Bond-dependent Crystal Response on Electric Field: Synchrotron Diffraction Study

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The interaction of a crystal with the permanent external electric field resulting in dielectric polarization and converse piezoelectric effect is well described on the macroscopic level. In last years the microscopic origin of these phenomena is actively studied by means of synchrotron diffraction technique. In this work, we present our recent investigations of the structural response of single crystals to an external electric field, and analyse the results in terms of the chemical bond in different structural units of the crystal.

Special attention will be paid to the study of bond specific structural response in α -GaPO₄. The experiment was carried out by modulation-demodulation technique at D3 beamline at HASYLAB. The measured diffraction intensities of 42 independent reflections were fitted to a structural model, validated on the basics of the developed theory of X-ray diffraction by a crystal in the external electric field [1]. The difference of field-induced deformations of GaO₄ and PO₄ tetrahedra is explained in terms of the different character of chemical bonds and by charge density features. Support by DFG and A.v.Humboldt-Foundation (V.T.) is kindly acknowledged.

[1] Gorfman S., Tsirelson V., Pietsch U., *Acta Cryst.*, 2005, A, *submitted*. Keywords: x-ray diffraction, dielectric properties, chemical bonding