Local structural properties of CuI at low temperatures

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Abstract
This study examined the local structural properties of CuI at low temperatures of 10–300 K by x-ray diffraction (XRD) and extended x-ray absorption fine structure (EXAFS) measurements at the Cu K edge. The XRD data were refined using two models, split (distorted zinc-blende structure) and non-split (zinc-blende structure), using a conventional Rietveld refinement combined with a maximum entropy method (MEM). MEM/Rietveld analyses showed that both the split and non-split models could fit the data. EXAFS revealed the split model fit to be better than the non-split model. The split distance of Cu–I pairs was approximately 0.03 Å at 15 K and increased to 0.07 Å at 300 K. XRD and EXAFS combined together suggested that the CuI crystal was in a metastable state with a distorted zinc-blende structure at low temperatures.

Q.2 (Some figures in this article are in colour only in the electronic version)

1. Introduction

Cuprous(I) halides (CuCl, CuBr, CuI), which are ‘binary’ (containing only two elements) metal halides, are representative ionic crystals with a rich phase diagram, and they exist in several crystalline forms. The structural behavior of cuprous(I) halides has been studied intensively, both experimentally and theoretically, and has been reported to show some interesting pressure-[1] and temperature-dependences [2–11]. Cuprous(I) halide crystals have three stable crystalline phases in different temperature regions, such as a zinc-blende (ZB) structure below 390 °C (γ-CuI), a wurtzite (WZ) structure between 390 and 440 °C (β-CuI), and a cubic structure above 440 °C (α-CuI). The structural transitions of cuprous(I) iodide depending on the temperature were examined by Raman spectroscopy [2], x-ray and neutron powder diffractions [3–10], and extended x-ray absorption fine structure (EXAFS) [11]. These measurements were analyzed using various crystalline structural models, including F43m, P6/mC, P6m2, and P3m1.

Previous studies concentrated mainly on superionic behavior [11] and structural transitions [1, 2, 5–10] at high temperatures above 300 °C, because cuprous(I) halides exhibit ionic conductivities comparable to those of molten salts while still in the solid phase (~0.1 Ω−1 cm−1) [12, 13]. On the other hand, Miyake et al reported that CuI did not have a cubic structure near 200 °C, suggesting the presence of metastable positions for copper atoms at the intermediate temperatures [3]. Recently, Adipranoto et al reported the possibility of split positions of copper atoms in a γ-CuI crystal at 300 K as well as in an α-CuI crystal at 773 K [14]. Those studies showed that the structural transition of ZB to WZ in CuI might not occur at a certain temperature but change gradually with increasing temperature. A ZB structure is cubic whereas a WZ structure is hexagonal. However, the local structures of the two phases are very similar. An atom in ZB has four neighboring atoms at the same distance whereas one neighboring atom distance is...
Table 1. XRD refinement of CuI powder for the non-split and split models at different temperatures. $T$ is temperature, $d$ is the mean distance of the iodine–copper pairs, $\chi^2$ and $R_p$ are the factors for the goodness of fit, and $P$ is the displacement of the copper position from the crystalline symmetry of a ZB structure, (1/4, 1/4, 1/4).

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Non-split model</th>
<th>Split model</th>
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<tr>
<td></td>
<td>$d$ (Å)</td>
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</table>

Figure 1. XRD pattern of CuI powder at different temperatures. The circles and lines are the data and best fits, respectively. The bars under the data indicate the positions of the calculated Bragg peaks by using the non-split model. The difference between the data and fit is shown at the bottom of each figure.

shorter than the others in WZ. The transition of ZB to WZ can be started by a slight position shift of the atoms.

ZB and WZ crystals are distinguishable simply by diffraction measurements. However, a small structural distortion can only be detected by precise measurements and analysis. This paper reports the local structural properties of cuprous(I) iodine below room temperature, which information will offer valuable insights into this interesting class of industrial materials. The structural properties were examined by x-ray diffraction (XRD) and EXAFS at low temperatures of 10–300 K. The powder XRD data were refined with a Rietveld refinement and a maximum entropy method (MEM) [15–17]. MEM/Rietveld analyses provide a local displacement of each atom, while EXAFS can detect the local structural properties around a selected specific element, including the bond length, bond length distribution, coordination number, and atomic species [18–20]. The distribution of atomic positions was examined by MEM/Rietveld analyses and the bond length distributions of atomic pairs were determined by EXAFS at low temperatures. XRD and EXAFS data were analyzed quantitatively with two models of split and non-split. A non-split model is identical to a ZB structure ($F\bar{4}3m$) and the locations of iodine and copper atoms were (0, 0, 0) and (1/4, 1/4, 1/4) in a ZB symmetry, respectively. However, for the split model, the copper position was displaced slightly from (1/4, 1/4, 1/4). In the split model based on a ZB structure, three bond lengths of the four Cu–I pairs are elongated when a Cu ion moves toward an I ion. This is similar to the local structure of atomic pairs in a WZ structure.

2. Experimental details

Commercial CuI powder (Aldrich) with a purity of 99.999% was used for the XRD and EXAFS measurements. Powder XRD measurements were performed at the 8C2 beamline of the Pohang Light Source (PLS). For the temperature dependent XRD measurements, CuI powder was filled uniformly into the sample holder cooled to 10 K in a closed-cycle-type refrigerator. For the XRD measurements, the x-ray wavelength of 1.5490 Å was used and the incident x-ray angle was fixed to 7°. The special resolution of the beamline was $\Delta d/d = \sim 10^{-5}$. For the EXAFS measurements, CuI powder was ground and sieved with a 25 μm sieve. The sieved powder was spread uniformly on a Scotch tape and folded to have the sample with absorption edge step of approximately 1.0. The powder sample was then placed inside a closed-cycle-type refrigerator and cooled to 15 K for EXAFS experiments. The EXAFS measurements were performed at the Cu K edge (8979 eV) in transmission mode at the 3C1 beamline of PLS. The incident x-ray energy was selected using a three-quarters turned Si(111) monochromator.

3. Results and discussion

Powder XRD data were obtained at various temperatures, and some representative data are shown in figure 1. The XRD data were analyzed using a conventional Rietveld method for the split and non-split models described above. Figure 1 shows that the XRD patterns agree with a ZB but WZ phase for all Q.3 temperatures. Table 1 lists the fitting results. Our analysis
Figure 2. Electron density distributions projected in (a) the (001) plane and (b) the (110) plane were determined by MEM of a CuI powder at 10 K. (c) The charge density distribution of the Cu site in the (110) plane and (d) the cross section of (c) along the vertical direction crossing the middle of the peak. (e) A ZB structure (F43m, γ-CuI).

demonstrates that both models of split and non-split fit the data equally well. The difference in the fitting results of the two models to the XRD data was negligible, when the $\chi^2$ and $R_p$ factors of the two models were compared. The bond length of the Cu–I pairs was elongated by 0.01 Å for the non-split model fit whereas it remained constant for the split model fit with increasing temperature. The bond length difference of the Cu–I pairs determined using the two models was approximately 0.04 Å.

Cu–I pairs have a tetrahedron structure in ZB CuI, as shown in figure 2(e). The charge distribution of Cu and I ions in a ZB structure is spherical symmetry. However, the charge distribution will be different from that of ZB CuI, if CuI has a distorted ZB structure. Figure 2 shows the charge density distributions obtained using a MEM-based pattern fit [15–17] in the Rietveld refinement with a split model. The middle atom with a circular shape in figure 2(a) is an iodine atom and the four square shaped atoms around the middle iodine atom are copper atoms. The charge density distribution of the copper site exhibits square and triangular shapes in the projections of the (001) and (110) planes, respectively, as shown in figures 2(a) and (b). MEM/Rietveld analyses with the split model showed that the charge density distribution was elongated slightly to the four iodine sites. This asymmetric charge density distribution of Cu ions agrees with a previous study using neutron diffraction measurements at higher temperatures [14]. Figures 2(c) and (d) show the intensity of the charge density distribution of a copper site in the projection of the (110) plane in figure 2(b). The intensity distribution demonstrates more clearly the displacement of copper atoms to the iodine atom sites. Since XRD detects average distance between atomic planes, it is intrinsically limited in describing the exact local structures of atoms in a distorted crystalline system.

Figure 3. (a) Normalized total x-ray absorption from CuI powder at the Cu K edge as a function of the incident x-ray energy at 15 and 300 K. The dotted line denotes the Cu foil measured at 300 K. (b) EXAFS ($k\chi$) at different temperatures as a function of the photoelectron wavenumber.

In order to probe possible local distortion and go beyond the limitations of XRD, we carried out EXAFS measurements. EXAFS can detect the local structural properties around a selected specific species atom. We examined the local structural properties around the copper atoms in the CuI crystal using EXAFS. Figure 3(a) shows the total x-ray absorption spectra from the CuI powder near the Cu K edge as a function of the incident x-ray energy. x-ray absorption near edge structure (XANES) is sensitive to the chemical valence state of the probe atom, and the energy band structure around the probe atom [21]. The XANES of the CuI powder was quite different.
The small bump at 4.2 of CuI, a Cu atom has four I atoms as the first neighbors at fully occupied mode, i.e. a ZB structure. In the ZB structure can be obtained by fitting the data to an EXAFS theory [25].

Increasing temperature. The detailed structural information however, the peak positions did not change significantly with increasing temperature. The EXAFS showed that the intensity decreased gradually with increasing temperature. The peak positions in the EXAFS were not counted. EXAFS showed that longer than the peak positions because the phase shift of the photoelectrons was not counted. EXAFS showed that the EXAFS was extracted from the measured data as a function of the photoelectron wavenumber, \( k \), the EXAFS was determined from that of Cu foil. The XANES data appear to be almost unchanged over the temperature range of 15–300 K, implying that the chemical valence state of Cu atoms and the energy band structure of the CuI remain unchanged in the temperature range.

Local structural information can be obtained by examining small oscillations (EXAFS) above the absorption edge [18–20]. After the atomic background was determined using the AUTOBK code (part of IFEFFIT package [22, 23]), the EXAFS was extracted from the measured data as a function of the photoelectron wavenumber, \( k = \sqrt{2m(E - E_0)/\hbar} \), where \( m \) is the electron mass, \( E \) is the incident x-ray energy, and \( E_0 \) is the edge energy. Three scans were taken at each temperature and appear to be identical, as shown in figure 3(b). The EXAFS signal changed gradually with increasing temperature. The EXAFS data in the region 2.5–11.0 Å\(^{-1} \) were Fourier transformed to \( r \)-space, as shown in figure 4(a).

The EXAFS data were analyzed using the IFEFFIT package [22, 23] and a standard analysis procedure [24]. The peak positions in the \( r \)-space correspond to atomic shells around a Cu atom in the CuI specimen. The true bond lengths of the atomic pairs were approximately 0.3 Å longer than the peak positions because the phase shift of the photoelectrons was not counted. EXAFS showed that the intensity decreased gradually with increasing temperature. However, the peak positions did not change significantly with increasing temperature. The detailed structural information can be obtained by fitting the data to an EXAFS theory [25].

For a start, we began our analysis by using a non-split and fully occupied mode, i.e. a ZB structure. In the ZB structure of CuI, a Cu atom has four I atoms as the first neighbors at 2.3 Å and 12 Cu atoms at 4.0 Å. The small bump at 4.5 Å in figure 4(a) is due to Cu–I–Cu multiple scattering and the peak at 4.9 Å is due to the next Cu–I single scattering. The data in the range of 1.5–5.5 Å were fitted. For the analysis, we included these four scatterings while varying \( E_0 \), bond lengths, and Debye–Waller factors (\( \sigma^2 \), including thermal vibration and static disorder) at the same time. The parameters (bond length and \( \sigma^2 \)) of multiple scattering were fixed to a combination of the Cu–I and Cu–Cu pairs. The fits were reasonably good at all temperatures, as shown in figures 4(b)–(e). From the fit, \( E_0 \) was determined to be 8984 eV, which was reasonable, as compared to the XANES shown in figure 3. Table 2 summarizes the results of the best fits.

EXAFS determined the first and second shell bond lengths to be 2.61 and 4.28 Å, respectively, at 15 K, as shown in figures 5(a) and (b). This agrees well with the XRD Rietveld result. The bond length of the Cu–I pairs decreased slightly with increasing temperature, whereas the bond length of the Cu–Cu pairs remained almost constant within uncertainty, as shown in figures 5(a) and (b). This result indicates that the volume of the CuI powder did not change much in the temperature range. The decrease of Cu–I bond length with increasing temperature could be due to the non-Gaussian

### Table 2

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<th>Model</th>
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<th>( d ) (Å)</th>
<th>( \sigma^2 ) (Å(^2 ))</th>
<th>( N )</th>
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distribution of the bond length. A non-Gaussian bond length distribution was examined in the fits but its contribution was negligible within uncertainty. At higher temperatures, the bond length of Cu–I pairs determined by EXAFS was slightly shorter than that of a non-split XRD fit. In general, a bond length determined by EXAFS is equal to or slightly longer than that of XRD because XRD measures the average distance of atomic planes whereas EXAFS detects directly the average distance of an atomic shell. The results of EXAFS and non-split XRD suggested that the non-split model might be incorrect. In the non-split model the bond lengths of Cu–I pairs cannot be varied individually. A split model fit was examined alternatively.

In the split model, one of the four neighboring iodine ions was located at a shorter distance from a Cu ion than the other three iodine ions in a ZB structure. The first peak at 2.5 Å in figure 3 was contributed by only Cu–I pairs. The Cu–I bond lengths could be determined independently from the atomic pairs. The split model also fitted to the data and was barely distinguishable from the non-split model fit by the naked eye, as shown in figures 4(b)–(e). The comparison of the goodness of fit factors of R-factor and reduced-χ²s for the two model fits can clarify which model fit is better than the other. The R-factor and reduced χ² of the fits were determined as follows:

\[ R_f = \sum_{i=1}^{N} \frac{|k^3 \chi_{\text{theory}}(r_i) - k^3 \chi_{\text{data}}(r_i)|^2}{|k^3 \chi_{\text{theory}}(r_i)|^2}, \]

\[ \chi^2_v = \frac{N_i}{N(N_i - N_{\text{var}})} \sum_{i=1}^{N} \frac{|k^3 \chi_{\text{data}}(r_i) - k^3 \chi_{\text{theory}}(r_i)|^2}{\epsilon^2(r_i)}, \]

where \( k^3 \chi(r_i) \) is EXAFS with a \( k^3 \) weight;

\[ \chi^2_v = \frac{N_i}{N(N_i - N_{\text{var}})} \sum_{i=1}^{N} \frac{|k^3 \chi_{\text{data}}(r_i) - k^3 \chi_{\text{theory}}(r_i)|^2}{\epsilon^2(r_i)}, \]

where \( N_i \) is the total number of independent data points, \( N_{\text{var}} \) is the number of fit variables, and \( \epsilon(r_i) \) is the total error at \( r_i \). The \( R_f \) and \( \chi^2_v \) values of the non-split model fit of the EXAFS data at 15 K were 0.016 and 8.0, respectively, whereas they were 0.007 and 4.0 for the split model fit, meaning that the split model fit is better than the non-split model fit. We have extended the analysis to other temperatures to find that the fits of the EXAFS data to the model fit were better than the fits to the non-split model over the entire temperature range, 15–300 K. Table 3 summarizes the goodness fit factors. The EXAFS data suggested that the Cu atoms in the CuI crystal were displaced slightly from the (1/4, 1/4, 1/4) site in the ZB structure below room temperature.

Figure 5(c) shows the short and long bond lengths of the Cu–I pairs determined by fitting the EXAFS data using the split model. The split model fits showed that the long bond length remained nearly constant in the temperature range 15–300 K, whereas the short bond length gets decreased gradually with increasing temperature. The difference in the two bond lengths increased with increasing temperature. The average bond length (closed circle) in figure 5(c) was obtained by summing the two bond lengths with a weight, as \( \langle d \rangle = \frac{1}{3} \times d_{\text{long}} + \frac{1}{3} \times d_{\text{short}} \). The average bond length decreased slightly above 250 K. We note that the short length of the Cu–I pairs is similar to the distance determined by XRD using the split model whereas the long and average lengths are larger than those of the XRD results. This is further evidence that the split model is better than the non-split model.

The peak intensities of the EXAFS data decreased dramatically with increasing temperature, as shown in figure 4(a), meaning that the thermal vibrations of the atomic pairs are substantially large. The measured \( \sigma^2 \) is affected by thermal vibrations and static disorder. The thermal vibrations depend on the temperature whereas the static disorder is independent of temperature. The thermal vibrations and static disorder can be determined by fitting the measured \( \sigma^2(T) \) to

Table 3. Goodness fit factors of EXAFS data obtained from the best fits with the two models described in the text at different temperatures. \( R_f \) and \( \chi^2_v \) are the R-factor and reduced-χ², respectively.

<table>
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<th>T (K)</th>
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<th>Split model fit</th>
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<td>( R_f )</td>
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<tr>
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the Einstein model,

\[ \sigma^2(T)_{\text{meas}} = \sigma^2_{\text{static}} + \frac{\hbar^2}{2\mu K_B \theta E} \coth \left( \frac{\theta E}{2T} \right), \]

where \( \mu \) is the reduced mass of an atomic pair, \( K_B \) is the Boltzmann’s constant, and \( \theta E \) is the Einstein temperature. Figures 6(a) and (b) show the measured \( \sigma^2 \) values and best fits with the Einstein model. The measured \( \sigma^2 \) values were determined by EXAFS data fits with the split and non-split models. The difference between the two models was negligible. The static disorders (\( \sigma^2_{\text{static}} \)) of the Cu–I and Cu–Cu pairs were 0.0 Å² and 0.0016 Å², respectively, suggesting that the static disorder of all atomic pairs in the CuI powder is negligible. EXAFS revealed no vacancy in any of the atomic sites, as summarized in table 2.

In a ZB structure, the bond lengths of four Cu–I pairs are equal. The crystal can have a distorted ZB structure that is similar to the WZ local structure, if one bond length is shorter than the others by moving a copper ion toward an iodine ion. In CuI crystals with a WZ structure (\( \beta \)-CuI), Cu(I) has four I(Cu) neighbors with one short and three long distances and 12 Cu(I) neighbors with six short and six long distances. XRD can show the difference between ZB and WZ structures. However, the difference between ZB and distorted ZB structures is not simple. The bond length of the Cu–I pairs is essential for distinguishing between ZB and distorted ZB structures. The EXAFS data were better fitted to the split model than the non-split model while the XRD data could be fitted to both models. We stress that EXAFS determines local structural properties more precisely than XRD because EXAFS detects the mean distance of an atomic shell from a selected atom whereas XRD measures the average distance between the atomic planes. Our EXAFS analyses indicated that the copper ions moved toward the iodine ions, which corresponded to our MEM/Rietveld analyses. We note that EXAFS revealed neither static disorder nor vacancies in a CuI crystal. These results strongly suggested that a CuI crystal has a distorted ZB structure at low temperatures. These results agree well with a previous report of a metastable state at low temperatures [3].

4. Conclusions

The structural properties of a CuI crystal were examined by XRD and EXAFS at 10–300 K. The XRD data were analyzed by MEM/Rietveld refinements using the split and non-split models for a copper site. The XRD data were refined well by both models. MEM/Rietveld analyses with the split model suggest that a copper atom moved toward an iodine site. EXAFS, which showed a better fit with the split model than the non-split model, confirmed the displacement of a copper atom to an iodine atom. EXAFS revealed neither static disorder nor vacancies in a CuI crystal. These XRD and EXAFS results suggest that the CuI crystal has a distorted ZB structure at low temperatures. EXAFS showed that the bond length difference of Cu–I pairs increased gradually with increasing temperature. This suggests that a structural phase transition from \( \gamma \)-CuI to \( \beta \)-CuI does not occur suddenly at a certain temperature.

Acknowledgments

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