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Recent Advances in Synchrotron Radiation Investigation of Ferroic Materials

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Abstract - Synchrotron radiation diffraction, scattering and absorption spectroscopy are among the most powerful tools employed today for the investigation of ferroic materials' fine structure. A comparative review of the mentioned techniques, as applied to bulk and nano-structured ferroelectric and magnetoelectric samples is presented and illustrated by means of practical examples.

The information contained in diffraction peaks gives the long-range space-time average structure. It provides the general structure diagram, precise lattice parameters and average atomic positions. In synchrotron applications, it is highly sensitive to symmetry breaking. Space/time deviations from mathematical periodicity decrease diffraction maxima and generate diffuse scattering.

The effect of single- and polycrystal symmetry on 2-D diffraction patterns and on physical properties is briefly reviewed. Associated software is presented.

Research using ferroelectric diffuse scattering in the three-dimensional vicinity of Bragg peaks represents a current tendency aimed at clarifying the static and dynamic characteristics of ferroelectrics above the Curie temperature T_c. The final objective is to elucidate the gestation of ferroelectricity from the paraelectric state.

Two models that represent extremes in the existing diversity of approaches are:

a) (Solid state physics) → Softening of the dynamic chains of correlated displacements that form the transverse optical (TO) modes.

b) (Quantum chemistry) → Static linearly ordered displacements that have short range in the paraelectric phase and show long-range order in the ferroelectric phase.

Representative case studies, performed by our group and from the literature, are discussed. Phonons in the cubic paraelectric phase of $PbTiO_3$, polarized nanoregions in PZN single crystals, ultra-thin layers of $PbTiO_3$ and linear disorders in $BaTiO_3$ and $KNbO_3$ are considered.

Measuring and processing the structured diffuse scattering leads to determination of the pair distribution function (pdf). Scattering-measured pdf is centered on an "average" atom, representative of the investigated phase.

X-ray Absorption Fine Structure (XAFS) investigation is briefly exposed. X-ray Absorption Near Edge Structure (XANES) offers information on oxidation state of the absorbing element and in general on the electronic structure of the target element's bonds. Furthermore, Extended X-ray Absorption Fine Structure (EXAFS) focuses on the determination of a few short-range structural characteristics invisible for the averaging eyes of diffraction techniques, like interatomic distances, coordination numbers and static and thermal disorder. In some cases it is capable of inter-bonds angle determination as well. Some recent applications of the technique to ferroic oxides are given.