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Structure of liquid copper halides under pressure

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Introduction

The pressure dependence of the local structure of liquid group 14 elements and liquid III-V compounds is different from that of crystal: The structural change occurs continuously in a wide pressure region below the transition pressure of crystal. And the local structure at high pressures is different from that of crystal [1, 2]. On the other hand, in liquid CdTe a structural transformation occurs in a narrow pressure width at almost the same pressure as the transition pressure of crystal [3]. The local structure of liquid copper halides at normal pressure was investigated and anomalous copper-copper pair distribution function was reported [4]. In the crystalline phase, super-ionic conduction indicates the broad distribution of copper-copper pair distribution function.

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

Fig.1 shows the *S(Q)* of liquid CuCl. For liquid CuCl, CuBr and CuI, *S(Q)* change their shape continuously with increasing pressure, in contrast with a sharp structural change in liquid CdTe [3], indicating anisotropic compression of the local structure. Fig. 2 shows the *g(r)* of liquid CuCl. With increasing pressure, the subpeak at about 4 Å shift towards smaller r, while the peak position of the first peak does not change. The pressure dependences of the coordination number *CN* and the peak position ratio r_2/r_1 of *g(r)* show that Cu atoms locate in the tetrahedral site and then in the octahedral site. The transition pressure of the copper position from the tetrahedral to the octahedral site increases from liquid CuCl to liquid CuI, similar to the crystals. At higher pressures, the local structure is similar to the intermediate structure between NaCl and CsCl structure. In liquid copper halides with large ionicity in the bonding between atoms, the pressure dependence of the local structure is similar to the crystals; the chemical order remains in the liquids.

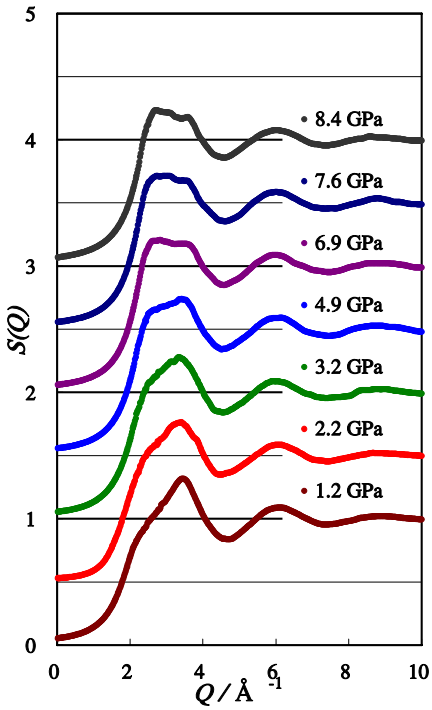

Figure 1. *S(Q)* of liquid CuCl at various pressures

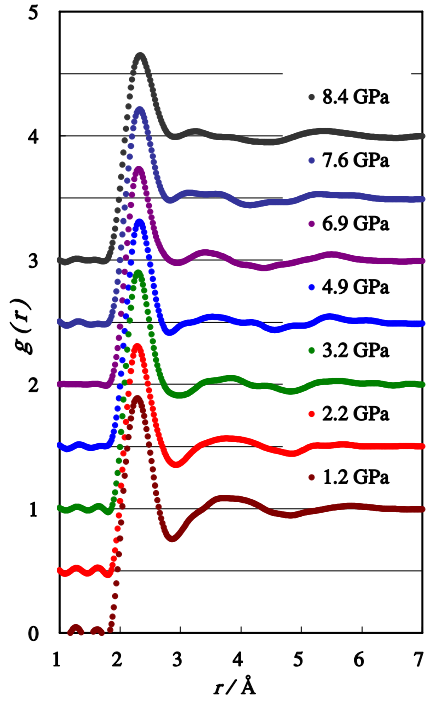

Figure 2. *g(r)* of liquid CuCl at various pressures

References

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