conference abstracts

s7'.m3.o3 **X-ray diffraction imaging of LiNbO₃ crystals with electric field induced modifications.** P. Pernot-Rejmánková[1], J. Baruchel[2], W. Laprus[3], *(1)LMGP-ENSPG, BP 46, F-38402 St Martin d'Heres, France, (2)European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France, (3)Polish Academy of Sciences, Swietokrzyska 21, P-00049 Warszawa, Poland*
Keywords: lithium niobate, ferroelectric domains, X-ray imaging.

An overview of diffraction imaging investigations of LiNbO₃ crystals will be given. Lithium niobate has a variety of significant technological applications due to its piezoelectric, elastic and non-linear optical properties. In particular, the knowledge of behaviour of this compound under an applied electric field is important for industrial applications.

Implantation by energetic (~ MeV) light ions such as hydrogen or helium has the effect of considerably lowering the refractive index in the implanted region, while the refractive index of the layer only traversed by the implanted ions generally remains approximately the same as the bulk one. The region of lower refractive index can thus define the boundary of a waveguiding area. The experiments with and without an electric field applied indicate that the implanted layer is single-crystalline and has the inverted polarization with respect to the bulk [1].

In addition, the diffracted intensity increases in the area of the sample under the electrodes and an expansion, or contraction, of the image of the bulk occurs according to the orientation of the applied field, for a given lattice plane. This **focusing effect** is associated with a curvature of the lattice planes under an applied field. Experimental evidence and a theoretical analysis based on the equations of the static electro-mechanical field in a piezoelectric medium, allow us to explain the reversed domain-related origin of the observed curvature [2].

Lithium niobate can achieve optical second-harmonic generation with enhanced efficiency when a periodic reversal of the sign of the non-linear optical coefficient d_{33} occurs in the phase matching period. This **periodically inverted domain structure** can be produced by applying an external electric field using patterned electrodes. Fresnel and Bragg diffraction were used simultaneously to visualize these ferroelectric domains within the bulk. The wavefront of the Bragg-diffracted X-ray beam is split by the phase difference between the structure factors of adjacent domains. This shift is measured through quantitative analysis of the image contrast as a function of propagation distance [3]. The internal distribution of domains can be investigated even at small sample-to-detector distances if an electric field is applied, due to additional distortions produced via the piezo-electric effect [4].

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[4] P. Rejmánková, J. Baruchel, P. Moretti, M. Arbore, M. Fejer and G. Foulon, J. Appl. Cryst. 31 (1998) 106

s7'.m3.o4 **Macroscopic and microscopic polarization in dielectrics.** R.Resta. *Dipartimento di Fisica Teorica, Università di Trieste, Italy*
Keywords: instrumentation, excited states.

The concept of macroscopic polarization is the basic one in the electrostatics of dielectric media: but for many years this concept has evaded even a precise microscopic definition, and has severely challenged quantum--mechanical calculations.

Textbooks usually visualize a polarized dielectric as an assembly of discrete microscopic polarization elements, à la Clausius-Mossotti. From this viewpoint, the macroscopic polarization looks like trivial matter. Unfortunately, the electronic distribution inside a real material is continuous, and often quite delocalized: the partition of the valence charge into localized contributions is highly nonunique.

The concept of dielectric polarization in condensed matter has undergone a genuine revolution in recent years. It is now pretty clear that---contrary to a widespread incorrect belief---macroscopic polarization has nothing to do with the periodic charge distribution of the polarized crystal: the former is essentially a property of the *phase* of the electronic wavefunction, while the latter is a property of its *modulus*. An outline of the modern theory[1,2], based on a Berry phase[3], will be presented.

Experiments invariably address polarization derivatives (permittivity, piezoelectricity, pyroelectricity,...) or polarization differences (ferroelectricity), and these differences are measured as an integrated electrical current: such current is the quantity which can be cast as a Berry phase. The modern theory has been very successfully particularly so in covalent materials.implemented, using first--principles ingredients, to the study of a large number of materials and phenomena.

The periodic polarization charge is the quantity that crystallography is able to measure, at least in principle. This *microscopic* quantity, although unrelated to macroscopic polarization, is interesting of its own. A few first--principles studies exist for some simple materials. Evidence will be given that even an extreme ionic crystal, like NaBr, is very far from the ideal Clausius-Mossotti limit.

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