MS40-1-4 A unique laboratory experimental setup for single-crystal X-ray diffraction under electric field #MS40-1-4

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Abstract
In the context of studies of multi-functional materials with piezo-ferro-electric properties, we are developing a device for the characterization of structural changes under static and alternating electric fields (of the order of 30 kV.cm-1) [1].
In this kind of materials, structural changes related to the application of an electric field take place at different physical scales, from the microscopic (atomic displacements, symmetry changes, crystal lattice distortion) to the macroscopic (microstructure, formation and displacement of domain walls, polarization switching). Single crystal X-ray diffraction is a well-adapted technique for exploring these structural changes. Accurate and complete mapping of the reciprocal space under electric field is an instrumental and methodological challenge. It can be achieved with the use of a 4-circles goniometer and a 2D detector such as the Cegitek RebirX 540 hybrid pixel detector [2]. Indeed, this detector has all the necessary specifications for this type of measurements (absence of readout noise, electronic shutter, fast readout time, adapted firmware).
The device developed in our laboratory [3] allows the generation of an alternating electric field and the positioning of the goniometer to be synchronized with the X-ray photons detection by the RebirX detector. The recorded diffraction images are multiplexed and summed directly in the detector using the firmware precisely developed for these experiments.
Applying an electric field in different directions to a single crystal suitable for XRD requires specific sample holders. They must be compact, adaptable to a usual goniometric head and allow a complete exploration of the reciprocal space. Different types of sample holders have been designed and built in the CRM2 laboratory and allow crystals of different size, morphology and nature to be subjected to an electric field according to chosen crystallographic orientations, with or without direct contact of the electrodes on the sample.
This experimental setup has been tested in different configurations, on an inorganic quartz crystal [3] but also on a molecular compound [4].

References
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Setup for SC-XRD studies under electric field