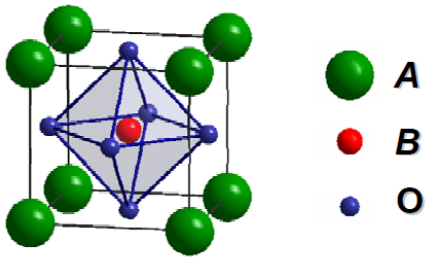
The term “multiferroics” is used to describe a class of very interesting materials, in which several qualitatively different long-range orderings coexist. They are very intensively investigated in the case of coexistence of ferroelectricity and magnetism because of fascinating fundamental properties as well as the potential for a wide range of applications. They are anticipated to be useful as memory elements, in which information would be stored in magnetic bits and the state of the bits could be changed by applying an electric field. They could also serve as magnetic field sensors, electrically switchable permanent magnets, as well as in magnonics – as spin waves amplifiers. One can think about using them as direct converters of variable magnetic field energy into electric energy stored in batteries powering wireless networks.

Studies of thermal, dielectric and magnetic properties of manganites $Sr_{1-x}Ba_xMn_{1-y}T_yO_3$ (where T = Ti, Fe), as well as of the structural and multiferroic phase transitions appearing in them are the main subject of the project. These compounds have deformed perovskite structure, Fig. 1, with general chemical formula ABO_3, where the large size strontium and barium ions are in A positions, while the small manganese and T ions occupy B sites. Each B ion is surrounded by six oxygen ions forming an octahedron, while A ions are located in the spaces between the octahedra. The $Sr_{1-x}Ba_xMnO_3$ compounds are antiferromagnetic insulators, which for $x \geq 0.45$ also exhibit spontaneous electric polarization, P_S, so they belong to the class of multiferroics. P_S occurs as a result of phase transition from cubic to tetragonal structure appearing below $T_C \sim 400$ K for $x = 0.5$, and similar to that observed in classic ferroelectric $BaTiO_3$. As a result of deformation, the Mn ions move from the center of the octahedron towards one of the oxygen ions. This is a unique behavior, since usually in perovskites containing magnetic B ions (e.g. Mn), the displacement of B ion from the octahedron center is energetically unfavorable. It is assumed that the cause of this shift is an elongation of the Mn-O bonds above equilibrium length, caused by replacement of some of Sr ions with larger Ba ions, as described by the 3-*dim* geometrical constraint in the form of increased value of the Goldschmidt tolerance factor above 1.



Rys. 1. Struktura krystaliczna idealnego perowskitu ABO_3.

It is expected that by use of tolerance factor argument, the improved ferroelectric and multiferroic materials could be obtained. Partial substitution of Ti ions with smaller magnetic Mn ions in $BaTiO_3$ should increase T_C and possibly induce magnetism. On the other hand, partial substitution of Mn ions with Ti ions in $(Sr,Ba)MnO_3$ should allow larger amount of Ba ions substituting for Sr, reinforcing the displacement of manganese ions, and thus increasing the value of the P_S in the magnetically ordered phase. In turn, partial substitution of Mn ions with Fe ions should enhance the magnetic ordering, i.e., raise the magnetic transition temperature. It is quite possible that Fe doping can also change the kind of magnetic ordering from antiferromagnetic to ferromagnetic one, being more desirable for applications.

In $Sr_{1-x}Ba_xMnO_3$, transition to the antiferromagnetic phase, which takes place at lower temperature then T_C, suppresses significantly the tetragonal deformation and displacement of the Mn ions from the centers of octahedra, i.e., it suppresses also the ferroelectric phase and P_S. The suppression, is not complete, thus the antiferromagnetic and ferroelectric phases coexist, and the compounds can be regarded as multiferroics.

The main goals of the proposed research there are:

1. Determining if it is possible to increase T_C and induce magnetism by substitution of Mn in $BaMn_{1-y}Ti_yO_3$.
2. Determining if it is possible to increase T_C and P_S, and minimize the decrease of the P_S in magnetic phase of $Sr_{1-x}Ba_xMn_{1-y}T_yO_3$ by a partial substitution of Mn with Ti and Fe and increasing Ba content.
3. Determining the kind of the magnetic order appearing in $Sr_{1-x}Ba_xMn_{1-y}T_yO_3$ and investigating if it is possible to change the character the ordering to the ferromagnetic by substitution of Mn with Ti and Fe.
4. Determining the phase diagram of the $Sr_{1-x}Ba_xMn_{1-y}T_yO_3$ system, in particular, investigating the influence of Ba content on the temperature, sharpness and the kind of the phase transitions from the paraelectric to the ferroelectric and from the paramagnetic to the magnetically ordered phase.

The specific heat measurement was chosen as the major experimental method, because this physical quantity is exceptionally sensitive to phase transitions of various kinds. The specific heat measurements will be carried out by relaxation method over the temperature range from 2 K to 400 K in the magnetic field up to 9 T, and by using Differential Scanning Calorimetry method, over the temperature range from 300 K to 800 K. Magnetization measurements over the temperature range from 2 K to 800 K in magnetic field up to 9 T, magnetization measurements under external pressure up to 10 kbar (1 GPa) over the temperature range from 3 K to 300 K in the field up to 5 T, as well as supplementary studies of dielectric properties will be performed too. In addition, Density Functional Theory calculations from first principles will be performed in order to understand properties of the studied materials.