Crystal and Magnetic Structure of Potentially Multi-Ferroic $PbFeO_3$

J.E. Greedan [1], T. Katsumata [2], T. Tsuchiya [2], Y. Inaguma [2] and S. Derakhshan [1]

[1] Brockhouse Institute for Materials Research and Department of Chemistry, McMaster University, Hamilton, ON, Canada L8S 4M1

[2] Chemistry Department, Gakushuin University, 1-5-1 Mejiro, Toshima-ku, Tokyo, Japan 172-8588

Multi-ferroics are materials that exhibit spontaneous electric and magnetic polarizations simultaneously. In the search for new multi-ferroic compounds, a popular strategy is to modify known ferroelectric materials by substitutions that introduce magnetic ions. For example,

$PbTiO_3$ is a well-known ferroelectric but is diamagnetic. Substitution of Ti with Fe will introduce magnetic properties. $PbFeO_3$ can be prepared only at high pressure (6 – 7 GPa) and temperature (1275 – 1575 K) in an anvil apparatus [1]. XPS data indicate that Pb^{2+}, Pb^{4+} and Fe^{3+} are present in this material. X-ray powder data are consistent with an orthorhombic pseudo cubic sub-cell with ac ~ 3.90 Å, but a complex supercell of $6a_c$ x $2a_c$ x $2a_c$ was found from electron diffraction. It was the goal of this study to determine the critical temperature for magnetic order and, if possible, the crystal and magnetic structures. The sample size was only ~ 700 mg. Data were taken from 2.8 K to 610 K. For measurements above room temperature, the sample was contained in a quartz tube backfilled with ~ 1 atm of oxygen as the sample is known to decompose above 720K in air. To search for magnetic reflections, the difference plot 296 K – 610 K was constructed as shown in Figure 1. Three magnetic reflections are marked with an asterix (*) at 2θ = 30.484(3)°, 59.89(1)° and 60.921(8)°. These can be indexed on the primitive orthorhombic cell as (1/2 1/2 1/2), (3/2 1/2 1/2) and (1/2 1/2 3/2) which indicates a G-type antiferromagnetic structure as was found for the related material, $PbFeO_2F$ [2]. The temperature dependence of the strongest magnetic peak (2θ = 30.48°) is shown in the inset which indicates T_c = 605(3) K for this material. Attempts to refine the crystal and magnetic structures are underway.

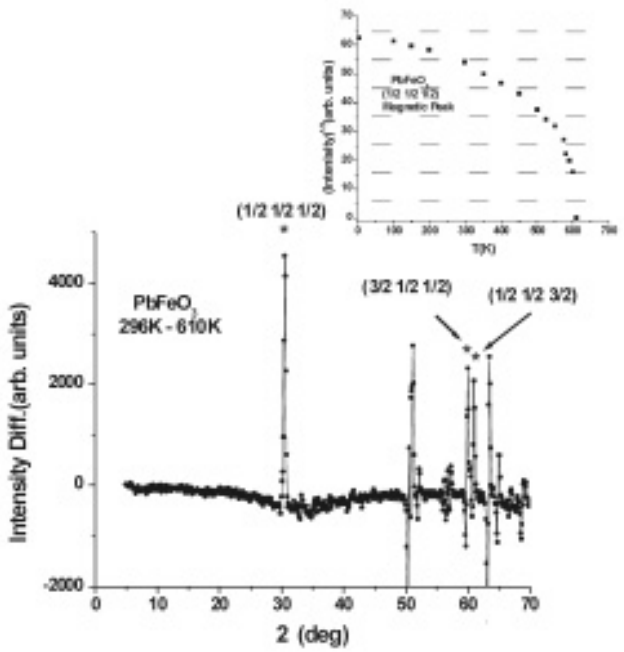

Fig. 1 The difference plot 296 K – 610 K for $PbFeO_3$. Magnetic reflections are marked with an asterix (*). The temperature dependence of the strongest magnetic peak at 30.48 deg ,(1/2 1/2 1/2), is shown in the inset which indicates T_c = 605(3) K.

References

[1] Takeshi Tsuchiya, Hiroyuki Saito, Masashi Yoshida, Tetsuhiro Katsumata, Tomonori Ohba, Yoshiyuki Inaguma, Takao Tsurui, and Masahiro Shikano, Mater. Res. Soc. Symp. Proc. Vol. 988 (2007) 0988-QQ09-16.

[2] Tetsuhiro Katsumata, Akihiro Takase, Masashi Yoshida, Yoshiyuki Inaguma, John E. Greedan, Jacques Barbier, Lachlan M. D. Cranswick, and Mario Bieringer, Mater. Res. Soc. Symp. Proc. Vol. 988 (2007) 0988-QQ06-03.