of liquid crystals on several types of alignment layers.

The results provide direct evidence for the structural dynamics responsible for laser-induced anisotropy as observed by polarisation holography [1], and gives an intriguing insight into the interaction of forces acting on liquid crystal molecular arrangements.

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Keywords: liquid crystals, laser-induced alignment, grazing incidence X-ray diffraction

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MS90 APPLYING NON-CRYSTALLOGRAPHIC ALGORITHMS TO CRYSTALLOGRAPHY
Chairpersons: Ralf W. Grosse-Kunstleve, Maryjane Tremayne

MS90.30.1
Acta Cryst. (2005). A**61**, C114
Cluster Analysis in Crystallography
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Cluster analysis is a well established tool in statistics, but one that is used surprisingly little in crystallography despite its considerable potential. We have established its use in several diverse areas of crystallography, in particular:
1. Pattern matching in powder X-ray diffraction: High throughput screening experiments designed to search for polymorphs and salts of drug candidates use PXRD to characterize the results, and this produces large quantities of data. We show how pattern matching methods based on appropriate correlation coefficients can be used in conjunction with clustering calculations to classify patterns automatically [1,2].
2. Databases: Database searching using the Cambridge Structural Database (CSD) [3] can produce thousands of 'hits' if a simple fragment is used, and as a result processing and interpreting the results becomes a considerable task. Cluster analysis using dendrograms, metric multidimensional scaling and suitable visualization tools can reduce the workload to a few hours of computer time with minimal user intervention.
3. Indexing powder patterns: In difficult indexing problems, it is possible to produce a large number of potential unit cells with figures of merit that are only marginally useful. Cluster analysis can be useful here, especially when self-organizing maps are utilised.

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Keywords: cluster analysis, pattern matching, databases

MS90.30.2
Acta Cryst. (2005). A**61**, C114
Crystal Structures from Powder X-ray Diffraction using Genetic Algorithms
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Contemporary advances of direct space strategies in solving crystal structures directly from powder X-ray diffraction data [1,2], and in particular, the success of the Genetic Algorithm method [3], have opened up a whole area of research which has hitherto been inaccessible even as recent as fifteen years ago. Applications to the study of synthetic products *in situ*, as well as the tackling of structural problems which have the complexity of more than one molecule in the asymmetric unit, are now at the forefront of these techniques. In addition to tackling such new challenges, structure solution strategies employing other analytical or computational methods have become a natural complement alongside the X-ray diffraction data. For example, multi-component molecular co-crystals have been prepared by an *in situ* solid state grinding process, yet have been solved using a combination of powder X-ray diffraction and solid state NMR techniques [4]. Moreover, the collection and assessment of reliable powder diffraction intensity prior to structure solution calculations is an avenue of study that shows considerable promise [5].

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Keywords: diffraction data, powder diffraction, X-ray crystallography of organic compounds

MS90.30.3
Acta Cryst. (2005). A**61**, C114
Powders, Prediction and Epitaxy: Applications of Differential Evolution
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Differential evolution (DE) is a robust and efficient global optimization algorithm based on evolutionary principles, which has been applied to a wide range of problems [1]. It shares the attractive features of other evolutionary algorithms but has a simpler implementation and fewer user defined control parameters enabling a greater insight into the control of the optimization process to be achieved.
Direct space methods of structure determination from powder diffraction is a field of rapid growth due to a number of computational and experimental developments [2, 3]. DE has been successfully applied to the determination of a number of organic and inorganic molecular structures from laboratory powder data.
The DE algorithm has also been applied to the prediction of crystal structures and epitaxial interfaces of organic crystals. In both cases, the lattice energy of the trial packing is calculated by an appropriate force field and then minimized by the DE algorithm. Utilization of a Beowulf cluster enables optimization of the DE algorithm control parameter to be performed in parallel.
In this talk, I will discuss these applications of DE with particular attention to the optimization of the performance of the algorithm, while highlighting areas of potential improvement and future developments.

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Keywords: optimization algorithms, ab-initio powder structure determination, epitaxy

MS90.30.4
Acta Cryst. (2005). A**61**, C114-C115
Refinement when Amplitudes aren't enough: Real-Space, H-Bonding & Electrostatics
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Methodological improvements have reduced, but not eliminated over-fitting in macromolecular structure refinement. It is well known that over-fitting depends on freedom in the atomic model compared to the quality and quantity of the experimental data. The latter depends on resolution – 3 Å usually being considered the minimum.
Our goal is to improve the robustness of refinements at resolutions that are at best marginal, by using fully the available data, or by adding stereochemical restraints to the model freedom. Real-space refinement is most advantageous when model-independent phases can be used as additional data. The local nature of the refinement eliminates the over-fitting due to compensating errors that occurs in reciprocal-space where all atoms depend on all data points. Atomic density functions that rigorously incorporate resolution limits allow

the method to be applied in both crystallography and electron microscopy at resolutions as low as 50 Å.

Additional stereochemical restraints have a modest positive impact in medium resolution crystallographic structures. A hydrogen-bonding restraint that is directionally targeted towards either dipolar or lone-pair interactions is beneficial, in contrast to prior attempts that optimized only dipolar effects. Minimization of the electrostatic potential energy is also beneficial, and more so when calculated by continuum methods rather than by the Coulombic methods previously used. This has been accomplished by combining refinement with numerical solution of the Poisson-Boltzmann equation.

Keywords: refinement, restraint, electrostatic potential

MS90.30.5
Acta Cryst. (2005). A**61**, C115
elNémo: **Using Normal Mode Analysis in Molecular Replacement**
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Normal mode analysis (NMA) is a powerful tool for predicting the possible movements of a given macromolecule. A newly emerging field of NMA in X-ray crystallography is the utilization of normal mode perturbed models as templates for diffraction data phasing through molecular replacement (MR), thus accounting for conformational changes arising for example from ligand binding or different crystallogenic conditions [1]. Given that half of the known protein movements can be modelled by displacing the studied structure using at most two low-frequency normal modes, NMA may have the potential to break tough MR problems in up to 50% of cases. Moreover, even in situations where a MR solution is available, NMA can be used to further improve the starting model prior to refinement, eventually reducing the time spent on manual model construction (i.e. when working with low resolution data sets). Here we present this approach at a number of examples where screening for MR solutions using NMA perturbed templates allowed to obtain a MR solution, whereas MR using the original template failed to yield a model that could ultimately be refined. We outline possible protocols of using NMA in MR and present the web- server *elNémo* [2] for online NMA template generation http://igs-server.cnrs-mrs.fr/elnemo/index.html.

[1] Suhre K., Sanejouand Y.H., *Acta Cryst.*, 2004, D**60**, 796-799. [2] Suhre K., Sanejouand Y.H., *Nucleic Acids Research*, 2004, **32**, W610-W614.
Keywords: crystallography, phasing, normal mode analysis

MS91 ELECTRON CRYSTALLOGRAPHY ON INORGANIC CRYSTALS
Chairpersons: Jacob Jansen, Vera Kletschkovskaia

MS91.30.1
Acta Cryst. (2005). A**61**, C115
Present Status of Electron Crystallography on Inorganic Materials
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The most promising alternative to X-rays for structural analysis of extremely small volumes are fast electrons, whose interaction with matter is several orders in magnitude stronger than of X-rays. Thus the two main branches of electron crystallography, electron diffraction structure analysis (EDSA) and (crystallographic) image processing of high-resolution electron microscopy images, are the methods of choice for structural characterisation of small samples and nanocrystalline materials.

Over the last years we have been witness of several new upcoming techniques on instrumentation that have pushed the frontiers of electron crystallography much further. The electron precession beam technique for example, considerably increases the obtainable resolution of any spot electron diffraction pattern and significantly reduces the dynamical contribution to the intensities of zone axis patterns. Thus this method is becoming a very attractive tool for scientists who want to determine crystal structures by EDSA. Another recent breakthrough took place in the field of high-resolution electron microscopy. A new generation of C_s-corrected FEG-TEM's and newly developed software enable to reconstruct the exit wave of crystals with resolution in the sub-Å range from through focus series.

These recent developments are now going to turn electron crystallography – more than 65 years after it's invention by Russian scientists – into a reliable and handy method for structure determination of tiny crystallites and nanosized materials.
Keywords: electron crystallography, inorganic materials, developments in electron crystallography

MS91.30.2
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Structural and Charge-density Studies of Transition-metal Oxides using Convergent-beam Electron Diffraction
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We developed a method to refine crystal structural parameters and charge density using convergent-beam electron diffraction (CBED) [1,2]. The method is based on the non-linear least-squares fitting between full dynamical calculations and experimental intensities of energy-filtered two-dimensional CBED patterns of zeroth-order Laue-zone (ZOLZ) reflections and higher-order Laue-zone (HOLZ) reflections. The HOLZ reflections are essential for the determination of atom positions and Debye-Waller factors and the ZOLZ reflections are utilized for obtaining charge density distributions.

For this purpose, we developed an energy-filter transmission microscope JEM-2010FEF [1], and an analysis program MBFIT [1]. A problem of long computation time needed for dynamical calculations was greatly eased by implementation of parallel computation on a computer cluster [3].

A nanometer scale probe in CBED has great advantages and can be used extensively. Our current targets are perovskite-type transition-metal oxides and related materials with strongly correlated electrons, in which very small domains of twin structures exist and characteristic phase separation occurs easily. In the present talk, analyses of perovskite transition-metal oxides using the CBED method are demonstrated.

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Keywords: CBED, structure refinement, charge density

MS91.30.3
Acta Cryst. (2005). A**61**, C115-C116
Incommensurate Modulated Structure Determination by Combining HREM and ED
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The incommensurate modulated structure can be treated as a multi-dimensional (MD) periodic structure cut with a three-dimensional hyper plane [1]. In the case of one-dimensional modulation the structural modulation reveals directly in the high-resolution electron microscope image projected in the direction perpendicular to the modulation wave vector, but the image resolution is usually insufficient for showing all atoms. In this work it is shown that the electron diffraction data can be utilized to enhance the determined structure resolution by means of the MD direct methods [2].

The electron diffraction pattern consists of main reflections and satellites. The main reflections correspond to the average structure. An arbitrary defocus image is averaged according to the unit cell of basic structure to obtain the average image, and the deconvoluted average image reveals the average structure. Fourier transform of the deconvoluted average image yields phases of low-resolution main reflections for the modulated structure. Phases of high-resolution main reflections for the modulated structure can be derived from the low-resolution phases obtained from the image and the amplitudes from the diffraction pattern. The MD direct-phasing method [2] can be used