the diffraction spots. Recently a CCD-based Laue diffractometer, CYCLOPS at the ILL, has been constructed which should provide a unique possibility for real-time exploration of reciprocal space and rapid data collection through phase transitions due to its fast readout system. Finally the Very Intense Polarized neutron diffractometer (VIP) at the LLB which combines a large area detector and a hot polarized neutron beam shows an unprecedented efficiency in the measurement of spin densities. In this talk a review of neutron instruments with area detectors, the receipts of the data reduction and trends of their development will be given.

Keywords: neutron, diffraction , monocristal

MS.68.4

Acta Cryst. (2011) A**67,** C155

Accurate data analysis for the koala and VIVALDI neutron Laue diffractometers

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The Koala (ANSTO) and VIVALDI (ILL) instruments are designed for relatively fast data collections using a minimal sample volume. This is possible due to large image-plates with ~3π steradian coverage and the use of unfiltered "white" neutron beams from high flux reactors. The historical difficulty with these instruments has been the processing of the multi-wavelength diffraction data into accurate corrected intensities useable by structure refinement programs. The Laue1234 software suite has been developed to address this problem and to allow accurate structural refinements[1], [2] for the Koala instrument. The software has now been extended to address the problem of the complex wavelength distribution found at the VIVALDI instrument.

Laue1234 runs on a conventional PC using new software and modified versions of the existing neutron Laue diffraction suite: lauegen and its associated programs [3] and argonne_boxes [4]. The peak integration software argonne_boxes has been modified to extend its applicability to lower peak intensities and to rigorously handle the propagation of errors. The algorithms were validated using simulated and observed data which has lead to the discovery of a new statistical effect due to detector crosstalk [5].

The program Laue4 was written to correct and merge the multi-wavelength peak intensities. The software corrects the intensities for beam variations between exposures, the incident beam wavelength distribution, wavelength dependent and time dependent efficiency corrections, secondary extinction and sample absorption corrections, and to a limited extent the effect of λ/2 peak overlap. The majority of these corrections are performed using a least squares approach where parameters in the correction model are adjusted to minimize a measure related to the R_{merge} of equivalent reflections. A non-parametric approach is used for the particularly complex and changeable wavelength distribution of the VIVALDI instrument. This approach optimizes the distribution using the observed intensities of equivalent reflections against a measure of the local complexity of the distribution compared to *a priori* distributions.

Of equal importance to the actual corrections is the incorporation of intensity uncertainties due to the limitation of the correction models. Without reasonable estimates of these systematic uncertainties the merging of intensities is dominated by long wavelength data where the counting statistics are best but the systematic errors due to extinction and absorption are worst.

Examples from Koala and VIVALDI will be presented to illustrate the capability of the software for refining structures with R_1 factors in the 2 to 5% range.

[1] A.G. Dikundwar, Ch. Venkateswarlu, R.O. Piltz, S. Chandrasekaran, T.N. Guru Row, *CrystEngComm* **2011**, *13*, 1531-1538. [2] P. Boyd, A. Edwards, M. Gardiner, C. Ho, M.H. Lemée-Cailleau, D. McGuinness, A. Riapanitra, J. Steed, D. Stringer, B. Yates, *Angew. Chem.-Int. Edit.* **2010**, *49*, 6315-6318. [3] C. Wilkinson, H.W. Khamis, R.F.D. Stansfield, G.J. McIntyre, *J. Appl. Cryst.* **1988**, *21*, 471-478. [4] N. Niimura, Y. Minezaki, T. Nonaka, J-C Castagna, F. Cipriani, P. Høghøj, M.S. Lehmann, C. Wilkinson, *Nat. Struct. Biol.* **1997**, *4*, 909-914. [5] C. Wilkinson, M.S. Lehmann, F.M. Matthew, P. Blakeley, D.A.A. Myles, S. Vogelmeier, M. Thoms, M. Walsh, G.J. McIntyre, *J. Appl. Cryst.* **2009**, *42*, 749-757.

Keywords: neutron_diffraction, data_analysis, laue_method

MS.68.5

Acta Cryst. (2011) A**67,** C155

Diffraction data quality analysis of EVAL15 integration

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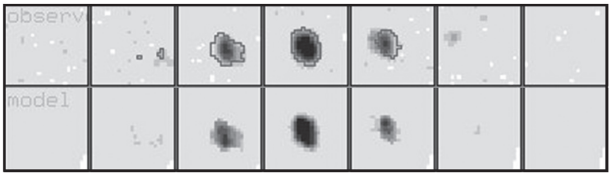
EVAL15 is a diffraction data integration method [1] that is implemented as part of the EVAL software package [2]. It simulates the complete diffraction process on the basis of only a few physical model parameters. The resultant reflection profiles are subsequently used in profile fitting of reflection intensities. This versatile method can cope with a range of complicated integration problems, e.g. of crystals with anisotropic mosaic spread or lattice distortion, overlapping reflections due to long axes or multiple lattices and aperiodic (incommensurate or composite) crystals. Moreover, the EVAL package can handle many types of goniometers, a large range of detectors, and various types of X-ray or neutron sources.

The general opinion on profile fitting is that the standard deviation of weak data is reduced, whereas for strong data it presents a disadvantage over summation integration. Methods that use ab initio generated models need a comprehensive description of the diffraction process. In this contribution we will describe the procedure for generating high quality profiles.



A detailed analysis of the data quality obtained by EVAL15 is given. The analysis comprises data sets of (metal)-organic compounds with a large dynamic range of reflected intensities, crystals with packing disorder and high resolution data. We use several quality indicators based on the statistical analysis of the data and on aspects of the refined structure.

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Keywords: data_quality, EVAL15, intensity_integration

MS.69.1

Acta Cryst. (2011) A**67,** C155-C156

Modelling thermal scattering and solving structures using Z-contrast imaging

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