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### Ordering effects in BiFeO<sub>3</sub>-based solid solutions

Pavel Teslenko,<sup>a</sup> Anatoly Pavlenko,<sup>b</sup> Larisa Reznichenko,<sup>b</sup> Olga Razumovskaya,<sup>b</sup> Yuri Kabirov,<sup>a</sup> <sup>a</sup>*Departament of Physics, Southern Federal University, SFEDU, Rostov-on-Don, (Russia)*. <sup>b</sup>*Institute of Physics, Southern Federal University, SFEDU, Rostov-on-Don, (Russia)*. E-mail: teslenko\_pavel@mail.ru

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In solid solutions of BiFeO<sub>3</sub> multiferroic and KNbO<sub>3</sub> ferroelectric or NaNbO<sub>3</sub> antiferroelectric the different order parameter interactions should occur: magnetic, ferro(-antiferro)electric, and of ferroelastic nature.

X-ray diffraction study in 20≤T≤800°C temperature range of (1-x)BiFeO<sub>3</sub>-(x)KNbO<sub>3</sub>(BFKNO) and (1-x)BiFeO<sub>3</sub>-(x)NaNbO<sub>3</sub>(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<sub>3</sub> with KNbO<sub>3</sub> doping lessen in transition temperature with the increase of X. The transition temperatures between Amm2, P4mm and Pm3m phases of pure KNbO<sub>3</sub> 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<sub>3</sub>, KNbO<sub>3</sub> and NaNbO<sub>3</sub> 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

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### Structural study of SrPrMRuO<sub>6</sub> double perovskites by symmetry-mode analysis

Edurne Iturbe-Zabaló,<sup>a,b</sup> Gabriel J. Cuello,<sup>a</sup> Josu M. Igartua,<sup>b</sup> <sup>a</sup>*Institut Laue-Langevin, Grenoble (France)*. <sup>b</sup>*Fisika Aplikatua II Saila, Zientzia eta Teknologia Fakultatea, UPV/EHU, Leioa (Spain)*. E-mail: iturbe@ill.fr

The natural way to study the phase-transitions is the use 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 SrPrMRuO<sub>6</sub> (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 (SXPDP) and Neutron Powder Diffraction (NPD) shows that these materials are double perovskites with a primitive space group:  $P2_1/n$  (No. 14, non conventional setting). In the four compounds Sr<sup>2+</sup> and Pr<sup>3+</sup> are totally disordered in A- and A'-sites; whereas M<sup>2+</sup> and Ru<sup>5+</sup> are completely ordered, in B- and B'-sites, respectively. For the refinements we have used AMPLIMODES for FullProf [3][5-6]. AMPLIMODES carries out a symmetry-mode analysis of a displace

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 ( $P2_1/n$ ), 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  $P2_1/n$  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]:  $P2_1/n-R-3-Fm-3m$ . HT neutron diffraction data of SrPrMgRuO<sub>6</sub> 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  $P2_1/n$  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.

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### High-pressure behavior of high silica ferrierite

Rossella Arletti,<sup>a</sup> Simona Quartieri,<sup>b</sup> Giovanna Vezzalini,<sup>c</sup> <sup>a</sup>*Dipartimento di Scienze Mineralogiche e Petrologiche, Università di Torino, (Italy)*. <sup>b</sup>*Dipartimento di Scienze della Terra, Università di Messina, (Italy)*. <sup>c</sup>*Dipartimento di Scienze della Terra, Università di Modena, (Italy)*. E-mail: rossella.arletti@unito.it

Ferrierite (FER framework topology) is a well-known aluminosilicate zeolite mineral. An understanding of the structure and properties of FER remains important because of its role as a catalyst in commercial reactions. For example, it is important in the petrochemical industry, where it has been used as a shape selective catalyst for the production of isobutene. The thermal behavior of this phase (in its high silica form) was recently studied by Bull et al [1], while its compressibility has never been investigated before.

The high pressure (HP) behavior of synthetic high silica zeolite ferrierite (FER) was investigated by means of in-situ synchrotron X-ray powder diffraction, with the aim to understand the P-induced deformation mechanism. The microporous material was synthesized starting from pure silica and pyridine and propyl-amine as structure directing agents. Here we report the preliminary results on the compressibility of the as synthesized phase. The study of the compressibility of the calcined one will be carried out in the following steps of the project.