Ordering effects in BiFeO$_3$-based solid solutions

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In solid solutions of BiFeO$_3$, multiferroic and KNbO$_3$, ferroelectric or NaNbO$_3$ antiferroelectric the different order parameter interactions should occur: magnetic, ferro-(anti)-ferroelectric, and of ferroelastic nature.
X-ray diffraction study in 20°≤θ≤30°C temperature range of (1-x)BiFeO$_3$-(x)KNbO$_3$ (BFKN0) and (1-x)BiFeO$_3$-(x)NaNbO$_3$ (BFNNO) solid solutions systems’ samples has allowed to make the (x,T) phase diagrams of the systems. It was established that in BFKNO system the R3c, Pbnm, Pm3m phases’ boundaries of pure BiFeO$_3$, with KNbO$_3$, doping lessen in transition temperature with the increase of X. The transition temperatures between Amm2, P4mm and Pm3m phases of pure KNbO$_3$, are also decreased with the decrease of X. The phase boundaries in BFNNO system’s solid solutions shift in a similar way.
The comparison of BFKNO and BFNNO phase boundaries shows that in these systems the ferroelectric phase transitions’ temperatures of BiFeO$_3$, KNbO$_3$ and NaNbO$_3$, decrease with the increase of secondary component’s content. This is also proved by preliminary results of permittivity-temperature dependencies investigations.

Keywords: ferroic, ferroelectricity, X-ray

Structural study of SrPrMnRuO$_4$ double perovskites by symmetry-mode analysis

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The natural way to study the phase-transitions is the usage of the symmetry-mode analysis, to understand in a proper way the microscopic mechanisms responsible for the phase-transitions. For that propose we have used the Bilbao Crystallographic Server [1][2][3] together with FullProf Suit [4].
The SrPrMnRuO$_4$ (M=Zn,Co,Mg,Ni) materials have been elaborated by the conventional Solid State Reaction Method. Rietveld analysis of laboratory X-ray Powder Diffraction (XRPD), Synchrotron Radiation Powder Diffraction (SRXRPD) and Neutron Powder Diffraction (NPD) shows that these materials are double perovskites with a primitive space group: P2/n (No. 14, non conventional setting). In the four compounds Sr$_2^n$ and Pr$_2^n$ are totally disordered in A- and A’-sites; whereas M$^o$ and Ru$^o$ are completely ordered, in B- and B’-sites, respectively. For the refinements we have used AMPLOMODES for FullProf [3][5]-6. AMPLOMODES carries out a symmetry-mode analysis of a displacive phase-transition. Starting from the experimental structures of the parent-phase (virtual or real, Fm-3m, No. 225 conventional setting) and knowing the metric of the low-symmetry phase (P2/n), the program determines the symmetry modes compatible with the symmetry break. In the NPD data analysis two modes have been identified as active: the ones responsible to yield the P2/n space group: GM$_4$, and X$_3$. These two modes are related to the rotation of the octahedra (oxygen movements): GM$_4$, generates a rotation around the monoclinic b axis and X$_3$, around the c axis.
The high-temperature (HT) laboratory XRPD analysis has revealed the following temperature-phase-transition sequence [7]: P2/n-R-3-Fm-3m. HT neutron diffraction data of SrPrMgRuO$_4$, material has been used to study the phase-transition by the symmetry-mode analysis. According to the theory, the two order parameters actuating in the monoclinic phase are expected to thermally stabilize and become zero at higher temperature. Taking into account that the amplitudes are different, it can be expected that one of them will become zero before the other and, thus, an intermediate phase will appear, before the cubic one. A first order phase-transition has been observed between P2/n and R-3 (No. 148 conventional setting). None of the amplitudes of the active modes will reach the zero value at the transition temperature. In the symmetry breaking from the prototype cubic phase into the trigonal intermediate (HT) phase a unique active mode has been identified: GM$_4$, which generates a rotation of the octahedra around the hexagonal c axis.

Keywords: transition-metal perovskites, phase-transitions, symmetry-mode analysis