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accelerating voltages. Since no information is assumed from any other determination and the results are very close to those found from equivalent X-ray analyses, it must be concluded that quantitative electron crystallography is not the stuff of fantasy and can be equally applied to centrosymmetric and non-centrosymmetric problems. It is even possible to use traditional structure refinement techniques after the initial model is obtained from the first set of phases. This may include Fourier techniques but, if there are enough data, least-squares refinement is also useful. When the only choice for collecting single crystal data is the electron diffraction option with microcrystalline samples, then there is every reason to attempt a structure analysis when intensity data are collected under known constraints to minimize the influence of multiple scattering. Research supported by NSF CHE91-13899 and NIH GM-46733.

MS–02.04.02 IMAGE DECONVOLUTION AND RESOLUTION ENHANCEMENT IN ELECTRON CRYSTALLOGRAPHY. By F. H. Li, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P. R. China.

An approach to crystal structure determination combining high resolution electron microscopy and electron diffraction has been established and applied to ordinary crystal structures as well as incommensurate modulated structures. A single high resolution electron microscope image and the corresponding electron diffraction pattern are used throughout the process which consists of two steps: image deconvolution and image resolution enhancement. In the first step, the defocus amount of the image is estimated on the basis of the Sayre equation or the maximum entropy principle. The image is then converted into the structure image with a resolution about 2Å, which is bounded by the resolution of the electron microscope. In the second step, the image resolution is enhanced by a phase extension technique based on the Sayre equation. Amplitudes of structure factors up to 1Å are measured from the electron diffraction pattern. Initial phases within 2Å are obtained by Fourier transforming the structure image resulted from the first step. The resolution of the structure image can be enhanced to about 1Å after the phase extension. The image can be further improved by Fourier recycling.

In dealing with incommensurate modulated structures the initial image is first averaged according to the unit cell of the basic structure and then converted into the average structure image by image deconvolution. Phases of main reflections are obtained from the Fourier transform of the average structure image. The phase extension from main reflections to satellite reflections is carried out based on a multi-dimensional direct method.

MS–02.04.03 FUTURE PROSPECTS FOR DIRECT STRUCTURE RETRIEVAL IN HIGH RESOLUTION ELECTRON MICROSCOPY. D. Van Dyck, University of Antwerp (RUCA), Belgium.

We are living in a very exciting period for structural research using high resolution electron microscopy (HREM). Indeed, the possibility to "see" the individual atoms of which matter is constructed seems within reach. Recent technological improvements allow to obtain a resolution of about 0.1 nm. However, the potential power of the technique is still severely limited by the problem of quantitative interpretation of the images. Thus far the only method to extract structural information from the images consists in comparing the experimental images with computer simulations for various trial structures. For this purpose the Schrödinger equation describing the dynamical electron diffraction as well as the image transfer has to be solved numerically. However this technique is very tedious, requiring a number of usually unknown parameters, and can only be applied with some success if the number of possible structure models is very limited. This makes HREM very much dependent on the availability of prior information obtained from other techniques. HREM would be much more powerful if a direct method exists to extract the structural information directly from the electron micrographs. Recently we proposed a new method to solve this inverse problem. In this method the electron microscope is computer controlled to capture images at very close focus values using a high resolution CCD camera so as to collect all information in 3D image space. By a suitable image processing algorithm it is then possible to retrieve the phase and hence the whole wavefunction in the image plane. From this the influence of the electron microscope aberrations can be eliminated straightforwardly and a projection of the atomic structure of the object can be obtained with a resolution of about 0.1 nm. Recently a Brite-Euram project has been approved for the period 1990-1994 to construct such a microscope. The first prototypes are now in operation and reveal direct 1 Å structural detail. The latest results will be presented and discussed.

MS–02.04.04 DIRECT PHASE DETERMINATION FROM FOURIER TRANSFORMS OF EM IMAGES Sven Hovmöller[1]*, Lars Eriksson[1], Xiaodong Zou[1], and Gunnar Svensson[2], Structural[1] and Inorganic[2] Chemistry, Stockholm University, S-106 91 Stockholm, Sweden.

The great advantage of electron microscopy (EM) over X-ray diffraction is that the structure factor phases are not lost. This was shown already in 1968 by DeRosier and Klug (Nature 217, 130-134). Fourier transform (FT) analysis is now a standard technique for EM images of protein crystals.

However, Fourier methods have until now not been much used for studying inorganic crystals by EM. There are two reasons for this, one theoretical and one practical.

From a theoretical point of view there has been doubts about what kind of phase information is available in the EM images and a skepticism about the quality of the amplitudes obtained from EM and electron diffraction. The main practical difficulty has been the lack of an easily available system for crystallographic image processing (CIP). It has been our aim to overcome both these theoretical and practical difficulties.

Images of $Ba_4Nb_{14}O_{23}$ (orthorhombic *Cmmm*, a=20.79, b=12.453, c=4.149 Å) were taken with a Philips CM 30, 300kV electron microscope. Thin areas near the edge were analyzed by our newly developed image processing system, CRISP (Hovmöller, Ultramicroscopy 41 (1992) 121-135). This structure had already been solved by single crystal X-ray diffraction (Svensson and Grins, in manuscript) and refined to an R-value of 3.1%. The amplitudes of the FT of the EM image showed a sharp decrease at 2.4 Å resolution. We interpreted this as being due to the first cross-over of the contrast transfer function of the EM. There were 17 unique reflections inside 2.4 Å resolution, and their phases were determined by CRISP. The phases from EM were compared to the structure factor phases calculated from the highly refined X-ray structure. They were all identical. This shows that the phases obtained in the EM are the same as the X-ray structure factor phases, also for inorganic crystals, provided thin crystals are used.

