Magnetic properties of α-HgI_2

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1. Introduction

Mercuric iodide has been studied for 40 years due to its efficiency as room temperature x (or γ) rays detector. Compared to commercial γ-ray detectors such as Ge semiconductor detectors, mercuric iodide does not need to cool down to liquid nitrogen temperature due to its large band gap (2.15 eV). In addition, mercuric iodide has other advantages such as high efficiency, low leakage current, less degradation, low electron-hole pair creation energy of 4.2 eV, and high atomic number (Hg : 80 and I : 53) [1-2]. On the other hand, mercuric iodide undergoes a structural phase transition from orthorhombic structure (yellow phase, β-HgI_2) to tetragonal structure (red phase, α-HgI_2) at 127 ℃. Interestingly, it is reported that the magnetic susceptibility of α-HgI_2 shows an anomaly around 60 ℃ [3]. They claim that the anomaly is related to the orange-red phase transition where the orange phase is a tetragonal structure with space group $I4_1/amd$ and has one dimensional disorder along c-axis. In this paper, we performed x-ray diffraction experiment at high temperatures and tried to reveal the relation between the magnetic susceptibility anomaly and the orange-red phase transition.

2. Methods and Results

α-HgI_2 was grown by an oil bath furnace, which is known as the best way to grow the high quality single crystals. For the structural analysis at high temperatures, we used an X-ray diffraction apparatus fabricated by PANalytical whose model name is Empyean. Since the X-ray diffraction patterns are obtained by a powder method, α-HgI_2 singly crystals are grinded and put on a glass. Figure 1(a) shows the X-ray diffraction pattern of α-HgI_2 single crystal at 25 ℃. A broad peak and high background below 30° may be originated by glass. All peaks are well coincide with the α-HgI_2 phase as shown in the index, indicating that the samples does not include any impurity phase. The X-ray diffraction patterns at 70 ℃ and 100 ℃ are shown in Fig 1(b) and Fig 1(c), respectively. Although overall feature of all the x-ray diffraction patterns is almost same, one can observe peak shifts and splitting due to temperatures. This will discuss later in conjunction with the magnetic properties of the mercuric iodide.

Fig. 2 shows the temperature dependence of magnetic susceptibility for the mercuric iodide. The magnetic susceptibility displays almost temperature independent up to about 350 K. Since the mercuric iodide does not contain partially filled d or f shell, it is natural that the diamagnetic signal appears from the low temperature to room temperature. Interestingly, when the temperature increases, the magnetic susceptibility increases rapidly over 350 K.

In order to investigate the magnetic susceptibility anomaly around 60 ℃, it is crucial to check a crystal structure changes by using x-ray at high temperatures. The overall x-ray patterns of α-HgI_2 at different temperatures are similar to all the range of the 2θ angle. However, the enlarged (102) peaks represent temperature dependences, as shown in Fig. 3(a). The (102) peak shows a left shift by increasing the temperature. Since the d-spacing becomes larger by increasing the temperature, the left shift is normal. The other interesting thing is that the peaks become sharper by increasing the temperature.

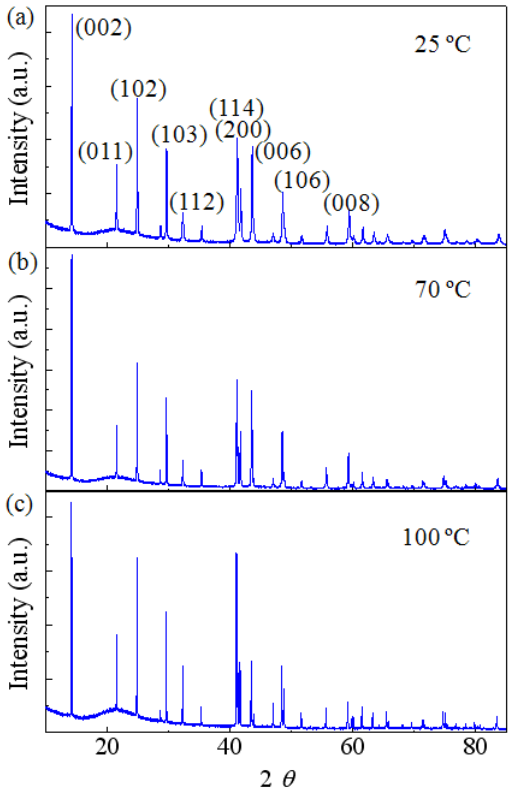

Fig. 1. X-ray diffraction pattern at 25 ℃ (a), 70 ℃ (b), and 100 ℃ (c)

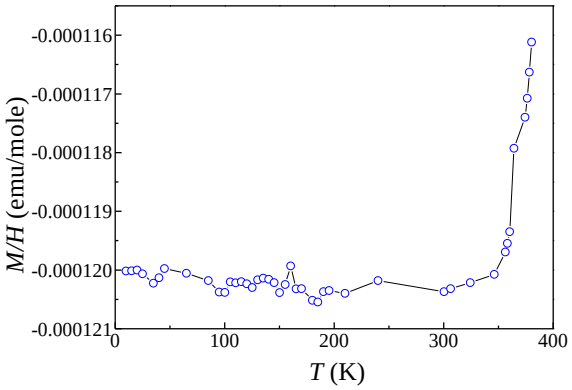

Fig. 2. Temperature dependence of magnetic susceptibility for the mercuric iodide.

This means that a better crystallinity is formed at higher temperature. On the other hands, some peaks such as (114) and (200) peaks display a clear separation by increasing the temperature, as shown in Fig. 3(b). This separation is not originated from the orange color phase, which can be found easily based on the X-ray powder diffraction database. In other words, the magnetic susceptibility anomaly around 60 ℃ may have another reason.

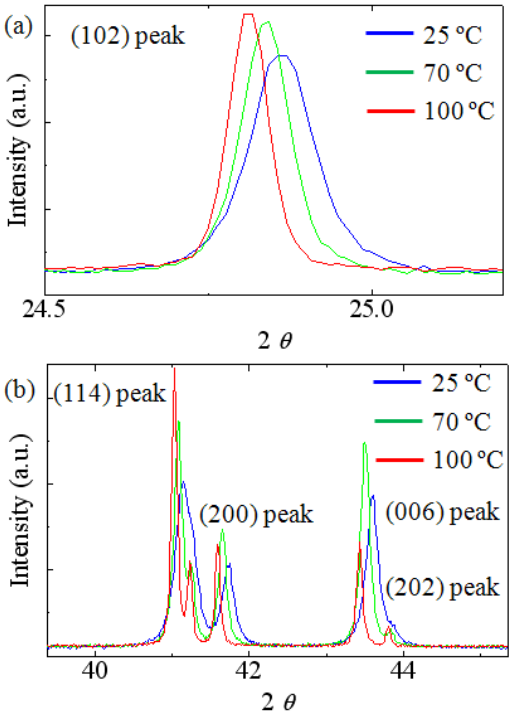

Fig. 3. X-ray diffraction pattern for (102) peak (a) and (114), (200), (006), and (202) peaks at different temperatures (b)

Generally speaking, when certain planes are mixed up, then most physical properties including magnetic susceptibility are compensated each other. And hence, at room temperature, the mixed plane and a coarse crystallinity give rise to the reduced diamagnetic susceptibility. In other words, the higher temperature yields the larger diamagnetic susceptibility due to the peak splitting and better crystallinity.

3. Conclusions

The high temperature x-ray diffraction patterns notify that the magnetic susceptibility anomaly of α-HgI_2 around 60 ℃ may originate from ordering (114) and (200) and (006) and (202) plane rather than orange-red phase transition. Generally, mixed crystal planes are compensated magnetic signals each other. And, hence, the ordered crystal planes and better crystallinity can be the reasonable origin for the enhanced diamagnetic susceptibility at high temperature.

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