Structure, electric and magnetic properties of Pb(V1-xMx)O3, 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, PbVO3 is quite interesting: it is isostructural to ferroelectric PbTiO3 (P4mm) and contains V4+ spin ½ cations [1]. However, previous studies have failed to observe magnetic order in PbVO3, 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 V4+ by Fe3+ or Ti4+ cations, aiming at a better understanding of the relations between structural, magnetic and electric properties. PbVO3 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 PbVO3, evidencing merohedral twinning related to ferroelectric domains also observed by SEM. For the Ti substitution, a complete Pb(V4+ 1-x Ti4+ x)O3 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(V4+ 1-2x V5+ x Fe3+ x)O3. 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.


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