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MS16-P04

Pre-transitional processes in lead zirconate doped by Ti studied by diffuse and inelastic X-ray scattering

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Lead-zirconate titanate ($PbZr_{1-x}Ti_xO_3$, PZT) is one of the most actively studied and widely used ferroelectric materials. One of the reasons of the interest is a complex phase diagram of lead zirconate and lead titanate solid solution, which illustrates variety of physical properties and crystal structures depending on titanium concentration. Other reasons of popularity are high piezolelectric properties, demonstrated by PZT around morthotropic phase boundary, and prospects of application of antiferrolectric properties [1], demonstrated by PZT with low Ti concentration.

Pure lead zirconate (x=0) is the prototypical antiferroelectric material. Between the cubic perovskite paraelectric phase and the antiferroelectric phase, in the narrow temperature range, intermediate ferroelectric phase exists. Addition of titanium increases the temperature range of stability of this phase. Cubic-to-intermediate phase transition is accompanied by doubling of the cell parameters of the paraelectric cubic lattice along two directions [2] and results in the appearance of M-superstructure with coordinate (H±1/2 K±1/2 0) in the diffraction pattern. Observation of additional satellites around M-point by electron diffraction [2] results in conclusion about complex domain pattern, characterized by antiphase domain boundary in lead displacement.

Recent studies [3] of pure lead zirconate reveals complex pattern of dynamical correlations in paraelectric phase. Diffuse scattering distribution indicates disordering of oxygen octahedral tilts and Pb displacements is shown in the high-temperature cubic phase. To study temperature behavior of these correlations X-ray diffuse scattering measurements have been done in wide temperature range in PZT with small titanium concentration ($x < 0.04$). To characterize dynamical origin of DS lattice dynamics have been studied using inelastic X-ray scattering. Obtained temperature evolution of DS and pre-transitional dynamical peculiarities will be shown in presentation and discussed in the context of mode coupling.

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MS16-P15

Interplay of cation disorder and thermoelastic properties of $MgGa_2O_4$

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Transparent semiconducting oxides are materials suitable for a wide variety of optoelectronic applications, such as UV-LEDs, Schottky diodes, high voltage transistors and transparent thin film transistors. Spinel structure $MgGa_2O_4$ was recently shown to have an appropriate carrier concentration and bandgap for such applications and it can be grown using various techniques from the melt as relatively large crystals[1]. Furthermore, it has a high chemo-physical stability and its conductivity can be controlled by adjusting the atmosphere during the growth process[1], making it an excellent candidate for future applications. However, spinel-like materials often exhibit anomalies in their physical properties at higher temperatures due to changes of their cation ordering (normal/inverse spinel). In fact, both heat capacity[1] and thermal diffusivity[2] of $MgGa_2O_4$ were shown to behave anomalously as a function of temperature.

We studied this issue by direct investigation of the cation ordering of annealed samples using single crystal X-ray diffraction. Additionally, we used inductive gauge dilatometry and resonant ultrasound spectroscopy to determine thermal expansion and the complete set of elastic constants, respectively, from 103 K to 1673 K to assess correlations between the changing structure and properties.

Thermal expansion and most stiffness coefficients show a discontinuity in their temperature dependence at about 820 K. Furthermore, the cation disorder is independent of temperature up to about 820 K and increases gradually at higher temperatures. Thus, the cation disorder in $MgGa_2O_4$ is most likely in equilibrium at high temperatures and undergoes a transition to a nonequilibrium state below 820 K, where the disorder cannot relax in laboratory timescales; a glass-like transition. This transition is likely also related to the anomalies in heat capacity[1] and thermal diffusivity[2]. The bond-valence model can qualitatively explain the relation between changing cation order and thermoelastic properties.

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