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The ultimate limit in resolution of protein crystal structures is determined by beam damage. Since electrons are about three orders of magnitude less damaging to biological materials than X-rays, we intend developing electron crystallography as an alternative to X-ray crystallography. Here, we discuss our progress in this endeavour:
Electron diffraction up to 0.2 nm resolution could be observed from 3D protein nano-crystals (up to 200 nm in size) and up to 0.1 nm for pharmaceutical nano-crystals;
By precessing the electron beam, a substantial fraction of spots could be made to fully pass the Ewald sphere, increasing the number of fully recorded reflections, whilst simultaneously reducing the effect of dynamical scattering;
By computer analysis of the spacings of randomly oriented diffraction patterns, we could determine the unit cells;
In favourable crystal settings, we could index the diffraction patterns; we are making progress in indexing all random diffraction patterns.
We anticipate that these steps will ultimately allow us to integrate the observed, indexed reflections, opening the way to full structure determination by cryo-electron diffraction.

Keywords: electron diffraction, structural biology, nanocrystallography

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Symmetry determinations from electron precession: Comparison and advantages with CBED

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The electron precession technique displays some interesting features connected with the crystal symmetry:
The integrated intensities of the diffracted beams present on electron precession patterns can be used to identify the "ideal" symmetry of the pattern, i.e. the symmetry which takes into account both the position and the intensity. It is shown that this "ideal" symmetry is connected with the Laue class;
The precession patterns exhibit a two-beam behaviour especially at large precession angle meaning that multiple diffractions are strongly reduced. This property can be used to identify the kinematical forbidden reflections due to screw axes and glides planes. It can also be used to detect reflections which exhibit weak differences of intensity. These reflections are very useful when dealing with the study of crystal displaying small symmetry departures;
The patterns display a large number of reflections in the Zero-Order Laue Zone (ZOLZ) but also in the High-order Laue Zone (HOLZ) whose observation allows an easy and sure identification of the shifts and periodicity differences of the reflections located in the HOLZ with respect to the ones located in the ZOLZ. These features are connected with the Bravais lattice and with the glide planes, respectively. A few possible space groups can be identified from all these observations. CBED and LACBED are also valuable techniques to deduce the point and space groups but the experiments are more difficult to perform since they require a perfect alignment of the zone axis and an adapted crystal thickness.

Keywords: electron diffraction, forbidden reflections, crystal symmetry

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Quantitative 3D electron diffraction data by precession and electron rotation methods

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We present a quantitative investigation of data quality using electron precession, compared to standard selected area electron diffraction (SAED), and present the new Electron Rotation Method for collecting 3D electron diffraction data. The SAED pattern of $K_2ONb_{14}O_{35}$ (projection symmetry 4*mm*, *a* = 27.5Å) (left) in the Figure goes to 1.10 Å resolution (h = 25), while the hk0 precession pattern (right) goes to 0.76 Å resolution (h = 36). The total number of unique reflections is doubled for precession compared to SAED. Precession patterns were obtained with SpinningStar from NanoMEGAS on a JEOL 2000CX TEM with a 16-bit CCD-camera and quantified by ELD from Calidris. Rmerge = 5%. The structure was solved by Sir97, both from SAED and from precession data, and refined with SHELX. Metal atom positions were refined; R-value 19% for precession and 28% for SAED. Niobium atoms were on average within 0.04 A from those obtained by X-ray diffraction for the isomorphous $Tl_2ONb_{14}O_{35}$. We are trying to localize the oxygen atoms. Reference: Oleynikov,P. Hovmoeller,S. and Zou,X.D. Precession electron diffraction: observed and calculated intensities. Ultramicroscopy 107 (2007), 523-533

Keywords: electron diffraction, precession, quantification

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Models for simplified treatment of precession electron diffraction

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Precession electron diffraction (PED) is an experimental approach to reducing the severity of dynamical effects in electron diffraction [1]. In PED, the incident beam is tilted along a cone about the zone axis; intensities from all orientations in the cone are integrated. This reduces the number of simultaneously excited beams as well as averaging over many orientations. It will be shown that PED reduces the complexity of the intensities vs. thickness {I(g,t)}, in a statistical sense using principal component analysis. Specifically, the number of parameters necessary to describe all variation within the set {I(g,t)} for a given zone axis is reduced with respect to a direct zone axis orientation. However, this reduction of complexity does not extend to an ability to accurately describe PED I(g,t)'s using accessible parameters such as spatial frequency |g| and structure factor amplitude (as in e.g. kinematical or 2-beam models)[2]. Thus, it is necessary to include at least some details of the interactions among simultaneously excited beams in order to develop anything beyond a fairly crude approximation of PED. This explains the limitations of 2-beam and Blackman models [2,3]. The development of more sophisticated models will be discussed. It will be shown that PED intensities are relatively insensitive to structure factor phases. The phase-insensitivity may provide a basis for close approximation