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# Structural Change in Liquid $SnI_4$ under High Pressure

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The objective of this report is to demonstrate that the liquid form of tintetraiodide, $SnI_4$, takes distinctively different structures in a relatively narrow pressure range at high pressures and high temperatures. At 1.3 GPa and 860K, the liquid consists of regular tetrahedral $SnI_4$ molecules, while they are heavily deformed or dissociated at 2.5 GPa and 980K. It is not yet clear whether the change in liquid structure is associated with a discontinuous 1st order phase transition as black phosphorous[1] or a sharp but continuous pressure evolution.

The melting curve of $SnI_4$ is known to have a sharp kink at ~1.7 GPa[2] and to show remarkable similarity with that of black P. This fact motivated us to search for structural change in liquid $SnI_4$. We have carried out synchrotron radiation x-ray diffraction study at PF-AR NE5C at KEK by using MAX80 and the energy dispersive method. A diamond capsule was used as a sample container to prevent chemical reaction of a sample with surrounding materials and to reduce background noise in diffraction patterns.

Typical structure factor $S(Q)$ for the high-pressure liquid is compared with that for the low-pressure liquid in Fig. 1. The effect of compression can be seen in shifts of the 1st and 2nd peaks to higher $Q$. The shift of the 4th peak from ~7.5 Å$^{-}$ to ~7.0 Å$^{-1}$ in the opposite direction must be associated with structural change in the short range order in the liquid state.

Figure 2 shows corresponding reduced radial distribution functions $G(r)$ obtained by Fourier sine-transform of $S(Q)$. The maxima of the 1st peak, 2.68 Å, and 2nd peak, 4.34 Å, in $G(r)$ at 1.1 GPa, respectively, agree with the Sn-I and the I-I atomic distances in the regular tetrahedral $SnI_4$ molecule. Obviously, the low-pressure liquid form has a molecular character. Note that the shoulder of the 2nd peak on the low $Q$ side arises from intermolecular I-I distances. The molecules are heavily deformed at 2.2 GPa. The ratio $r_2/r_1$ is obtained as 1.35, being much smaller than $(8/3)^{-1/2}$=1.63 for a regular tetrahedron. Structural characterization of the high-pressure liquid form using MD simulation is now in progress[3].

We have revealed the evidence for change in short range order in liquid $SnI_4$ under pressure. Precise measurement of pressure evolution of liquid structure is under way as well as the measurement of the density.

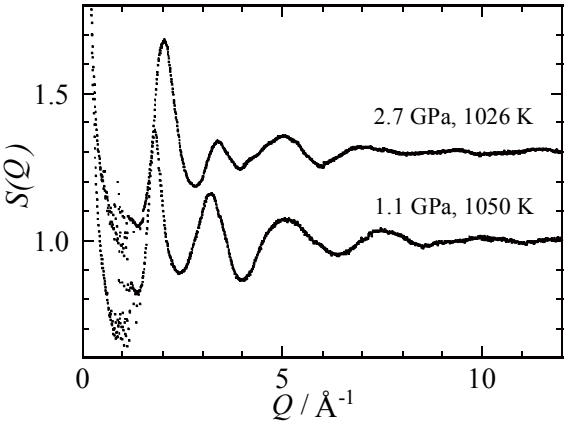


**Figure 1** Structure factor $S(Q)$ for low- pressure and high-pressure liquid forms.

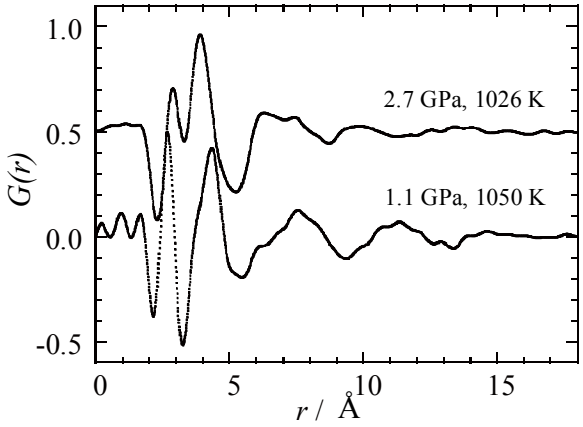


**Figure 2**. Reduced radial distribution fanction $G(r)$ for low-pressure and high-pressure liquid forms.

## References

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