

Structure of Liquid HgTe under Pressure

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Introduction

In order to elucidate the effects of the ionicity in chemical bonding on the structure of covalent liquids, we have investigated the structure of liquid HgTe under pressure. Recently we reported the structure of liquid III-V compounds; GaSb [1], liquid InAs [2] and liquid InSb [3] under pressure. The ionicity of the chemical bonding of HgTe is higher than that of these liquid III-V compounds.

Experimental

X-ray diffraction patterns were taken by an energy-dispersive method using the synchrotron radiation. Pressure was generated by using the multi-anvil high-pressure apparatus, MAX80, installed at AR-NE5C.

Results and Discussion

The static structure factors, $S(Q)$ of liquid HgTe at high pressures are shown in Fig. 1. There exists two main peaks at 2.2 \AA^{-1} and 3.0 \AA^{-1} at low pressures. With increasing pressure, the height of the peak at 2.2 \AA^{-1} increases and the position shifts towards a higher Q -value while the height of the peak at 3.0 \AA^{-1} decreases. On the other hand, the second peak at 4.9 \AA^{-1} shifts towards a lower Q -value in spite of volume contraction. These results show that the local structure of liquid HgTe does not contract uniformly. The ratio of the second peak position to the first peak positions, Q_2/Q_1 , decreases with increasing pressure, which is similar to those of group 14 elements and III-V compounds. It changes from 2.25 at 0.3 GPa to 2.05 at 8 GPa. Typical values of the ratio are 2.6-2.7 for liquids with the zincblende-like local structure, 2.09-2.12 for liquids with the NaCl-like local structure and about 1.92 for liquid Sn between 2 GPa to 19 GPa and for liquid InSb above 10 GPa.

The pair distribution functions, $g(r)$ was obtained by the Fourier transformation of $S(Q)$. The first peak position, r_1 , of $g(r)$ does not change or rather shifts towards a larger r -value and its height increases with increasing pressure. It suggests that strong covalent bonds between atoms remain under high pressure. The second peak shifts towards a smaller r -value with volume contraction. With increasing pressure, a hump, which appears on the right hand side of the first peak, becomes small and approaches the first peak. The coordination number CN_1 of liquid was evaluated by integrating the radial distribution function $4\pi r^2 n g(r)$ up to r_1 and multiplying two. The value of CN_1 increases continuously from four at 0 GPa to six at 8 GPa.

These results suggest that the local structure of liquid ZnTe changes continuously from the NaCl-like structure

to another high-pressure local structure. Candidates for the local structure may be the CsCl structure, which is a bcc structure without chemical ordering, and the high pressure form of liquid tin or liquid III-V compounds.

The pressure dependence of the local structure is alike among liquid HgTe, CdTe and ZnSe, although the pressure width where structural changes occur is different. The local structure changes from the zincblende-like structure to the NaCl-like structure, and then into another high-pressure form. The pressure dependence of the local structure of liquid compounds with high ionicity in the bonds is similar to those of crystals. This is in contrast with the quite different pressure dependence of the liquids from that in the crystals with less ionicity in the bonds.

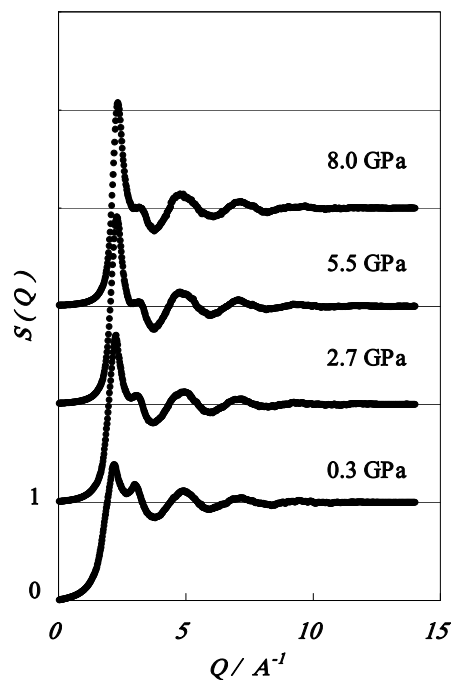


Fig. 1. $S(Q)$ of liquid HgTe at several pressures.

References

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