

This will be demonstrated on a number of molecular structures solved from laboratory data and validated later with the use of synchrotron and/or neutron data.

**Keywords:** crystal structure determination X-ray powder data, synchrotron powder diffraction, neutron powder diffraction

### MS25.25.3

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#### Close Contact Penalty Functions in Direct Space Methods and Energetic Considerations in Structure Refinement

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When solving crystal structures from powder diffraction data using direct space methods, all available information such as molecular structures and space group symmetry is used to limit the number of degrees of freedom. When limited quantity of information is available from a powder diffraction pattern (e.g., broad peaks, preferred orientation, positions of weak scatters) and/or the number of degrees of freedom is large, it may be necessary to add extra chemical information in order to obtain a solution. This chemical information can be that the generated structures should be energetically stable, where the potential energy contributes to a combined figure of merit alongside the powder pattern similarity,  $R_{wp}$ .

Considering the fact that viable solutions should not contain overlapping atoms, adding a simple close contact penalty that prevents solutions with non-viable intermolecular interactions from being generated is adequate for the global optimization process, which aims at locating a rough, refinable solution.

During Rietveld refinement an accurate description of the potential energy should be used in combination with the  $R_{wp}$  in a weighted optimization process. The a priori determination of the weighting factor might not be intuitive; in such cases a Pareto optimization (a posteriori preference articulation) can be used to obtain an appropriate value so as to ensure that structures that are both chemically viable and in close agreement with the experimental powder pattern.

**Keywords:** ab-initio structure determination, Rietveld structure refinement, potential energy

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#### Differential Thermal Expansion and Laboratory Capillary X-ray Powder Diffraction: Progress, Practicalities and Performance

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The challenge for experimental XRPD applied to crystal structure determination, is to obtain the best possible estimates of diffracted intensities. The chance of achieving this is enhanced by using (i) low- $T$  data collections to decrease thermal vibration and therefore boost the intensities seen at higher diffraction angles and (ii) new PSD detector technologies yielding improved signal-to-noise and count-rates. Importantly, significant improvements to the extracted intensity information available from overlapping peaks may be gained by using multiple low- $T$  data collections, thereby exploiting differential thermal expansion (DTE) [1,2]. Here we present the exploitation of DTE to retrieve an immense amount of accurate intensity data from a series of laboratory capillary X-ray powder diffraction data sets collected at several temperatures. We describe a validated method for intensity extraction and include details on the impact of improved PSD detectors and high intensity laboratory X-ray sources on this approach.

[1] David W. I. F., Shankland K., McCusker L. B., Baerlocher Ch. in *Structure Determination from Powder Diffraction Data*, Ch. 1, David et al. (Eds), Oxford University Press, Oxford, 2002. [2] Zachariasen W. H., Ellinger F. H., *Acta Crystallogr.*, 1963, **16**, 369.

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### expansion, crystal structure determination

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#### Rapid Structure Solution using Global Optimisation and Distributed Computing

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The use of global optimisation methods has helped to increase the size and complexity of molecular organic structures that can be solved directly from powder diffraction data. These methods require many repeat runs to be performed in order to confirm the location of the global minimum in parameter space; this is particularly true for very complex structures, where success rates in locating the minimum may fall to only a few percent. Fortunately, these multiple runs can be performed independently of each other and as such, they are ideally suited to the notion of grid-type computing. We have recently adapted the DASH [1] program to run under the GridMP [2] distributed computing system; the current setup allows up to eighty DASH simulated annealing runs to be executed in parallel on *existing* desktop resources. Initial results show not only impressive performance gains but also indicate that new computational routes that were previously closed to us (due to their compute-intensive requirements) are now open. For example, full characterisation of a hybrid Monte Carlo (HMC) method of structure determination from powder diffraction data required many months of CPU time; the work was performed in a matter of days using a grid-adapted version of the HMC code [3].

[1] David W.I.F., Shankland K., Shankland N., *Chem. Commun.*, 1998, 931-932. [2] <http://www.ud.com> [3] Markvardsen A.J., Shankland K., David W.I.F., Didlick G., *J. Appl. Cryst.*, 2005, **38**, 107-111.

**Keywords:** powder diffraction, structure determination, parallel computing

### MS26 RECENT ADVANCES IN QUASICRYSTAL RESEARCH

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### MS26.25.1

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#### Fabricating Novel Symmetry Nanoscale Systems using Quasicrystal Surfaces

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Quasicrystals are metallic alloys which have unusual structural properties: they are aperiodic and may display symmetries not observed in periodic materials. The surfaces of these materials offer opportunities for the fabrication of nanostructures and thin films which themselves have unusual symmetries and structures. In turn, measurements of such nanostructured systems may offer insights into the larger question of the relationship between physical properties and aperiodicity. Several such systems have been fabricated and are under investigation in our laboratory, and some examples will be shown.

One spectacular case is that of an ultrathin film grown by the deposition of copper atoms on the five-fold surface of the icosahedral  $Al_{70}Pd_{21}Mn_9$  quasicrystal [1]. STM images show that the in-plane structure comprises rows having separations of  $S=4.5\pm 0.2$  Å and  $L=7.3\pm 0.3$  Å, whose ratio is the Golden mean  $\tau=1.618...$  within experimental error. The sequences of such row separations form segments of terms of the Fibonacci sequence, indicative of the formation of a pseudomorphic Cu film. We have recently demonstrated that such films can also be grown using magnetic elements such as Co, Fe and Ni. Characterisation of their magnetic properties has also been undertaken and will be discussed.

[1] Ledieu J., Hoefft J.T., Reid D.E., Smerdon J.A., Diehl R.D., Lograsso T.A., Ross A.R., McGrath R., *Phys. Rev. Lett.*, 2004, **92**, 135507.

**Keywords:** quasicrystals, nanostructures, scanning tunnelling microscopy