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Structure, electric and magnetic properties of $Pb(V_{1-x}M_x)O_3$, $M=Ti, Fe$ compounds

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It is well known that ferroelectricity and magnetic order are considered as hardly compatible in perovskite compounds. In this respect, $PbVO_3$ is quite interesting: it is isostructural to ferroelectric $PbTiO_3$ ($P4mm$) and contains V^{4+} spin $\frac{1}{2}$ cations [1]. However, previous studies have failed to observe magnetic order in $PbVO_3$, which was attributed either to a 2D magnetic behaviour or to magnetic frustration on a square lattice [2]. We present here the study of the substitution of V^{4+} by Fe^{3+} or Ti^{4+} cations, aiming at a better understanding of the relations between structural, magnetic and electric properties. $PbVO_3$ single crystals and powders of substituted compounds were prepared at 6GPa, 950°C in belt and Conac type systems. A single crystal diffraction experiment confirmed the proposed structure for $PbVO_3$, evidencing merohedral twinning related to ferroelectric domains also observed by SEM. For the Ti substitution, a complete $Pb(V^{4+}_{1-x}Ti^{4+}_x)O_3$ solid solution is observed for $x = 0$ to 1, while the Fe substitution stops at $x=0.5$ due to heterovalent cation replacement, the formula being $Pb(V^{4+}_{1-2x}V^{5+}_xFe^{3+}_x)O_3$. The cation oxidation states were checked by XANES (FAME-ESRF). The structures were studied by joint refinements of NPD (D1B-ILL) and XPD (Laboratory and ID31-ESRF) data, yielding the coordinations of V and M cations and the spontaneous polarization using a point charge model. A decrease of tetragonality, domain size along the c-axis and polarization is observed with increasing substitution. For the Ti series, the magnetic behaviour progressively changes from 2D to Curie-Weiss with increasing x. In the case of Fe, a broad peak in magnetic susceptibility is observed, at temperatures increasing from 12K to 30K for x going from 0.1 to 0.5. This was checked as due to a spin glass behaviour. No sign of magnetic order was observed by NPD. At the same time, a broad, frequency dependent anomaly of the dielectric constant is observed, reminiscent of a relaxor behaviour.

[1] R. V. Shpanchenko, V. V. Chernaya et al. *Chem. Mater.*, 16 (17), 3267, 2004, [2] A. A. Tsirlin, A. A. Belik, R. V. Shpanchenko et al. *Phys. Rev. B* 77, 092402, 2008

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