

## Poster Sessions

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Borinic complexes with N,O and N, N chelate ligands are known to have very interesting optical features [1] desirable for applications in organic light emitting diodes (OLEDs).

First complexes have been obtained and characterized by Letsinger and Skoog in 1955 [2]. Since then, the chemistry of boronic derivatives has been vigorously studied. It is focused on development of new synthetic methods, triggering wavelength of emission, improving efficiency of emission and tuning stability of these compounds. Properties of borinic complexes results from the properties of bonds formed with boron atom (especially B-N bonds) [3].

Recently, a new group of complexes with the boron atom in asymmetrical coordination has been synthesised and characterized [4]. Our preliminary DFT calculations and analysis have shown that one can expect correlation between the observed physical features and structural and electronic parameters of borinic complexes. Hence, in this contribution we will present the experimental and theoretical structural properties of borinic derivatives in the context of their applications in functional materials.

[1] A. Nagai, Y. Chujo, *Chem. Lett.* **2010**, *39*, 430-435; F. Jäkle *Coordination Chemistry Reviews*, **2006**, *250*, 1107-1121. [2] R.L. Letsinger, I. Skoog, *J. Am. Chem. Soc.* **1955**, *77*, 2491. [3] C.H. Chen, S. Jianmin, *Coordination Chemistry Reviews*, **1997**, *171*, 161-174. [4] L. Jastrzębski, P. Kurach, S. Luliński, J. Serwatowski, G. Wesela-Bauman, K. Woźniak, *unpublished results*.

**Keywords:** optoelectronics, coordination, boron

### MS28.P02

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#### Microhardness and dopant concentration in GaSe:In and GaSe:S crystals

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The unit cell of GaSe consists of two bonded planes of Ga in which every atom is surrounded by three atoms from adjacent Se layer. The strong bonding inside the fourfold atomic planes and weaker Wan-der-Vaals bonding between the stacks results in the polytypism and perfect cleavage. A semiconducting  $\epsilon$ -GaSe may become an important material for light frequency conversion into IR and THz ranges. However the cleavage and poor hardness considerably limits its application.

In and S are known to be the promising dopants which are able to improve mechanical, optical and other properties of GaSe.

But there is a lack of published data on the distribution of the doping impurities along the ingot. Much of the papers correlate the changing properties of GaSe just with the impurity concentration in the charge.

In this work GaSe:S and GaSe:In crystals were grown by modified Bridgman technique [1]. The doping was performed by adding of the impurity in the charge both in elementary state (In or S) and in the form of GaS and InSe. Molar ratio between GaSe and the impurity was 1, 5 and 20%. The crystals were cut orthogonal to the growth direction for investigation of chemical composition, Vicker's microhardness and optical properties.

Doping by the elementary impurity is preferable if desirable concentration in the crystal does not exceed 2 mol.% of S or 0.2 mol.%

of In. In that way the impurity distribution is very homogeneous along the crystal. For the crystals of solid solutions GaSe-GaS and GaSe-InSe higher concentrations of S and In are possible. However the impurity content increases gradually to the tail of the crystal, so the length of the sample with uniform composition becomes critical. On the other hand, gradient concentration of impurity in GaSe is a desired result for frequency conversion of ultra-short pulses with broad spectral bandwidths and for pulse widths compression [2].

The microhardness increment of GaSe is well correlated with impurity concentration. The maximum values were measured to be 3 times larger than that for pure GaSe crystals.

Variation of optical properties and the application perspectives of double doped GaSe:In,S crystals will be discussed in the report.

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[1] K.A. Kokh, B.G. Nenashev, A.E. Kokh, G.Yu. Shvedenkov, *J. Cryst. Growth* **2005**, *275*, E1964-E1967. [2] J.J. Huang, W. Gao, T. Shen, B.L. Mao, Yu.M. Andreev, A.V. Shaiduko, G.V. Lanski, U. Chatterjee, V.V. Atuchin, *JOSA*, **2007**, *24*, P.3081-3090.

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#### Effects accompanying GaN substrate misorientation in growth of InGaN and AlGaN layers

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InGaN and AlGaN layers are used in many electronic and optoelectronic devices as LEDs (light emitting diodes), laser diodes emitting in violet/blue/green spectral region, and high electron mobility transistors (HEMTs). These devices form a multibillion market, the largest from all compound-semiconductor devices.

In the presentation, we will show experimental results of microstructural examinations performed on AlGaN and InGaN layers grown on misoriented (off-axis) GaN substrates by Metalorganic Chemical Vapour Phase Epitaxy (MOVPE). The following effects accompany the application of off-cut substrates with respect to the on-axis ones: i) morphology of the layers is much better, ii) p-doping is more effective, iii) cracking of AlGaN layers happens at higher layer thickness and larger Al content, iv) unit cells of the ternary layers are not tetragonally deformed any more- the deformation is trigonal, v) indium incorporation into InGaN layers is smaller.

These results were obtained using High Resolution X-ray Diffractometry (HR XRD), Atomic Force Microscopy (AFM), and photoluminescence (PL) and explained using an elasticity theory and theory of MOVPE growth. In particular, the problem of indium incorporation will be explained in details by analysis of atomic step flow during the growth of InGaN layers.

Some of the effects, as better morphology, p-doping, less-cracks, have a positive impact on the device performance. Smaller effectiveness of indium incorporation makes fabrication of true-blue and green emitters more difficult, but, on the other hand, gives an unique possibility of constructing multicolor laser diode arrays on GaN substrates laterally patterned to obtain a variable misorientation across the wafer.

**Keywords:** semiconductors, GaN, epitaxy