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

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***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.

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Keywords: crystallography, phasing, normal mode analysis

MS91 ELECTRON CRYSTALLOGRAPHY ON INORGANIC CRYSTALS

Chairpersons: Jacob Jansen, Vera Kletschkovskaia

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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

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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

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Incomensurate 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