

**o.m1.o3** **Micro-structured ferroelectrics for advanced optical applications.** F. Laurell, V. Pasiskevicius, H. Karlsson, R. Clemens, J. Hellström and S. Wang, *Laser Physics and Quantum Optics, Royal Institute of Technology 100 44 Stockholm, Sweden, tel. 46-8-7911327, fl@optics.kth.se.*

Keywords: ferro-electricity, NLO materials.

Ferroelectric materials are frequently used in optical applications to provide advanced functions to lasers and micro-optical components. The primary properties utilized are related to the acousto-optical, electro-optical and nonlinear optical properties, which allows light to be spatially and temporally modulated, as well as shifted in wavelength.

It was recently found that several ferroelectric crystals could be domain engineered by electric field poling after growth, i.e. a structure of oppositely oriented domains can be artificially made in an original single domain crystal. This is a flexible technique, which gives a new dimension of freedom to the design of optical components. Most the work has so far been focused on nonlinear optics to provide tailor made crystals for second harmonic generation and optical parametric oscillation. The crystals are then patterned on one of the c-faces with a lithographically defined periodic electrode with a grating pitch of a few  $\mu\text{m}$ , while the other side is patterned with a continuous electrode. An electric field higher than the coercive field is applied and oppositely oriented domains can nucleate under the electrode and grow straight through the substrate to the other side of the sample. The grating period is in this case chosen to compensate for phase velocity differences between the interacting optical waves and allows for generation of any wavelength within the transparency range of the material. For the materials explored to date,  $\text{LiNbO}_3$ ,  $\text{LiTaO}_3$  and crystals from the KTP family, this means wavelength from about 380 nm to 5  $\mu\text{m}$ . In this case established materials have been tailored for use at new wavelengths which is one of the great advantages with the so called quasi-phase matching (QPM) technique. There are several other advantages with the QPM scheme, which has made it revolutionise nonlinear optics. Probably the most important is that the flexible design allows any nonlinear tensor components to be utilised. Compared to birefringent phasematching which is the technique previously used an improvement of typically a factor 10 can be obtained for the conversion efficiency in the low power regime which can make conventional diode lasers useful in nonlinear optics.

The same arguments can in principle be used for redesigning electro- and acousto-optics, and work is presently in progress to investigate the possibilities in this field.

This presentation will review the basics of domain engineered ferroelectric materials for optical applications and the possibilities these opens in the next generation of optical systems.

**o.m1.o4** **PSEUDO -- a program for a pseudosymmetry search.** E. Kroumova, M.I. Aroyo, J.M. Pérez-Mato, J.M. Igartua, S. Ivantchev. *Departamentos de Física de la Materia Condensada y Física Aplicada II, Universidad del País Vasco, Apdo 644, 48080 Bilbao, Spain*

Keywords: pseudosymmetry, displacive ferroelectrics, supergroups.

The existence of pseudosymmetry in a crystal structure is indicative of a slightly distorted structure of higher symmetry. If the distortion is small enough, it can be expected that the crystal acquires this more symmetric configuration at a higher temperature after a phase transition. Using this type of reasoning Abrahams<sup>1</sup> developed structural criteria for the prediction of ferroelectricity in inorganic crystals. Its application to the structural data given in Inorganic Crystal Structure Database<sup>2</sup> for several polar groups resulted in the prediction of a number of new ferroelectric materials, some of which have already been experimentally verified.

Recently, we have developed a general procedure<sup>3</sup> for the systematic search of pseudosymmetry which is based on the determination of all possible minimal supergroups of the structure space group. For each of the minimal supergroups a transformed structure is obtained by applying the supergroup additional operations to the initial structure. Pseudosymmetry is detected when all atomic displacements necessary to make the transformed structure coincident with the original one can be chosen within a certain range. The efficiency and correctness of the approach has been checked on the compounds with Pnma,  $P2_12_12_1$ , and Pba2 symmetry.

For a structure specified by its space group  $H$ , the cell constants, and by one representative from each of the occupied Wyckoff positions, the program PSEUDO calculates the displacements of the atoms necessary to obtain a structure with higher symmetry given by the space group  $G_i > H$ , where  $G_i$  is a minimal supergroup of  $H$ . The output consists of the groups  $G_i$ , for which the maximal displacement is less than some previously given threshold. Also, the displacements for all of the atoms which would give the structure with the higher symmetry are listed.

The program PSEUDO, forms part of the Bilbao Crystallographic Server<sup>5</sup> and is available on-line at <http://www.cryst.ehu.es/pseudo.html>

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