

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, in which bonds between atoms have large ionicity, a structural transformation occurs in a narrow pressure width at almost the same pressure as the transition pressure of crystal [3]. Anomalous copper-copper pair distribution function of liquid copper halides 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

Static structure factor $S(Q)$ of liquid CuCl, liquid CuBr and liquid CuI 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.

The ratio of r_2/r_1 is plotted in Figure 1 for liquid CuI, liquid CuBr and liquid CuCl. When the copper atom locates in the tetrahedral site of the fcc sublattice of the anions (zincblende structure), the ratio of r_2/r_1 is 1.63. The ratio is 1.55 for tetrahedral site of the bcc sublattice (alpha-AgI structure) and is 1.41 for octahedral site of the fcc sublattice (NaCl structure). With increasing pressure, r_2/r_1 ratio decreases continuously indicating the transition of the position of copper atoms from the tetrahedral site to the octahedral site. As the value of $g(r)$ at the first minimum increases with increasing pressure, it is difficult to evaluate the coordination number from the integration of the radial distribution function. Therefore, to analyze the local structure, the value of $g(r)$ at the $1.41 r_1$, $1.55 r_1$, and $1.63 r_1$ are plotted in Figure 2 for liquid CuI. Below 6 GPa, the value at $1.63 r_1$ for tetrahedral site of the fcc sublattice and the value at $1.55 r_1$ for tetrahedral site of the bcc sublattice have large values and begin to decrease at about 6 GPa. Above 6 GPa, the value at $1.41 r_1$ for octahedral site of the fcc sublattice has a large value

suggesting the six-fold coordination structure. 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.

References

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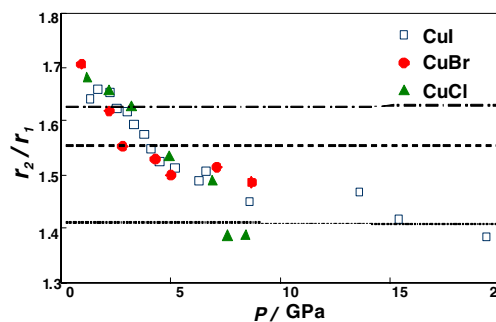


Figure 1. Pressure dependence of r_2/r_1 of liquid CuI, liquid CuBr and liquid CuCl. The chain line: the value for the tetrahedral site in the fcc sublattice (zincblende structure). The dashed line: the value for the tetrahedral site in the bcc sublattice (alpha-AgI structure). The dotted line: the value for the octahedral site in the fcc sublattice (NaCl structure).

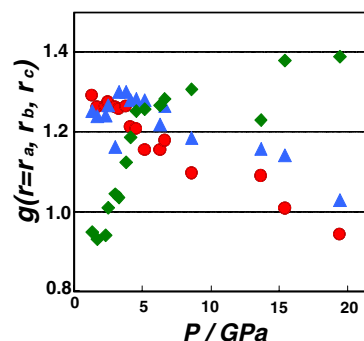


Figure 2. The values of $g(r)$ at $r_a=1.63 r_1$ (circle), $r_b=1.55 r_1$ (triangle), and $r_c=1.41 r_1$ (square) of liquid CuI.