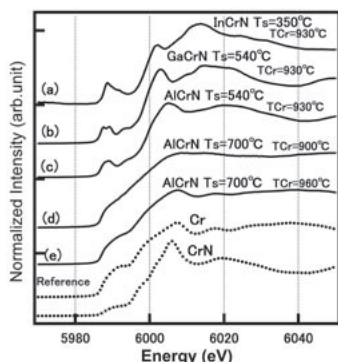


about growth mechanisms and structural properties of III(Al, Ga, and In)-Cr-Nitride. Those layers were grown on Al₂O₃ (0001) with GaN (0001) templates by radio frequency plasma assisted molecular beam epitaxy. Structural properties were studied by XANES and XAFS analysis. Fig.1 shows XANES spectra. Cr 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

Acta Cryst. (2008). A64, C218

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

David A Langs, Herbert A Hauptman

Hauptman-Woodward Medical Research Institute, Structural Biology, 700 Ellicott Street, Buffalo, NY, 14203, USA, E-mail: langs@hwi.buffalo.edu

“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_{min} 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_{min} 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

Acta Cryst. (2008). A64, C218

NRCVAX revisited: Reusing existing software

Peter S White

University of North Carolina at Chapel Hill, Department of Chemistry, CB#3290 Caudill Hall, Chapel Hill, NC, 27599-3290, USA, E-mail : pwhite@unc.edu

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

Acta Cryst. (2008). A64, C218-219

Workflow and metadata in OLEX2

Richard J Gildea, Luc Bourhis, Oleg V Dolomanov, Judith AK Howard, Horst Puschmann

Durham University, Department of Chemistry, Science Laboratories, South Road, Durham, Durham, DH1 3LE, UK, E-mail : r.j.gildea@durham.ac.uk

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