



**Photorefractive Materials,  
Effects and Devices**

**Light in Structured Nonlinear Materials**

**October 13-15, 2011**

**Ensenada, Mexico**

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**Cornelia Denz (University of Münster, Germany)**

Structured light fields for complex photonic lattices and optical manipulation

**Jack Feinberg (University of Southern California, USA)**

Self-pumped phase conjugation and laser resonator cavities

**Peter Günter (ETH-Zurich/Rainbow Photonics, Switzerland)**

Past, present and future of photorefraction

**Jean-Pierre Huignard (Jphopto - Consultant Photonics, France)**

Photorefractives and other types of nonlinearities for applications to dynamic holography and laser beam control

**Ponciano Rodríguez-Montero (INAOE, Mexico)**

Adaptive photodetectors: from ultrasonic waves to heartbeat detection

**Alexandr Shumelyuk (Institute of Physics, National Academy of Sciences, Ukraine)**

Photorefractive wave mixing in monoclinic crystals with bipolar conductivity (Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub>)

**David C. Smith (University of Southampton, Great Britain)**

Non-linear Control of Surface Plasmon Polaritons with Photorefractive Liquid Crystal Cells

**C. Y. J. Ying (University of Southampton, Great Britain)**

Local electro-optic coefficient enhancement in LiNbO<sub>3</sub> channel waveguides by domain engineering

## Preface

The proceedings in this volume are the summaries of works to be presented at the 13<sup>th</sup> conference on Photorefractive Materials, Effects and Devices, which will take place in Ensenada, Mexico, on October 13-15, 2011. This is the first conference of the series to be held in Latin America; however, this could hardly be called a Latin-American conference: there are contributions from over 20 countries from North and South America, Europe and Asia.

Many of the materials in which the photorefractive effect is observed are used in other fields of nonlinear optics: quasi-phase-matching in periodically poled materials, photonic crystals, slow and fast light propagation in structured materials, among others; furthermore, many of the researchers that work - or previously worked - in the field of the photorefractive effect are now involved in other fields of nonlinear optics but with the same materials (and in many cases rely on their expertise in the photorefractive effect to avoid it altogether). We therefore found it appropriate to gather these topics in the same conference and to give it the subtitle "Light in Structured Nonlinear Materials."

In 2011 two important and productive figures in the field of the photorefractive effect, Prof. Peter Günter and Prof. Jean-Pierre Huignard, have retired. They were kind enough to accept crossing the Atlantic to give plenary talks at this conference. In addition, this year is the 30th anniversary of the discovery of the self-pumped phase conjugator, better known as the "Cat conjugator," by Prof. Jack Feinberg, who will also honor us with an invited talk.

This is the first conference of the series to introduce a tutorial session, which will take place on October 12, one day before the conference starts, directed towards undergraduate and graduate students interested in nonlinear optics. We would like to thank Germano Montemezzani, Klaus Meerholz, Sakellaris Mailis and Serguey Odoulov for accepting the invitation to give these talks.

We would like to thank CICESE, INAOE, CONACYT, the AFOSR and the organizers of the previous conference, Karsten Buse and Cornelia Denz, for financial (and even emotional) support. Finally, we would like to thank the international organizing committee and all of the attendees for their confidence in us and in Mexico to organize and hold the conference here. We hope you will find this conference interesting, stimulating and, of course, fun.

Sincerely,

Roger, Serguei and Rubén  
Ensenada, October 2011

# Topics and Session Chairs

**Charge transport effects** (Mercedes Carrascosa, Universidad Autónoma de Madrid, Spain)

**Lithium niobate and related materials** (Jingjun Xu, Nankai, University, China)

**Wave-mixing processes** (Serguey Odoulov, Institute of Physics, Ukraine)

**Information processing and storage** (Kazuo Kuroda, Tokyo University, Japan)

**Interferometric applications** (Jaime Freilich, Universidad Campinas, Brazil)

**Polymer, liquid crystal and other materials** (Malgosia Kaczmarek, University of Southampton, UK)

**Ferroelectric nano-particle and hybrid materials** (Dean Evans, Air-force Research Laboratory, Dayton, USA)

**Beam and pulse nonlinear propagation** (Wieslaw Krolikowski, Australian National University, Australia)

**Periodic and aperiodic nonlinear ferroelectric structures** (Robert Eason, University of Southampton, UK)

**Photorefractive waveguides and periodic structures** (Detlef Kip, Helmut Schmidt University, Germany)

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# Mechanochemically synthesized LiNbO<sub>3</sub> nanocrystals

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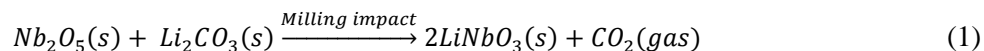
**Abstract:** LiNbO<sub>3</sub> nanocrystals were prepared by mechanochemical-calcination method using Li<sub>2</sub>CO<sub>3</sub> and Nb<sub>2</sub>O<sub>5</sub> as precursors. Synthesis of LiNbO<sub>3</sub> occurred during the ball milling but not to a completion. Subsequent heating to complete the LiNbO<sub>3</sub> synthesis was needed.

## Introduction

Lithium Niobate (LiNbO<sub>3</sub>) has good piezoelectric and non-linear optics properties and polarization along crystallographic c-axis [1]. There exist several synthesis methods for LiNbO<sub>3</sub> such as: Czochralski, powder laser deposition, solid state reaction and mechanical alloying [2-4] the application of the material will determine the preparation route to take. The present research work describes the obtention of LiNbO<sub>3</sub> by a mechanochemical reaction using lithium carbonate (Li<sub>2</sub>CO<sub>3</sub>) and niobium oxide (Nb<sub>2</sub>O<sub>5</sub>) as precursor agents, followed by a heat treatment at 650°C. The obtained samples were analyzed using X-ray diffraction, DTA-TGA, Raman Spectroscopy and HRTEM techniques.

## Sample Preparation and Characterization

Stoichiometric (equimolar quantity) lithium niobate (LN) powders were prepared by high-energy ball milling (SPEX 8000 mixer) in a nylon vial with Al<sub>2</sub>O<sub>3</sub> balls. Several samples were prepared at different milling times of 3, 9, 30, 45, 90, 210, 300, 600, 900 and 1200 min in order to observe the mechanochemical effect. The source materials were Li<sub>2</sub>CO<sub>3</sub> and Nb<sub>2</sub>O<sub>5</sub> of high purity 99.99 %, commercially available from Alfa Aesar, they were weighted according to the following reaction:



Products were analyzed by DTA-TGA using TA Q600 in the temperature range between 30°C to 1100°C, these analysis provide information about the temperature formation of crystalline LN, after that powders were heated at 650°C. Then X-ray diffraction (XRD) was recorded for all samples using a Pananalytical X-Pert system with source of CuK $\alpha$  radiation at 40 keV and 30 mA in the 2 $\theta$  range between 20° and 90°, at 0.02° steps every 4 seconds. The Raman spectrum was recorded on a Jobin Yvon (Horiba grup) Raman spectrometer (lexc = 632.8nm). The spectra samples were obtained in the range 100-1000 cm<sup>-1</sup>. Morphology and structure of the LN powders were examined in a HRTEM Jeol JEM-2200FS.

## Results and Discussion

Formation of pure crystalline LiNbO<sub>3</sub> phase by mechanochemical process and subsequent calcination was confirmed from XRD peaks and Raman spectrum as shown in Figure 1. Crystallographic indexation was obtained using JCP: 00-074-2238 for trigonal (R3c) indicating (012), (104), (110), (024) and (116) as principal directions with FWHM of 25  $\pm$  5nm.

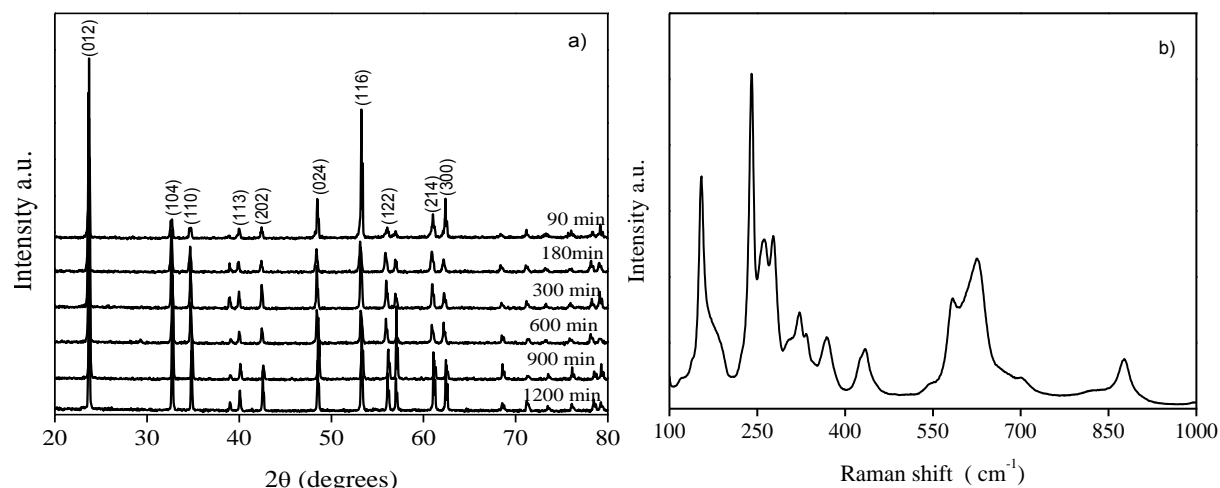


Fig. 1. a) XRD peaks of LN as prepared at different milling times and heated at 650°C. b) Raman spectrum of LN nanopowders

Figure 2 shows high resolution TEM image and selected area diffraction pattern (SAD) of the LiNbO<sub>3</sub> samples after calcination process. In the image more details on *LiNbO<sub>3</sub>* crystallographic structure are observed. The interatomic distances as measured were 0.4140 nm. Select area diffraction pattern (SAD) shows principal diffractions directions at [110], [116] and [312].

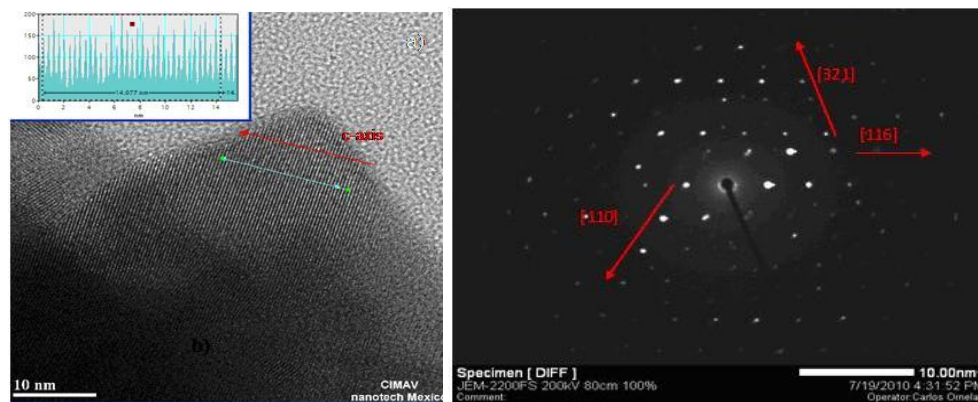


Fig. 2. Transmission electron and select area diffraction for LiNbO<sub>3</sub> samples after calcination process

## Conclusions

An effective synthesis method to produce LiNbO<sub>3</sub> nanocrystals using lithium carbonate ( $Li_2CO_3$ ) and niobium oxide ( $Li_2CO_3$ ) as precursors was developed during this research work. XRD measurements, Raman spectrum, HRTEM images and electron diffraction confirmed the formation of crystalline phases.

**Acknowledgements:** The authors thank: PROMEP-SEP for the project F-PROMEP-39/REV-03 SEP-23-005 and to the NANOTECH-CIMAV.

## References

- [1] Tatyana Volk, Manfred Wöhlecke, "Lithium Niobate: Defects, Photorefraction and Ferroelectric switching", Springer series in materials science 115 (2008).
- [2] Jie Zhan a,n,1, DongxuLiu, WeiDub, ZeyanWanga, PengWanga, Hefeng Cheng, Baibiao Huang, Minhua Jiang, "Synthesis and characterization of high crystallinity, well-defined morphology stoichiometric lithium niobate nanocrystalline", Journal of Crystal Growth 318 (2011) 1121–1124.
- [3] de Figueiredo RS, Messai A, Hernandez AC, Sombra ASB. "Piezoelectric lithium niobate by mechanical alloying". J Mater Sci Lett 17 (1998) p 449–51.
- [4] L.B. Kong, T.S. Zhang, J. Ma b, F. Boey. "Progress in synthesis of ferroelectric ceramic materials via high-energy mechanochemical technique" Prog. Mater. Sci. 53 (2008) 207–322.

# Oxygen vacancies effect in magnetic moment of LiNbO<sub>3</sub>: Theoretical study

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**Abstract:** Spin polarized DFT calculations exposed that magnetic nature emerges in LiNbO<sub>3</sub> unit cell, magnetism arising from the oxygen vacancies at the NbO<sub>6</sub> octahedron.

In the last decades ferroelectric Lithium Niobate (LN) has attracted great interest in optoelectronics applications, because of photorefractive and non-linear optics properties [1]. The fact of the off centering Nb<sup>5+</sup> originated from its d<sup>0</sup> electronic states, contradicts the possibility of magnetism that arises from local magnetic moments associated with the occupation of d-states at the Nb sites [2]. Recent studies have demonstrated the room temperature ferromagnetism in Ln:Co single crystal films [3], also room temperature ferromagnetism has been observed in nanoparticles of otherwise nonmagnetic materials has been attributed to point defects at the surface of the nanoparticles [4-6]. In order to expose a magnetic behavior of LN we carried out a systematic calculation of its electronic structure when oxygen vacancies are present in its crystalline structure; thus in this work we present our results in the spin polarized electronic energy band structure, density of states and magnetic moment of LN, calculated with the local density approximation in CASTEP code [7].

## Crystal structure and calculation method

Calculations of band structure and density of states were carried out for the crystalline structure without vacancies and then with oxygen atom vacancies in different crystallographic positions. The starting lattice parameters were  $a = 5.148$  and  $c = 13.840$  and the space group for this material is R3c. Local density approximation (LDA) and Ceperly-Alder parameterized by Perdew and Zunger (CA-PZ) functional were used in the calculus. The geometry was first optimized using BFGS algorithm, in order to start the electronic energy band and density of states calculations with the spin polarized option, using the high spin as initial values. The cut off energy was 260 eV, with SCF tolerance of  $2 \times 10^{-6}$  eV/atoms. The k point mesh parameters were 3x3x2, with ultrasoft pseudopotentials used for all atoms. All calculations were carried out under trigonal symmetry constrains.

## Results

The figure 1 shows the calculated spin polarized DOS for the crystal structure of LiNbO<sub>3</sub> without O vacancies (a) and with O vacancies (b). As can be observed in Fig. 1(a), there is not spin polarization found in our calculations. However, the fig 1(b) shows a spin polarization which gives a magnetic moment of 0.44  $\mu_B$  to the LiNbO<sub>3</sub> unit cell when O vacancies are present in the NbO<sub>6</sub> octahedron; in this case, the d orbital has one electron unpaired because the O vacancy. A deepest analysis exposed a p and d orbital's spin polarization as the underlying origin for this magnetic moment; where spatial rearrangement of electrons, when O vacancies are present, is proposed as the principal contributor to magnetic behavior.

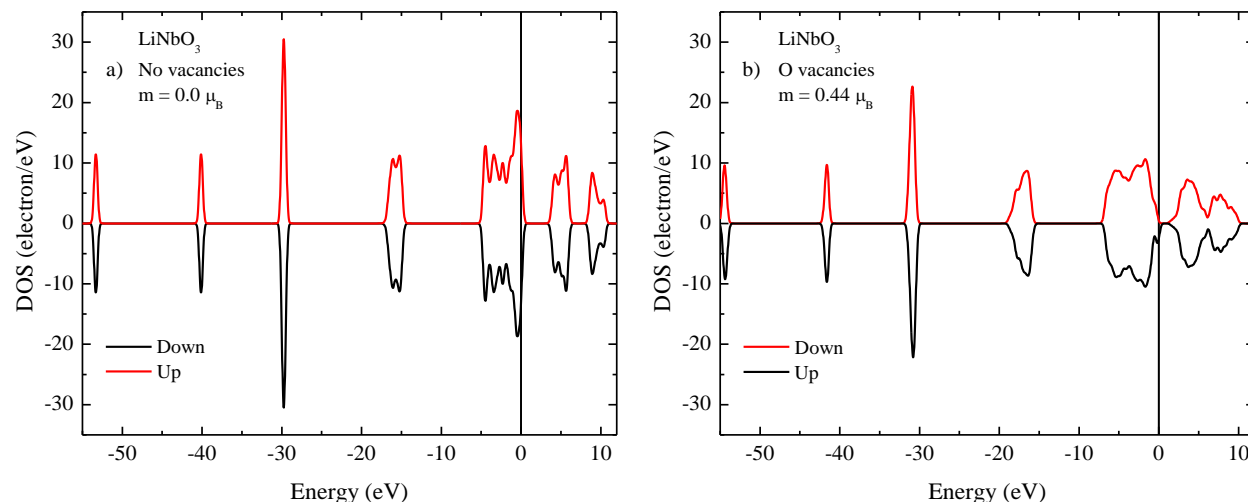


Fig. 1. The density of electronic states of the LN: a) without vacancies, and b) with oxygen vacancies at the  $\text{NbO}_6$  octahedrons.

## Conclusions

The present study exposed a new magnetic property in nanocrystalline LN. The magnetic nature is rendered possible by the oxygen vacancies in the  $\text{NbO}_6$  octahedron.

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## References

- [1] Tatyana Volk, Manfred Wöhlecke, "Lithium Niobate: Defects, Photorefractive and Ferroelectric switching", Springer series in materials science 115 (2008).
- [2] T. T. M. Palstra, G. R. Blake, "Multiferroic Materials: Physics and Properties" in Encyclopedia of Materials: Science and Technology, Elsevier (2006).
- [3] J A. Sundaresan, C.N.R. Rao, "Ferromagnetism as a universal feature of inorganic nanoparticles", Nano Today 4 (2009) 96-106.
- [4] R.V.K. Mangalam, Nirat Ray, Umesh V. Waghmare, A. Sundaresan, C.N.R. Rao, "Multiferroic properties of nanocrystalline  $\text{BaTiO}_3$ ", Solid State Comm. 149 (2009) 1-5
- [5] Min Wang, Guo-Long Tan, and Qingjie Zhang, "Multiferroic Properties of Nanocrystalline  $\text{PbTiO}_3$  Ceramics", J. Am. Ceram. Soc., 93 (2010) 2151-2154.
- [6] Cheng Song, Changzheng Wang, Xuejing Liu, Fei Zeng, and Feng Pan\*, "Room Temperature Ferromagnetism in Cobalt-Doped  $\text{LiNbO}_3$  Single Crystalline Films", Crystal Growth & Design, 9 (2009) 1235-1239.
- [7] S. J. Clarck, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. J. Probert, K. Refson, M. C. Payne, "First principle methods using CASTEP", Zeitschrift fuer Kristallographie, 220 (2005) 567-570