measurements. White x-rays ranging energy up to 150 keV from a bending magnet were used.

Pressure was generated with the two stage compression method, where the first stage is a the six anvils mounted on the DIA guide-block and the second stage consists of eight anvils of tungsten carbide with truncated edges. An octahedral shaped pressure medium of MgO was compressed by the second stage anvils.

To measure the diffraction in a wide angle range, channels were dug on the guide-block and the press was rotated around the vertical central axis. The highest scattering angle, 2θ, where diffraction was measured is 15°.
To check the ability of the collimator for eliminating the diffraction from the surrounding materials around the sample, the x-ray diffraction was measured for liquid silicon with a small x-ray absorption coefficient. Result is shown in Fig. 1.

A sample of tellurium and NaCl mixture was compressed to a disk and then put in a NaCl capsule. The capsule was embedded in the pressure medium. Measurements was done at 7 scattering angles from 3° to 15°.

In Fig. 2, the static structure factor, S(Q), of liquid tellurium measured with a load of 1500 ton is shown. The first peak position of S(Q) is 2.46 A^{-1}, which is larger than that at normal pressure, 2.11 A^{-1}. The sub-peak of S(Q) at 3.1 A^{-1} of liquid tellurium at normal pressure, which corresponds to the correlation between atoms on the same chain, disappears at 18.1 GPa.

Detailed analysis is in progress.

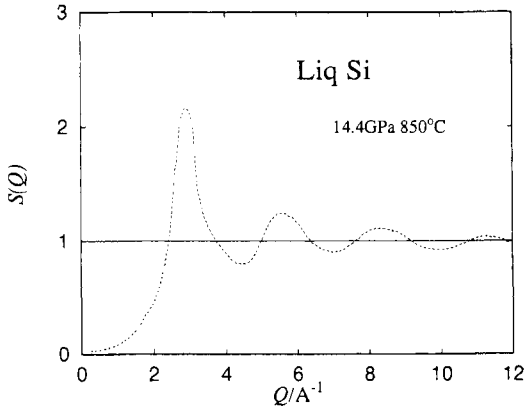

Fig.1 S(Q) of liquid silicon at 14.4 GPa and 850℃.

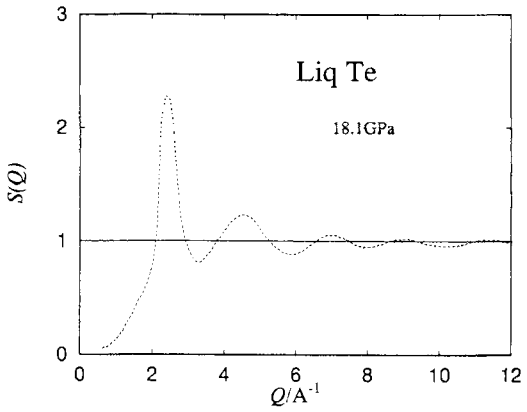

Fig.1 S(Q) of liquid tellurium at 18.1 GPa and 800℃