for phase extension and refinement of main reflections, and then used for phase extension from main reflections to satellite reflections.

[1] De Wolff P.M., *Acta Cryst. A*, 1974, **A30**, 777. [2] Hao Q., Liu Y.W., Fan H.F., *Acta Cryst*. 1987, **A43**, 820.

Keywords: incommensurate modulated structure, high-resolution electron microscopy, electron diffraction

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Electron Dynamical Diffraction Imaging and Diffuse Scattering by Small Dislocation Loops

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Effects of dynamical scattering of high-energy electrons by elastic fields of interstitial or vacancy loops in a crystalline material provide a convenient means for diffraction contrast imaging. In this presentation we describe new developments in the methodology of simulation of diffraction images and *dynamical* diffuse scattering by small dislocation loops. To simulate diffraction images, a many-beam Howie-Basinki equation approach has been developed where strong dynamical effects as well as the non-parallel propagation of diffracted beams in the crystal are treated using a combination of the adaptive spatial mesh and wave field interpolation techniques. The significance of dynamical diffraction as well as practical applications of the new approach are illustrated by the comparison of simulated and experimentally observed images. The treatment of diffuse scattering includes effects of Kikuchi diffraction on Huang diffuse scattering patterns that we simulate using the atomic displacement fields evaluated using anisotropic elasticity solutions and atomistic modelling.

Keywords: electron microscopy and diffraction, quantitative electron diffraction, dynamical diffraction

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Characterization of Nanophases in HRTEM: Fourier Transform and Simulation

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High resolution transmission electron microscopy (HRTEM) was applied to study the microstructure of biomaterials based on calcium phosphates: α-tricalcium phosphate, octacalcium phosphate (OCP) and hydroxyapatite (HAP). Phase analysis at nanolevel was required to evaluate whether the final product included one or several Ca phosphate modifications. Due to high sensitivity of all these compounds to irradiation of the convergent electron beam such local analysis was performed by processing diffractograms (Fourier transform) from HRTEM images with Digital Micrograph software (Gatan). Interpretation of the experimental results was done by the means of simulation of selected area electron diffraction patterns and HRTEM images using JEMS [1], which allows to perform large calculations of dynamical diffraction patterns and HRTEM images for big multiatomic crystallographic unit cells.

HAP nanocrystals (5-20 nm) randomly oriented relatively to each other were identified in plasma sprayed coatings on different substrates. OCP crystals were found to contain HAP inclusions and their sizes were dependent on crystal growth regime. Phase transformation during high temperature synthesis of α-tricalcium phosphate from the β-form has been studied.

[1] JEMS: http://cimewww.epfl.ch/people/Stadelmann/jemsWebSite/jems.html Stadelmann P..

Keywords: electron microscopy and diffraction, simulation, calcium compounds

MS92 EMERGING TECHNOLOGIES FOR STRUCTURAL BIOLOGY

Chairpersons: Sine Larsen, Michael Becker

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Diffraction from a Laser-aligned Beam of Hydrated Proteins

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The aim of this work is to solve proteins which cannot be crystallized. An apparatus is under construction at ASU physics (electrons) and at the Advanced Light Source in Berkeley (X-rays) to obtain diffraction patterns from a single-file submicron droplet stream [1]. Each water droplet contains, on average, one protein. The droplets freeze by evaporative cooling to vitreous ice, most of which is allowed to sublimate. The molecules are aligned by a 100 watt CW fiber laser. All three beams , laser, X-rays and droplets, run continuously, and diffraction data is aquired continuously by CCD camera until adequate signal-to-noise is achieved. The laser polarization is then rotated into a new orientation using a quarter-wave plate, allowing tomographic diffraction data collection for three-dimensional reconstruction. The phase problem for the continuous diffraction pattern is solved by novel iterative Gerchberg-Saxton-Fienup methods [2]. Waves scattered by different molecules don't interfere. The requirements of laser power and droplet temperature needed to achieve sub-nanometer resolution and so observe the secondary structure of proteins will be described in detail. Factors which affect the damping of oscillations in the laser beam and momentum transfer by elastic diffraction to a levitated molecule.

[1] Spence J., Doak B., *Phys. Rev Letts*, 2004, **98**, 198102. [2] Spence J. et al, *Acta Cryst A*, 2005, in press. [3] Marchesini S. et al., *Phys Rev.*, 2003, **B68**, 140101(R).

Keywords: proteins, structure, laser alignment

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Protein Structures without Crystals

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Many proteins are inherently difficult to crystallize, due to various physical properties, e.g. membrane proteins, due to their large hydrophobic area, or amyloid-forming peptides and proteins due to very strong hydrogen bond networks in combination with hydrophobic interactions. Novel light sources (X-ray free electron lasers) may enable us to obtain structural information from small non-crystalline samples if we are able to gather enough scattering data before radiation damage destroys the sample. On the other end of the spectrum computer simulations of molecular dynamics may be able to predict structures of small proteins based on force fields within the near future. In the current presentation I give an overview of our work in both areas and how they are connected.

Keywords: X-ray, fel, gromacs

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Structural Proteomics using NMR in RIKEN Structural Genomics/Proteomics Initiative

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RIKEN Structural Genomics/Proteomics Initiative (RSGI) (http://www.rsgi.riken.jp) was organized by RIKEN Genomics Sciences Center and Harima Institute at SPring-8 in 2001. RSGI has been integrated into the National Project on Protein Structural and Functional Analyses ("NPPSFA" or "Protein 3000"), organized by the Ministry of Education, Culture, Sports, Science, and Technology (MEXT), as one center of the program for comprehensive studies. We are now focusing on proteins involved in phenomena of biological and