s3.m2.o1 **Modelling and Refinement in Crystallography: An Overview.** S. Parsons, *Department of Chemistry, The University of Edinburgh, Edinburgh, Scotland. S.Parsons@ed.ac.uk.*.
Keywords: computing, refinement, modelling.

Until recently data collection formed the most time-consuming stage of a crystal structure determination. Nowadays, though, modern area detector systems based on image plates and ccd's are capable of collecting two or three data sets a day. In laboratories where such instruments are available the rate-limiting step is data processing, and the most time-consuming stage of this is undoubtedly refinement. This presentation will focus upon features of crystal structure determination, which, if present, can hinder refinement, or stop it altogether.

Disorder is the most common of these, and nicely illustrates the contrast between modelling and fitting approaches. X-rays are diffracted by electrons, which are distributed in both time an space and treatment of disordered regions in crystal structures with part-weight discrete-atom models is really only efficient and meaningful when the disorder can be modelled over two or three sites. It rapidly becomes inefficient in the case of truly diffuse solvent regions. The BYPASS or SQUEEZE procedure implemented in the excellent and widely used programme PLATON has largely solved this problem by directly transforming disordered electron density out of the data set.

Pseudo-merohedrally twinned crystals often used to be discarded at the data collection stage, when it proved impossible to index the diffraction pattern. This is a problem encountered fairly frequently in our own work on low-melting compounds. Again, software has come to the rescue and programmes such as Dirax and Twindx have solved this problem, making it necessary to take account of twinning during refinement. If twinning is untreated refinements can appear to get stuck with high R-factors and noisy difference maps. The twin law is often evident from the output of the indexing programmes, but in cases where it is not it can be inferred from the geometry of the unit cell and/or trends in the indices of poorly-agreeing data.

Limited data can also pose significant difficulties during refinement, and this will be illustrated by high-pressure crystal structure determinations in which the pressure cell can obscure much of reciprocal space (data completeness of ca 30% is far from unusual). In high-pressure structure determinations choice of parameters can have a critical effect on the path of refinement; again illustrative examples will be given.

s3.m2.o2 **Incommensurate structures: modeling beyond the 3rd dimension.** G. Chapuis, *Institut de Cristallographie, Université de Lausanne, BSP Dorigny, 1015 Lausanne, Switzerland*,
Keywords: superspace groups, aperiodic crystals, incommensurate structures.

The resolution of incommensurate and composite structures in the superspace formalism is now well established. The success of this field is due to ground breaking works from P.M de Wolff, A. Janner and T. Janssen in the seventies who established the basic theory of quasiperiodic systems and presented some real examples of applications in the field of structural crystallography.

The domain of quasiperiodic or aperiodic crystals has further evolved since the establishment of the complete list of superspace groups in 3+1 dimensions which are published in vol. C of the International Tables of Crystallography. Systems of software programs for the refinement of incommensurate structures in superspace are also available [1,2].

With more than two decades of experimental research in this domain, what did quasicrystallography contribute to the structural sciences?

Our views on crystalline structures has greatly evolved by realizing that long range order can not only by be realized in nature by three dimensional periodicity but also by other unexpected means. In addition, many structures classified as "disordered" have been reinterpreted as perfectly ordered aperiodic crystals. Perhaps one of the most interesting aspect of the reinterpretation of crystals concerns some new insight into the atomic interactions which govern the formation of (quasi-)periodic structures.

[1] W.A. Paciorek, MSR - The program system for 1-dimensional incommensurate structure refinement, (1995).
[2] V. Petricek and M. Dusek, JANA2000 - Crystallographic Computing System, (2000).