LInBO$_3$-type Polar Antiferromagnet InVO$_3$ Synthesized under High-Pressure Conditions

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ABO$_3$-type oxides exhibit various structures with different combinations of A- and B-site ions. Their structures can be empirically predicted by Goldschmidt’s tolerance factor $t$, $t = (r_A + r_O) / \sqrt{2(r_B + r_O)}$, where $r_A$, $r_B$, and $r_O$ are the radii of the A, B, and oxygen ions, respectively [1]. As shown in Figure 1, the Ln$^{3+}$V$^{3+}$O$_3$ (Ln: lanthanides) crystallizes in the GdFeO$_3$-type distorted perovskite structure with a tolerance factor, $t$, from 0.786 to 0.843 [2-4]. While ScVO$_3$ ($t = 0.744$) crystallizes in a bixbyite-type structure, which is described as (Sc$_{0.5}$V$_{0.5}$)$_2$O$_3$ with disordered Sc$^{3+}$ and V$^{3+}$ [5]. Interestingly, the bixbyite-type ScVO$_3$ undergoes cation ordering to the GdFeO$_3$-type perovskite phase by applying high-pressure and high-temperature conditions [6]. InVO$_3$ was also reported to crystallize in a bixbyite-type structure upon reduction of InVO$_4$ [7]. Although the ionic radius of In$^{3+}$ (0.80 Å) is between that of Lu$^{3+}$ and Sc$^{3+}$, the GdFeO$_3$-type perovskite phase has not been reported yet.

In this study, we applied high-pressure and high-temperature technique to synthesize the perovskite phase for InVO$_3$. Instead, we have found that the polar LInBO$_3$-type structure is stabilized under 9 GPa and 1373 K. Figure 2 shows the synchrotron X-ray diffraction (SXRD) pattern of newly obtained InVO$_3$. LInBO$_3$-type structure with space group R3c can considerably fit the SXRD pattern, giving the lattice parameters $a = 5.29139(3)$ Å and $c = 13.98160(7)$ Å [6]. The crystal structure, polar and magnetic properties will be discussed in the conference.

References