

Poster Sessions

new system makes use of interactive interfaces and state-of-the-art visualization tools. To date, the project has delivered a sequence and ligand processing workflow, supported by a graphical user interface and managed by a workflow engine. The functional and interface design incorporates feedback collected from depositors and annotators.

During 2011 the project will develop the new user interface for deposition. The overall design of the system, completed modules and the prototype for the deposition interface will be presented.

The wwPDB members are: RCSB PDB (supported by NSF, NIGMS, DOE, NLM, NCI, NINDS and NIDDK), PDBe (EMBL-EBI, Wellcome Trust, BBSRC, NIGMS, and EU), PDBj (NBDC-JST) and BMRB (NLM).

Keywords: database, macromolecule, annotation

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An overview of solvent use and solvate formation in the CSD

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As part of an ongoing investigation into solvate formation [1], [2], a database of over 90,000 solution-based crystallisation experiments has been extracted from the Cambridge Structural Database [3]. For each compound crystallised, the solvent(s) used and any solvent(s) included in the resulting crystal are listed.

Three categories of solutes were distinguished in the initial analysis of the data: organometallic compounds, organic salts and neutral organic molecules. The most frequently used solvents for organometallic compounds are hexane, dichloromethane, diethyl ether, toluene, pentane and their binary mixtures. Organic salts are most frequently crystallised from methanol, ethanol, water and acetonitrile, with the use of mixed solvents being less common for this group. Common solvents for neutral organic compounds include methanol, ethanol, hexane, dichloromethane, ethyl acetate and acetone.

The overall frequency of solvate formation is higher for organic salts and organometallic compounds than for neutral organic molecules. Surprisingly, this trend also holds for solvate formation with apolar solvents, which do not interact more strongly with ions than with neutral molecules.

The most frequently included solvent is water, which is often present in crystals grown both from water and from organic solvents. The relative frequencies of solvates with various organic solvents are similar to those found earlier by Görbitz [4]. Solvate formation propensities are obtained from these frequencies by taking into account the frequency of using each solvent for crystallisation [5]. There is a large variation in these propensities: 18% of the crystals grown from water are hydrates, but only 0.4% of the crystals obtained from ethyl acetate include solvent molecules. In fact, hydrates are more frequent than ethyl acetate solvates even among crystals grown from solutions in ethyl acetate.

Solvate formation propensities depend on whether crystals with only metal-coordinated solvent molecules are counted as solvates or not. For strongly coordinating solvents (e.g., ethanol, DMF), the difference can be more than twofold.

Data on crystallisation from mixed solvents can be used to test competition between different solvents and to make small differences between similar overall solvate formation propensities more clearly visible. Unfortunately, the exact composition of solvent mixtures is rarely reported, so these results may be biased if mixtures rich in one of the components are used more frequently than mixtures rich in other(s).

[1] L. Infantes, L. Fábrián, W. D. S. Motherwell, *CrystEngComm* **2007**, *9*, 65-

71. [2] L. Fábrián, *Acta Crystallographica* **2008**, *A64*, C93. [3] F. H. Allen, *Acta Crystallographica* **2002**, *B58*, 380-388. [4] C. H. Görbitz, H. P. Hersleth, *Acta Crystallographica* **2000**, *B56*, 526-534. [5] A. Nangia, G. R. Desiraju, *Chemical Communications* **1999**, 605-606.

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A new interface to the cambridge structural database (CSD) in crysAlis^{Pro}

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Instrument time is a valuable commodity which can often be wasted with the accidental recollection of known samples. In order to avoid such mistakes cross checking unit cells with those in databases of crystal structures such as the CSD [1] prior to data collection is a useful exercise. To facilitate this we have, in conjunction with the Cambridge Crystallographic Database Centre (CCDC), developed module within CrysAlis^{Pro} [2] which provides a simple user friendly interface to the CSD allowing fast and easy unit cell checking within our data collection software. The module and its functionality are presented herein.

[1] F.H. Allen, *Acta Cryst.* **2002**, *B58*, 380-388. [2] Agilent Technologies, CrysAlis^{Pro} Software system, **2010**, Agilent Technologies UK Ltd.

Keywords: software, instrumentation, diffraction

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Computer-readable database for magnetic space groups

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We have developed a magnetic space-group database and made it freely available over the internet. Settings for both the nuclear cell (Opechowski-Guccione setting) and magnetic cell (Belov-Neronova-Smirnova setting) are listed, as well as the transformations between them. For each space group and setting, the operators and the Wyckoff positions are given. These data are consistent with existing tables [1,2]. Both human-friendly and computer-friendly versions of the tables are available.

[1] D. Litvin, *Acta Cryst.* **2008**, *A64*, 419-424. [2] C. J. Bradley and A. P. Cracknell, *The Mathematical Theory of Symmetry in Solids* **1972** (Oxford University Press, London).

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Boronic complexes-towards applications in functional materials

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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

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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 ϵ -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