

Structure of liquid I-VII 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 I-VII compounds under pressure. Recently we have reported the pressure dependence of the local structure of liquid III-V and II-VI compounds [1-6]. The ionicity of I-VII compounds is higher than that of III-V compounds. The local structure of liquid CuX (X=Cl, Br and I) is known to be different from that of the typical ionic liquids, in which the pair correlation functions between cation-cation correlation function and anion-anion correlation function is same. In the crystalline phase, CuI has a superionic conductive phase in which Cu ions distributed in disordered structure. Presence of ionic bonding and covalent bonding is expected in both crystalline and liquid phases. It is interesting to investigate the pressure dependence of the local structure of liquid CuX.

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 factor $S(Q)$ of liquid CuI at several pressures is shown in Fig. 1. With increasing pressure, the peak position of the first peak shifts towards higher Q . On the other hand the peak position of the second peak shifts towards higher Q up to 4.1 GPa and then shifts to lower Q above 5.1 GPa. If the structure of liquid contracts uniformly, the shape of $S(Q)$ expands to higher Q without changing its height. Therefore, above change of the second peak suggests that the drastic change in the local structure of liquid CuI occurs between 4.1 GPa and 5.1 GPa. The ratio of Q_2/Q_1 changes from 1.70-1.66 below 4.1 GPa to 1.60 above 5.1 GPa.

The pair distribution functions, $g(r)$ was obtained by the Fourier transformation of $S(Q)$. The change in the value of r_1 , the first peak position of $g(r)$ of liquid is small while r_2 , the second peak position of $g(r)$ decreases and becomes narrow with increasing pressure. The ratio of r_2/r_1 decreases from 1.63 at 0.8 GPa to 1.44 at 6.6 GPa. The value of r_2/r_1 is 1.63 for the zincblende structure and 1.41 for the α -AgI structure. It suggests that Cu ions locate in the space of tetrahedral site between I ions below 4.1 GPa and other site above 5.1 GPa such as tetrahedral site of α -AgI structure.

X-ray diffraction of liquid CuBr and liquid CuCl was also measured under high pressure. Detailed analysis is in progress.

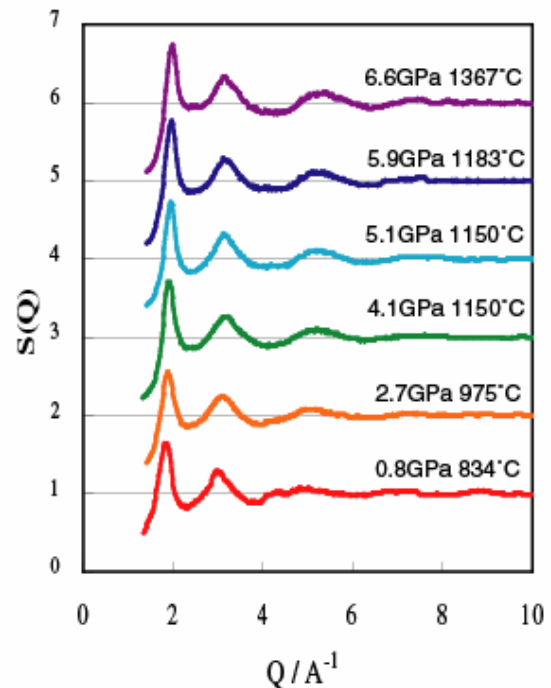


Fig. 1. $S(Q)$ of liquid CuI at several pressures.

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