

Machanism of Phase Transformation in AgBr at High Pressure: Revisit

Chia-Hui Lin (林佳蕙) and Jennifer Kung (龔慧貞)

Department of Earth Sciences, National Cheng Kung University, Tainan, Taiwan

AgX (X=F, Cl, Br) adopt B1 (NaCl) structure under ambient conditions. By computational investigation, a dense B2 (CsCl) structure is clearly favored at high pressure for silver halides[1]. AgF and AgCl have shown to undergo a pressure-induced transition from B1 structure to B2 structure at high pressure condition[2,3]. However, AgBr has not yet observed being transforming to the B2 structure experimentally. In general, The B1 structure $\rightarrow$ B2 structure phase transformation is a reconstructive transition. But for experimental evidences, several binary AB compounds with B1 structure are known to transform into B2 structure via intermediate phases under high pressure[4]. Under compression experiment, AgF was observed directly transformed from the B1 structure to the B2 structure. AgCl transformed into B2 structure but via two intermediate phases, the KOH-type structure and the TII-type structure experimentally[3]. Current experimental results indicate that AgCl and AgBr have a common high pressure phase - the KOH type structure[5]. The aim of the present work is to find if AgBr have a common transition pathway as AgCl does across the B1/B2 transition.

AgBr has been studied in a diamond anvil cell (DAC) by angular dispersive X-ray diffraction with a synchrotron source at room temperature. The pressure was determined by the ruby luminescence method and the equation of state of Au[6]. The high-pressure structural behavior of AgBr has been investigated up to ~ 18 GPa. The selected X-ray diffraction patterns from AgBr are shown in Fig.1. With increasing pressure, B1 structure transformed to an unknown structure (X phase) with pressure range about 3 GPa which is not KOH-type structure as previous study described[5]. At elevated pressure KOH-type structure and TII-type structure were found. However, during the decompression we observed the KOH-type structure reverted to B1 structure directly without via an "X phase" observed in compression.

The results of experimental studies using AgBr are summarized in Fig.2. The KOH-type structure was observed in all of the three runs, which was in good agreement with previous study[5]. The "X phase" is an intermediate phase between B1 structure and KOH-type structure in AgBr which is never found before. However, the current data of X-ray diffraction was limited to identify the structure of "X phase". Above 15.6 GPa, we found the TII-type structure in AgBr for the first time. The pathway of KOH-type structure transformed to TII-type structure in AgBr was the same as it is in AgCl[3]. The B2 structure has not observed in AgBr even at high pressure ~ 18 GPa and room temperature. Due to the pressure range is not high enough to observe the complete B1 $\rightarrow$ B2 transformation, the high pressure research of AgBr is still worth pursuing.

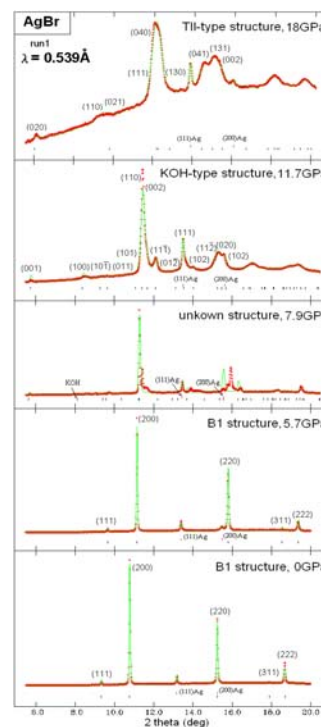


Fig.1: Selected X-ray diffraction patterns of AgBr (run1) collected at high pressure under compression condition. An additional diffraction peak of Ag was found in AgBr at both ambient and elevating pressure condition. Experimental (red line) and calculated (green line) profiles from Rietveld and La Bail refinement are indicate in the pattern, where the short ticks indicated modeled reflection position.

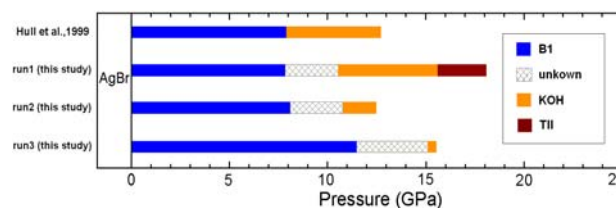


Fig. 2: Phase transition pressures observed in AgBr during the compression. The X-ray powder diffraction measurements on AgBr were carried out with synchrotron radiation at the SP12 (run1 and run2) and 01C (run3) beam line, respectively.

References

- [1] G. S. Nunes, P. B. Allen, and J. L. Martins, Phys. Rev. B **57**, 5098 (1998).
- [2] S. Hull and P. Berastegui, J. Phys. Condens. Matter **10**, 7945 (1998).
- [3] K. Kusaba, Y. Syono, T. Kikegawa, and O. Shimomura, J. Phys. Chem. Solids. **56**, 751 (1995).
- [4] P. Toledano, K. Knorr, L. Ehm, and W. Depmeier, Phys. Rev. B **67**, 144106 (2003).
- [5] S. Hull and D. A. Keen, Phys. Rev. B. **59**, 750 (1999).
- [6] S. H. Shim, T. S. Duffy, and K. Takemura, Earth Planet. Sci. Lett. **203**, 729 (2002).