

MS16-P15**Assessment of Pyroelectricity in Polar Oxides from Atomic Displacements**

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The phenomenon of pyroelectricity is known since 2000 years and describes the temperature dependency of the spontaneous polarization in non-centrosymmetric crystals. The origin is based on displacements of the atomic positions induced by temperature variations. These structural changes are measurable with common structural analysis methods, e.g. single crystal X-ray diffraction (XRD). However, in addition electron density redistributions play a crucial role.

This work shows an approach how to use measurable structural changes in combination with electronic structure modeling to determine pyroelectric coefficients of materials. Atomic displacements have been determined with XRD for the crystal structures of the pyroelectric standards and well-known material systems lithium niobate (LiNbO₃) and lithium tantalate (LiTaO₃) in a temperature range from 80 K to 400 K. As a result, the spontaneous polarization and the pyroelectric coefficient have been calculated and show a high comparability with theoretical and experimental data. Furthermore, the newly developed Resonant X-ray Diffraction method *REXSuppress* [Richter2018] provides increased sensitivity for very small displacements of the atoms. Hereby, destructive interference of the intensity at specific Bragg reflections is used to detect structural deviations at picometer accuracy. This is particularly important for tiny structural changes, as shown for the recently discovered pyroelectric migration-induced field-stabilized polar (MFP) phase in normally non-polar cubic strontium titanate (SrTiO₃) [Hanzig2013, Hanzig2015].

This work may be of wide interest for the pyroelectric community, presenting an alternative approach to determine pyroelectric properties from structural data and for the characterization of structural and physical properties of new materials or phases.

References:

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MS16-P16**Crystal structure**

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In course of extensive investigations of the Al - Cr phase diagram AlCr₂ was commonly assigned as Cr-richest binary compound, however, stable below about 900°C only [1]. Based on powder diffraction data MoSi₂ structure type was assigned, but no detailed structural analysis has been described till now. The phase diagram is indicating particular problems to obtain single crystals of this particular intermetallic compound. In a multi-step sintering procedure, carefully monitored by powder diffraction as well as scanning electron microscopy (SEM), finally well-defined samples were obtained. Within these samples large grains measuring up to 100 µm could be identified and selected ones were cut out using focused-ion beam (FIB) methods. Those pieces proved to be single crystals with good quality and allowed for the first detailed structural investigation of AlCr₂. Lattice parameters a = 3.0056 and c = 8.6449 Å for the body-centered tetragonal unit cell are in excellent agreement with those given in [1] for the ideal composition. The structural model refines well in space group *I4/mmm* without indications of mixed or anti-site occupancies. The c/a ratio at 2.876 is much larger than the typical value for MoSi₂ at 2.437 and quite close to the ideal value for a three-fold bcc-type superstructure. The disordered solid solution of Al in Cr existing at higher temperatures adapts indeed a bcc-type structure. A detailed comparison with the structure of MoSi₂ is currently hampered by the fact that structural parameters given by different authors are varying quite significantly [2, 3].

In an optional way the structural arrangement may be discussed on the basis of hexagonal AlCr₂ layers, which are stacked in *ABAB* sequence along [110] direction. This allows for interesting comparison with hexagonal CrSi₂ and orthorhombic TiSi₂ type arrangements in which the same type of layers is stacked in *ABCABC* or *ABCDABCD* sequence, respectively.

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