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Analysis of Structural Phase Transition of New Oxide Ion Conductor, $Ba_2In_2O_5$ –Significance of Synchrotron X-Ray Diffraction at High Temperatures-

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Although $Ba_2In_2O_5$ shows low oxide ion conductivity below 910 °C, abrupt conductivity increase is observed at the temperature, resulting in higher conductivity than that of yttria stabilized ZrO_2 above 910 °C. The increase in oxide ion conductivity has been attributed to structural phase transition from brownmillerite with ordered oxide ion vacancy to cubic perovskite with random distribution. However, crystal structure of $Ba_2In_2O_5$ at high temperature is not clear because so far reported X-ray diffraction measurements on $Ba_2In_2O_5$ have insufficient sensitivity and resolution to identify slight distortion from ideal cubic perovskite structure. In addition, we have discovered another second order phase transition at 1060 °C in $Ba_2In_2O_5$ using thermal analyses and concluded that the phase above 1060 °C is the most promising oxide ion conductor [1, 2]. However, diffraction measurements above 1060 °C have not been reported. In this study, structural phase transition of $Ba_2In_2O_5$ has been investigated by synchrotron X-ray diffraction with high sensitivity and resolution. For analysis of crystal structure at high temperatures, originally designed furnace equipped at BL-3A or 6C in PF was employed [3, 4].

Fig. 1 shows the synchrotron X-ray diffraction patterns of $Ba_2In_2O_5$ at (a) 700 °C, (b) 1000 °C and (c) 1200 °C. For comparison, diffraction patterns obtained with CuKα radiation are also depicted. The diffraction patterns at 700 °C could be indexed as orthorhombic brownmillerite regardless of X-ray source. X-ray diffraction patterns at 1000 °C indicated that structure of this phase was not cubic. By using synchrotron X-ray radiation, minor peaks were clearly observed. The diffraction pattern obtained with CuKα radiation at 1200 °C can be apparently indexed assuming cubic structure. However, minor peaks were observed in the diffraction pattern obtained with synchrotron radiation, indicating that slight distortion from cubic perovskite in $Ba_2In_2O_5$ at 1200 °C. Thus, it is concluded that diffraction measurements using CuKα radiation is not sufficient but those employing synchrotron radiation with higher sensitivity and resolution is required for precise determination of crystal structure and phase transition of $Ba_2In_2O_5$.

References

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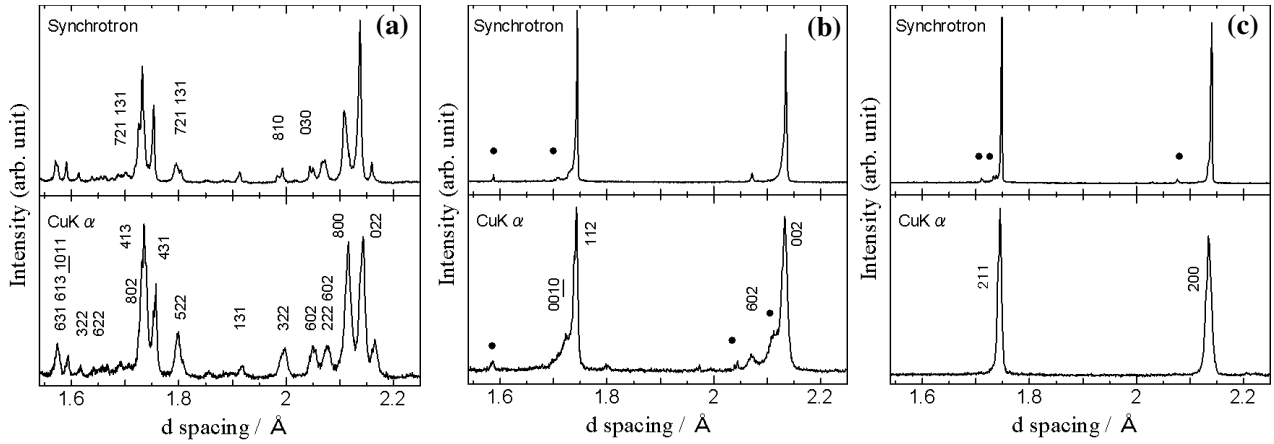

Fig. 1 X-ray diffraction patterns of $Ba_2In_2O_5$ obtained using synchrotron X-ray and CuKα radiation at (a) 700 °C, (b) 1000 °C and (c) 1200 °C. The peaks are indexed as (a) orthorhombic, (b) tetragonal and (c) cubic symmetry. • represents unidentified peaks.