

Structure of liquid II-VI compounds 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 II-VI compounds; liquid CdTe, liquid HgTe and liquid ZnSe under pressure. Recently we reported the structure of liquid III-V compounds; liquid GaSb [1], liquid InAs [2] and liquid InSb [3] under pressure. The ionicity of the chemical bonding of II-VI compounds is higher than that of these 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 II-VI compounds at several high pressures are shown in Fig. 1. We can see the similarity in the shape of $S(Q)$ among liquid ZnSe, liquid CdTe and liquid HgTe [4-6].

The pair distribution functions, $g(r)$ was obtained by the Fourier transformation of $S(Q)$. The value of r_1 , the first peak of $g(r)$ of liquid ZnSe at 1.7 GPa and 4.3 GPa is almost the same as the value of crystalline ZnSe with zincblende structure. For liquid CdTe below 2 GPa, it is almost the same as its crystalline value with the zincblende structure and above 2 GPa it is almost the same as its crystalline value with the rocksalt structure. For liquid HgTe, at low pressure it is almost the same as its crystalline value with the rocksalt structure and increases with increasing pressure.

From the comparison of the pressure dependence of $S(Q)$ and $g(r)$ it is concluded that 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 rocksalt-like structure and then to 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 local structure of liquids from that in the crystals with less ionicity in the bonds.

For liquid HgTe, the structural change occurs continuously in contrast with the sharp change in liquid CdTe. This may be related to the presence of the

intermediate structures between the zincblende structure and the rocksalt structure and above the rocksalt structure.

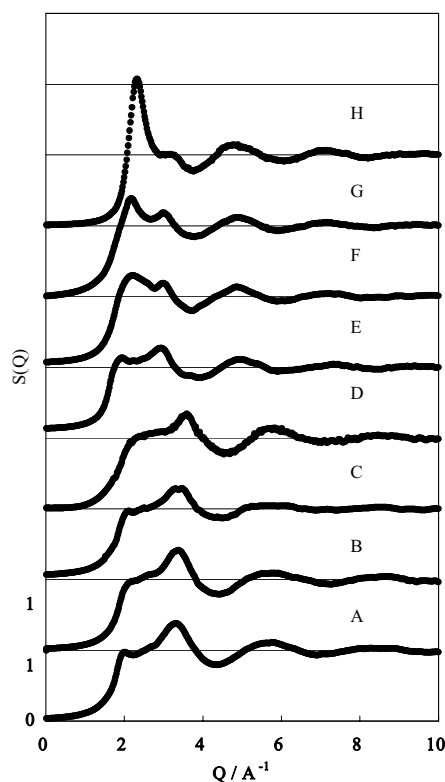


Fig. 1. $S(Q)$ of liquid II-VI compounds. A: liquid ZnSe at 1.7 GPa, B: liquid ZnSe at 4.3 GPa, C: liquid ZnSe at 5.5 GPa, D: liquid ZnSe at 7.3 GPa, E: liquid CdTe at 0.5 GPa, F: liquid CdTe at 3.0 GPa, G: liquid HgTe at 0.3 GPa and H: liquid HgTe at 8 GPa.

References

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