Microsymposia

common defect type, while in the non-polar a-GaN layers most of the defects are (0001)-oriented stacking faults [1].

We developed a method for the determination of the densities of individual defect types both in c- and a-oriented GaN layers, based on diffuse x-ray scattering and reciprocal space mapping. In the c-GaN layers the method is based on the comparison of the reciprocal space map of the diffusely scattered intensity measured both in standard and grazing-incidence geometry, with simulations based on a numerical Monte-Carlo procedure [2], [3]. The density and type of stacking faults in a-GaN layers can be determined from the intensity distribution along [0001]-oriented streaks in reciprocal space perpendicular to the fault planes.

We have measured a series of GaN layers of both orientations with various defect densities and compared the densities resulting from our procedure with results of other independent methods (transmission electron micrography, etching techniques) and we obtain comparable total densities of defects.

[1] M.A. Moram, M.E. Vickers, *Reports on Progress in Physics* **2009**, *72*, 036502. [2] M. Barchuk, V. Holý, B. Miljevic, B. Krause, T. Baumbach, J. Hertkorn, F. Scholz, *J. Appl. Phys.* **2010**, *108*, 043521. [3] M. Barchuk, V. Holý, B. Miljevic, B. Krause, T. Baumbach, *Appl. Phys. Lett.* **2011**, *98*, 021912.

Keywords: gallium nitride, diffuse X-ray scattering, defects

MS.28.3

Acta Cryst. (2011) A67, C74

Lithium niobate: a smart material for various applications in ontoelectronics

Marc D Fontana, Sabrina Mignoni, Rachid Hammoum, Patrice Bourson, Laboratoire Matériaux Optiques, Photonique et Systèmes, Université Paul Verlaine – Metz and Supélec, 2 rue Edouard Belin, 57070 Metz (France). E-mail: fontana@metz.supelec.fr

LiNbO₃ (LN) is a widely studied optoelectronic material useful for a great variety of applications in non linear optics, integrated optics and solid state lasers [1], [2]. It can be grown in large single crystals, usually by Czochralski technique, and generally in the congruent composition [3]. Therefore it presents a Li deficiency and thus can be easily doped with various impurities. Doping these crystals can suitably change their optical properties [2]. Thus doping LN with rare earth ions or Cr is appropriate to induce luminescence. The introduction of Fe gives rise to a large photorefractive effect, whereas doping with Mg or Zn provides electrooptic coefficients with an efficient use [1], [2].

In fact the incorporation of dopants induces a change in the local structure of intrinsic (lattice) defects related to non-stoichiometry [4]. The congruent composition corresponds to a composition of nearly 0.94, meaning that about 6% of Li sites are empty. Since Nb5+ ions have a radius close to Li⁺, they can go fill these empty sites (they are called antisites defects). Different models were proposed to describe the intrinsic defects in the nominally pure crystals with different compensation mechanisms: Li vacancy model or Nb vacancy model for the congruent composition [3] and coexisting Li and Nb vacancies with a content varying with the composition from congruent to stoichiometric [5]. The incorporation of dopants in the LN lattice does not have the same effect since it enters the A site (generally occupied by Li ions) or the B site (generally occupied by Nb ions) according to the nature and the concentration of the dopants. As a consequence, it induces different changes in the dynamics of intrinsic defects: Nb and Li vacancies, Nb antisites.

Here are pointed out the dependencies of several linear and non linear optical properties on the dopant content. The electrooptic and photorefractive [6-8] properties recorded in LN crystals doped with Mg, Fe, Zn or Hf [9], [10] are especially reported and discussed. The

link between the mechanism and site of incorporation of dopants and the non-monotonous behaviour of optical properties is demonstrated. Thus the remove of antisite defects is related to a threshold in the behaviour of some optical properties.

At last is shown how the optimization of the structure can be used in applications in optoelectronics.

[1] E. Kratzig, O.F. Schirmer, Photorefractive Materials and Their Applications, Topics in AppliedPhysics, Springer-Verlag, Berlin, 1999, 62, 131-166. [2] T. Volk, M. Wöhlecke, Lithium Niobate Defects, Photorefraction and Ferroelectric Switching, Springer Berlin Heidelberg, 2008. [3] A. Räuber, Chemistry and physics of lithium niobate, Current Topics in Material Sciences, Ed. by E. Kaldis, North Holland, Amsterdam, 1978, 481-601. [4] Y. Zhang, L. Guilbert, P. Bourson, K. Polgar, M.D. Fontana, J. Phys.: Condens. Matter 2006, 18, 957-963. [5] F. Abdi, M.D. Fontana, M. Aillerie, P. Bourson, Applied Physics A 2006, 83, 3, 427-434. [6] M. Abarkan, M. Aillerie, J.-P. Salvestrini, M.D. Fontana, E. Kokanyan, Applied Physics B: Lasers and Optics 2008, 92, 603-608. [7] R. Mouras, M.D. Fontana, M. Mostefa, P. Bourson, J. Opt. Soc. Am. B 2006, 23, 3, 1867-1871. [8] F. Abdi, M. Aillerie, P. Bourson, M.D. Fontana, Journal of Applied Physics, 2009, 106, 033519. [9] R. Hammoum, M.D. Fontana, M. Gilliot, P. Bourson, E. Kokanyan, Solid State Communications, 2009, 149, 1967-1970. [10] S. Mignoni, M.D. Fontana, M. Bazzan, M.V. Ciampolillo, A.M. Zaltron, N. Argiolas, C. Sada, Applied Physics B: Lasers and Optics, 2010, 101, 541-546.

Keywords: defect, optoelectronics, doped

MS.28.4

Acta Cryst. (2011) A67, C74-C75

Study of the thermal anisotropy of KLu(WO₄)₂ for high power laser applications

M. Aguiló, M. C. Pujol, X. Mateos, J. J. Carvajal, F. Díaz, Física i Cristal·lografia de Materials i Nanomaterials (FiCMA-FiCNA-EMAS), Universitat Rovira i Virgili (URV), Campus Sescelades, c/ Marcel.lí Domingo, s/n, E-43007 Tarragona, (Spain). E-mail: Magdalena.aguilo@urv.cat

KLu(WO₄)₂ crystal belongs to the monoclinic system, with the space group C2/c. This material is a well known interesting laser host material for optically active lanthanides ions, such as Yb3+ and Tm3+. Successful laser action of both ions, at 1.1 microns and 1.9 microns has been already demonstrated, in different configurations such as slab, waveguide and thin disk and also, in continuous-wave (cw) and pulsed regimes. Nevertheless, the complete knowledge of the physical anisotropy of this material and its application in laser action can lead to further improvements in laser efficiency or new applications. In relation with this aspect, the study of the thermal anisotropy of this material is crucial. Thermal conductivity in this crystal is a symmetrical second-rank tensor and as the crystal is monoclinic it has four nonzero components in the crystallo-physical frame $X_{l\kappa}//a$. $X_{2\kappa}//b$, $X_{3\kappa}//c^*$. With the measurement of the thermal diffusivity along four crystallographic directions (a, b, c) and c^*), and the specific heat capacity, the thermal conductivity tensor has been calculated.

KLuW is grown from high temperature solutions. The solvent used by us is $K_2W_2O_7$ and the growth method was the Top Seeded Solution Growth by Slow Cooling (TSSG-SC). Samples for each measurement are crystallographically oriented to be cut and polished to optical grade quality. The eigenvalues of the thermal conductivity are κ '₁₁=2.95 Wm ¹K-¹, κ '₂₂=2.36 Wm ¹K-¹, and κ '₃₃=4.06 Wm ¹K-¹, with the maximum value along a direction in the *a-c* crystallographic plane, at 40.75° from the N_g principal optical axis (22.25° from c crystallographic axis), figure 1 shows the location of the tensor. KLuW is a optical biaxial crystal, in which the reference system for laser applications and linear optics is the real refractive index part, so the three principal optical directions,