

[o.m1.p11] Pinning effects and the dynamic behavior of ferroelectric domains in $\text{Sr}_{0.61}\text{Ba}_{0.39}\text{Nb}_2\text{O}_6:\text{Ce}$. T. Granzow¹, M. Imlau¹, Th. Woike¹, W. Kleemann², M. Wöhlecke³, R. Pankrath³, ¹ *Institut für Kristallographie, Universität zu Köln*, ² *Angewandte Physik, Universität Duisburg*, ³ *Fachbereich Physik, Universität Osnabrück*.
 Keywords: ferro-electricity, NLO materials.

Strontium-Barium-Niobate (SBN), $\text{Sr}_{0.61}\text{Ba}_{0.39}\text{Nb}_2\text{O}_6$, crystallizes in the unfilled tungsten-bronze-structure and undergoes a relaxor-kind phase-transition from the paraelectric high-temperature phase (PSG 4/mmm) into the ferroelectric low-temperature phase (PSG 4mm). A 'random-field Ising-model' has been proposed to explain this behavior.

In the ferroelectric phase only 180°-domains are present, which are oriented parallel or antiparallel to the polar c-axis. Investigations of the dynamic behavior of these domains are of interest for both the theoretical understanding of the relaxor-type phase-transition and for technological applications, e.g. the electric fixation of holograms for holographic data storage.

The dynamic behavior of the ferroelectric domains under the influence of an externally applied electric field is investigated by observing the electric polarization. Macroscopic polarization is measured by detecting electric charges on the crystal surface. Variation of the external field results in a ferroelectric hysteresis loop.

This ferroelectric hysteresis loop shows a pronounced 'aging', which depends on temperature, doping of the crystal and on the frequency used for measuring the hysteresis loop. The influence of the conductivity on the aging process is demonstrated by illumination of the crystal, whereby the photoconductivity increases by three orders of magnitude. This behavior can be explained by pinning-effects due to the influence of internal electric fields in the bulk of the crystal. Comparison with measurements of the time-dependent behavior of the electric polarization in a constant external electric field supports this model.

The characteristics of the ferroelectric domains of SBN:Ce which result from these measurements are presented for different temperatures and doping concentrations. They are discussed on the basis of the 'random-field Ising-model' to explain the relaxor behavior.

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[o.m1.p12] Polymorphism of nonlinear optical materials. Tatiana V. Timofeeva¹, Vladimir N. Nesterov¹, Ronald D. Clark¹, Mikhail Yu. Antipin^{1,2}, ¹ *Department of Physical Sciences, New Mexico Highlands University, Las Vegas, New Mexico 87701, USA*; ² *Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilov St., B-334, Moscow, Russia*.
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Three NLO materials 1,1-dicyano-4-(4-dimethylaminophenyl)-1,3-butadiene (I), 3-methoxy-dicyanovinylbenzene (II), and 2-adamantylamino-5-nitropyridine (III) have been thoroughly investigated to find polymorphs with acentric structure and molecular orientation optimal for second harmonic generation. We choose these compounds since for analogous materials acentric crystals were observed before. It was found that compounds I and II crystallize in two forms from the same solvent (concomitant or one-pot polymorphism). For compound III two forms were also obtained. Form IIIa was crystallized by zone melting technique [1] and by sublimation, and form IIIb was obtained from solution. Some characteristics of these polymorphs are listed below:

Compound	Space group	Z	Color
Ia	P2 ₁ /c	4	red
Ib	P2 ₁ /n	4	dark
Iia	P2 ₁	6	yellow
Iib	P-1	4	colorless
IIIa	Pna2 ₁	4	yellow
IIIb	Pca2 ₁	4	yellow

Crystal energy for both modifications of compound I was found to be almost equal, and that explains in part that they crystallize from the same solvent under the same conditions. Polymorphs of I are built of similar molecular layers with different layers superposition. The same situation was found for polymorphs of II. So polymorphs of I and II might also be described as organic polytypes.

For compound III acentric form (IIIa) was found and described in the literature before [1]. We found another acentric form IIIb. Results of crystal energy calculations show that in this case only introduction of hydrogen bond interactions allows to reproduce relative stability of polymorphs IIIa and IIIb.

Powder test of second harmonic generation revealed NLO activity of polymorphs IIIa and IIIb, but no activity was found for acentric Iia form, due to its pseudocentrosymmetric structure.

Results of powder X-ray diffraction, UV spectroscopy, quantum chemical calculations of molecular hyperpolarizability of polymorphs are also discussed.

[1] Yokoo, A., Tomaru, S., Yokohama, I., Itoh, H., Kaino, T. "A new method for long-rod organic nonlinear optical crystals with phase-matched direction", *J. Crystal Growth*, 1995, 156, 279-284.