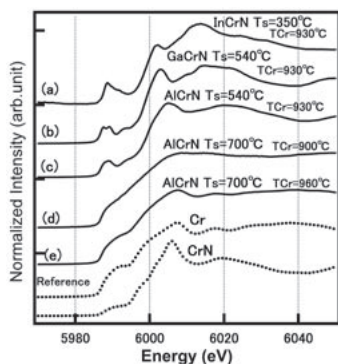


about growth mechanisms and structural properties of III(Al, Ga, and In)-Cr-Nitride. Those layers were grown on Al<sub>2</sub>O<sub>3</sub> (0001) with GaN (0001) templates by radio frequency plasma assisted molecular beam epitaxy. Structural properties were studied by XANES and XAFS analysis. Fig.1 shows XANES spectra. Cr foil and CrN spectra also are given. In Fig.1, the comparison of the spectra (d) and (e) of AlCrN grown at 973K with that of Cr foil indicates that the Cr clusters with a nano-size, which could not be detected in XRD, are formed in AlCrN grown at 973K. In the other hand, we have reported Cr atoms substitute Ga-site in GaCrN grown at 813K (b). Comparing the spectra (b) to (c), Cr atoms substitute Al-site in AlCrN grown at 813K. In a similar way, Cr atoms substitute In-site in InCrN grown at 813K (a). Low temperature MBE enables the growth of AlCrN, GaCrN and InCrN without CrN segregation or Cr cluster. The structural properties and electric states will be discussed in the conference in detail.



Keywords: diluted magnetic semiconductor, XAFS, III-Cr-N

## P02.02.59

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### Efforts to improve the phase convergence of the shake-and-bake (SnB) algorithm towards solutions

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“Shake and Bake” procedures attempt to determine crystal structures from random atom starting models by phase refinement algorithms that operate in both real and reciprocal space. The reciprocal space module uses a parameter shift procedure to minimize R<sub>min</sub> for the individual phases for each real/reciprocal space refinement cycle. The majority of the reciprocal space refinement cycles, however, do not actually move the phases towards the solution, but rather perturb the phases so they might escape from local false minima until by chance a downhill pathway to the solution is found. Recent work has surprisingly shown that it is possible to analyze these intermediate non-solution stages of the refinement to identify subgroups of phases that have a significantly lower mean phase error than the remaining reflections in the direct methods trial sets. We are currently examining various methods to exploit this information and accelerate the rate convergence of the SnB process towards solutions. This will be exceedingly important for the more intransigent structure determinations in which all trials constantly languish in the non-solution R<sub>min</sub> optimization state. Research support from the Human Frontier Science Program (HFSP) is most gratefully acknowledged.

Keywords: direct methods, shake-and-bake algorithm, phase refinement

## P03.01.01

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### NRCVAX revisited: Reusing existing software

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This project came about after trying to use a commercial package in a service environment. The software provided, although functional, proved cumbersome especially once one tried to ensure that the resulting structures were easily publishable using CifCheck and could be formatted as readable reports for the users. The intent is to produce a flexible program system that provides error checking throughout the structure solution and refinement process thereby reducing the problems that have to be handled during the report production process. The NRCVAX software package(1) was designed to run interactively on small computers. Most other programs at the time were batch oriented and designed for mainframes, although in later years many of them have been wrapped in interactive user interfaces. One of the more obvious differences was that NRCVAX was a set of discrete programs that each performed a distinct crystallographic task. These programs were connected by binary files and the underlying operating system. The other major difference was that the user interacted with the programs via a question and answer dialog where reasonable defaults were suggested. The current approach is to provide as seamless a connection as possible from the data collection routines to NRCVAX. The programs have been repackaged so that as little user interaction as possible is required in routine situations. For more complex structures the full power of the system is still available. At the moment this is not an attempt at an automated structure determination package, rather it is assumed that a competent crystallographer is in control who can make intelligent decisions as required.

(1) Gabe, E.J., Le Page, Y., Charland, J.-P., Lee, F.L. and White, P.S. (1989) *J. Appl. Cryst.*, 22, 384-387.

Keywords: computer applications, single-crystal structure analysis, software design

## P03.01.02

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### Workflow and metadata in OLEX2

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Olex2 is an open source molecular graphics program [1] for solution, refinement and manipulation of small molecule crystal structures. There is an emphasis on usability and work-flow, which is achieved through a customisable and intuitive graphical-user-interface. The work-flow in Olex2 is designed to take a structure right from space group determination and solution through to refinement and preparation of the final structure report as simply as possible. Olex2 makes many complex crystallographic tools available to the user in a way that is intuitive for novice and experienced crystallographers alike. The program uses its own structure model, which can then be passed to structure solution and refinement programs such as ShelX. In addition, the program has its own structure solution and refinement methods based on the cctbx, which are available as a plug-in. Integration of the cctbx project with Olex2 is seen as key to future development of new and exciting features. The innovative history feature creates a history-tree for each individual solution of the structure, along with each stage of the refinement process. This enables the user to return transparently to an earlier point at any time, without having to concern themselves with saving and

renaming copies of files. The metadata module automatically collates information from the data collection and processing steps. This can then be edited and added to, before merging with the information generated by the refinement program employed to create a complete and correct cif file, if possible. The precompiled Olex2 executable can be downloaded free of charge by academic users from <http://www.olex2.org>.

1. <http://sourceforge.net/projects/olex2>.

Keywords: crystallographic software, small molecules, graphical display and rendering of molecules

### P03.01.03

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#### OLEX2: A portable molecular graphics toolset for crystallography

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Olex2 consists of two main parts: a flexible and easy-to-use Graphical User Interface (GUI) and comprehensive crystallographic library. The GUI provides intuitive access to all aspects of the underlying crystallographic library as well as external programs and libraries such as the computational crystallographic toolbox (cctbx)[1] and the ShelX[2] package. It is designed to make working with crystal structures as easy as possible for users with different experience. The GUI is easily extensible and written in extended HTML; it is designed to highlight possible problems with the structure and implements an easy to follow solve-refine-report workflow. Many other, more specialised tools, can be accessed through the GUI also, and a fully functional, command-line interface is provided at all times. Many of these tools are written in the Python scripting language and can be modified and extended by the user. The Olex2 GUI is also portable (currently tested to work on MS Windows and several 32/64 bit versions of Linux). The crystallographic library provides a portable platform for crystallographic software development and contains various tools for file I/O and structure model manipulation. Apart from these basic features, many more high-level features are included: geometric hydrogen placement, space group determination, tests for missing symmetry elements, calculation of voids and surfaces, pattern matching, report generation are only a few to mention. Olex2 is an open source project located at [www.sourceforge.net](http://www.sourceforge.net). The Windows distribution is maintained by us and compiled executables are available from [www.olex2.org](http://www.olex2.org). We acknowledge the financial support of EPSRC (EP/C536274/1).

1. CCTBX: <http://cctbx.sourceforge.net>

2. ShelX: G.M. Sheldrick, *Acta Cryst.* (2008). A64, 112-122

Keywords: visualisation, GUI, crystallographic programming library

### P03.01.04

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#### NORM - a program for performing normal probability plots and half-normal probability plots

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The program NORM primarily was written to obtain normal probability plots [1] from the data contained in a .FCF-file of the wide-spread used SHELXL program [2]. Furthermore normal probability plots and half-normal probability plots of arbitrary quantities can be obtained. Therefore the program can be used to estimate the reliability of the standard deviations and to identify significant geometric differences of two similar molecules in the asymmetric unit or of the same molecule in two different crystal structure determinations [3]. The difference between two independently determined interatomic distances generally is normally distributed and crystallographically independent molecular geometries can be compared using the powerful method of normal probability plot analysis [4]. Further capabilities of NORM are to plot  $\Delta(F^2)/\sigma(F^2)$  vs.  $F_c^2/\max(F_c^2)$  or to plot  $\text{SQRT}(w)\Delta(F^2)$  vs.  $\sin(\theta)/\lambda$ . Finally a normal probability plot of  $\Delta m = (F1 - K * F2) / \text{SQRT}[\sigma(F1)^2 + K^2 * \sigma(F2)^2]$  can be obtained in order to compare the observed structure factors F1 and F2 (or measured intensities) of two data sets, e. g. the measurements of two crystals of the same compound [1]. The scale factor K between the two data sets is computed to minimize  $\sum (\Delta m)^2$ . The plots produced by NORM can be viewed on the screen or included into Microsoft Word. Some examples for the use of NORM will be discussed.

[1] Abrahams S. C., Keve E. T., *Acta Cryst.*, 1971, A27, 157. [2] Sheldrick, G. M., SHELXL-97. Program for the Refinement of Crystal Structures. Univ. of Göttingen, Germany, 1997. [3] Johansson M. H., Otto S., Oskarsson Å., *Acta Cryst.*, 2002, B58, 244. [4] Albertsson J., Schultheiss P. M., *Acta Cryst.*, 1974, A30, 854.

Keywords: data analysis, normal probability plot, software

### P03.01.06

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#### Computational challenges in wide-angle X-ray solution scattering (WAXS)

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The advent of third-generation high-brilliance synchrotrons brings not only opportunities for investigating molecular structure, but also challenges for data analysis. Measurements of X-ray scattering from proteins in solution, for instance, are now of high quality even at wide angles. Presently, WAXS experiments represent a valuable, but largely complementary tool to other experimental methods. Realizing the full potential of WAXS rests on meeting two primary challenges: characterizing the structural information contained in WAXS data, and developing methods to enable quantitative interpretation in terms of molecular structure. We address these challenges simultaneously using an integrated approach that combines experiment with molecular modeling. We have investigated several computational approaches for calculating the scattering from a protein in solution, given either a single set of atomic coordinates or sets of coordinates as calculated using techniques like molecular dynamics. Although calculating small-angle scattering patterns from structures is well established, our focus is development of techniques flexible and efficient enough to allow an exploration of a wide range of models for scattering (e.g., structure of the hydration layer) with sufficient accuracy at wide angles that the simulated patterns are truly representative of the molecular model under consideration. This will substantially increase the power of WAXS as a tool for biophysical characterization of protein structure and dynamics. Improving our understanding of the nature