

More detailed analysis reveals, however, how compositional disorder sets up a local strain field and couples to soft modes preventing their condensation into a low symmetry phase. We study, by means of DS experiments and atomistic modelling different ferroelectric compounds that exhibit this type of behaviour [1]. In the case of $\text{KNb}_{1-x}\text{Ta}_x\text{O}_3$ substituting ferroelectrically active Nb atoms with Ta (up to high values of x) does not alter significantly the tendency for the system to host polar BO_6 chains. It does however constrain the transverse correlation of chains (the fact observed experimentally for similar, BaTiO_3 -related compounds [2]). For $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ molecular dynamics simulations for different realizations of B-site partial disorder enables extraction of the conditions necessary for the existence of polar order. At the same time it is shown that the DS observed for this compound is not directly related to so-called polar nano-regions. $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ and $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ are among the other materials being analyzed.

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Orbital Ordering of Co^{3+} Intermediate-Spin State in RT ferromagnet $\text{Sr}_3\text{YCo}_4\text{O}_{10.5}$

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$\text{Sr}_{1-x}\text{R}_x\text{Co}_4\text{O}_{10.5}$ ($R = \text{Y}$ and lanthanide, $0.2 < x < 0.25$) has been found recently as a room temperature ferromagnet with $T_C \sim 340$ K, which is the highest T_C among perovskite Co oxides [1]. The crystal structure is formed with the CoO_6 octahedral layers and the $\text{CoO}_{4.25}$ layers, which stack along c axis alternatively. By powder x-ray diffraction, the orbital state of Co^{3+} ($3d^6$) was evaluated from the anisotropy of the CoO_6 octahedron in the ferromagnetic phase, and the e_g orbital ordering of intermediate spin (IS) state was proposed as an origin of the ferromagnetism [2]. Therefore, the orbital ordering and spin-state of Co^{3+} have been investigated using a resonant x-ray scattering technique [3].

A resonating signal with a $\sigma \rightarrow \pi$ scattering component was observed at $(h\ 0\ 0)$, where $h=2n+1$ (n : integer), near the $1s \rightarrow e_g$ transition energy of Co. This provides direct evidence of not only e_g orbital ordering but also the existence of the IS state. Moreover, we suggest that the ferrimagnetism is induced by the e_g orbital ordering of the IS state of Co^{3+} . The peculiar e_g orbital, spin-state, and magnetic orderings are also discussed.

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Total neutron scattering in the α -quartz type materials for piezoelectric applications.

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Quartz type materials belong to the $P3_121$ or $P3_221$ space group with formula $A^{\text{IV}}\text{O}_2$ or $A^{\text{III}}B^{\text{V}}\text{O}_4$. The structure consists of a helical chain of tetrahedra along the z -axis. In the quartz family of materials, the thermal stability of the α -phase is linked to the tilt of the tetrahedra around a two-fold axis, which is the mechanism of the α - β phase transition. This behaviour depends on the nature of the cations at the center of the tetrahedra. Thermal stability in the α -quartz type materials was studied by total neutron scattering on the GEM diffractometer at the ISIS spallation neutron source. Average structures have been refined and atomic pair distributions have been generated. Analysis by reverse Monte Carlo modelling of our total scattering experiments in this group of materials show that the degree of disorder in the instantaneous structure increases well before the phase transition for materials exhibiting an α - β phase transition. This dynamic disorder in the oxygen sub-lattice is at the origin of the rapid decrease of the piezoelectric properties at high temperature. This occurs for example at close to 500K in α -quartz, well below the α - β transition at 846K. We show that the chemical nature of the cations (size, number of electrons) in the tetrahedra can be used to improve the thermal stability of these materials [1], [2]. In the case of GaAsO_4 , which contains the largest cations and is the most distorted in this group of materials, the degree of dynamic disorder is limited even at temperatures up to the decomposition of the material around 1300K.

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News on mullite and mullite-type compounds

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Synthetic forms of the mineral mullite represent one of the most important constituents of high-temperature ceramics. It can be synthesized in a solid-solution series with general composition $\text{Al}_{4+2x}\text{Si}_{2-2x}\text{O}_{10-x}$ where x ranges between 0.18 and 0.88 [1]. Within this compositional range, there are two thermodynamically stable compounds with $x = 0.25$ (3:2-mullite, $3\text{Al}_2\text{O}_3 : 2\text{SiO}_2$, $\text{Al}_{4.5}\text{Si}_{1.5}\text{O}_{9.75}$, so-called sinter-mullite) and $x = 0.4$ (2:1 mullite, $2\text{Al}_2\text{O}_3 : 1\text{SiO}_2$, $\text{Al}_{4.8}\text{Si}_{1.2}\text{O}_{9.6}$, so-called fused-mullites). Sinter-mullites are usually produced by solid-state reactions and fused-mullites by melting or crystal-growth techniques. About six years ago, Fischer and Schneider [2] did the first attempt to define the mullite-type family of crystal structures for a class of compounds having the same arrangement of