DESY SUMMER STUDENT PROJECT

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Simulations towards Coherent X-ray Diffractive Imaging of a colloidal crystal with a stacking fault

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ABSTRACT

In order to reveal the structure of a colloidal crystal the simulated diffraction patterns were inverted using phase retrieval methods. A full 3D reconstruction was retrieved showing the stacking fault as well as 200 nm colloid balls.

INTRODUCTION

To reveal the structure of periodic crystals coherent x-ray diffractive imaging (CXDI) [1] was used. CXDI is a lensless technique for 2D and 3D reconstruction of the image of nanoscale structures. The basic idea of CXDI is that a sample of finite size is illuminated by a coherent x-ray beam and the corresponding diffraction pattern can be uniquely inverted, to yield the electron density of the sample. The advantage of using no lenses is that the final image is aberration-free and so the resolution is only diffraction and dose limited. The objective lens from a typical microscopy is replaced with an algorithm to convert the reciprocal space diffraction pattern into a real space image.

In order to calculate electron densities within the crystal from a diffraction experiment we need two information – the amplitudes of the diffraction pattern and the phase values of the diffraction pattern. Only the intensities can be determined directly by an experiment. Information about phase is lost. Without knowledge of the phase, it is not possible to reconstruct a real space image. This is also called the phase problem. Iterative phase retrieval methods [2] solve this problem and enable us to recover detailed information about the structure of object.

Using high energies or a big lattice spacing will result in a 2D diffraction pattern with several Bragg peaks that can be mapped on a single 2D detector. Such diffraction patterns are then used to reconstruct an image via an iterative algorithm [3].

By these experiments we measure only diffracted intensities. If a diffraction pattern is sampled sufficiently finer than the Nyquist frequency so that the number of correlated intensities is more than the number of unknown variables in real space, phases are usually uniquely encoded in the diffraction intensities. Then the inversion of this diffraction pattern can reveal the arrangement of crystallic particles, the 3D structure of a sample in the real space image. The scattered intensity for a small sample at high energies from coherent x-ray's can be expressed as a Fourier transform of the shape function which is directly related to a projection of electron density [4].

Measurements of the sample were performed at synchrotron PETRA III. Experiment carried out at the coherent scattering beamline P10 with incident x-ray energy of 7.9 keV. The experimental arrangement is illustrated in Fig. 1. The sample was coherently illuminated by an x-ray beam and could rotate around the vertical axis (φ) perpendicular to the incident x-ray direction. The total size of the sample was about 7 μm and consisted of 200 nm colloidal balls with stacking faults. Colloid crystal was positioned at a distance 5 m in front of detector. The diffraction pattern of the object was recorded by charge-coupled device (CCD) with a size of 16 mm and the number of pixels was 1300x1300.

SIMULATING THE DIFFRACTION PATTERNS

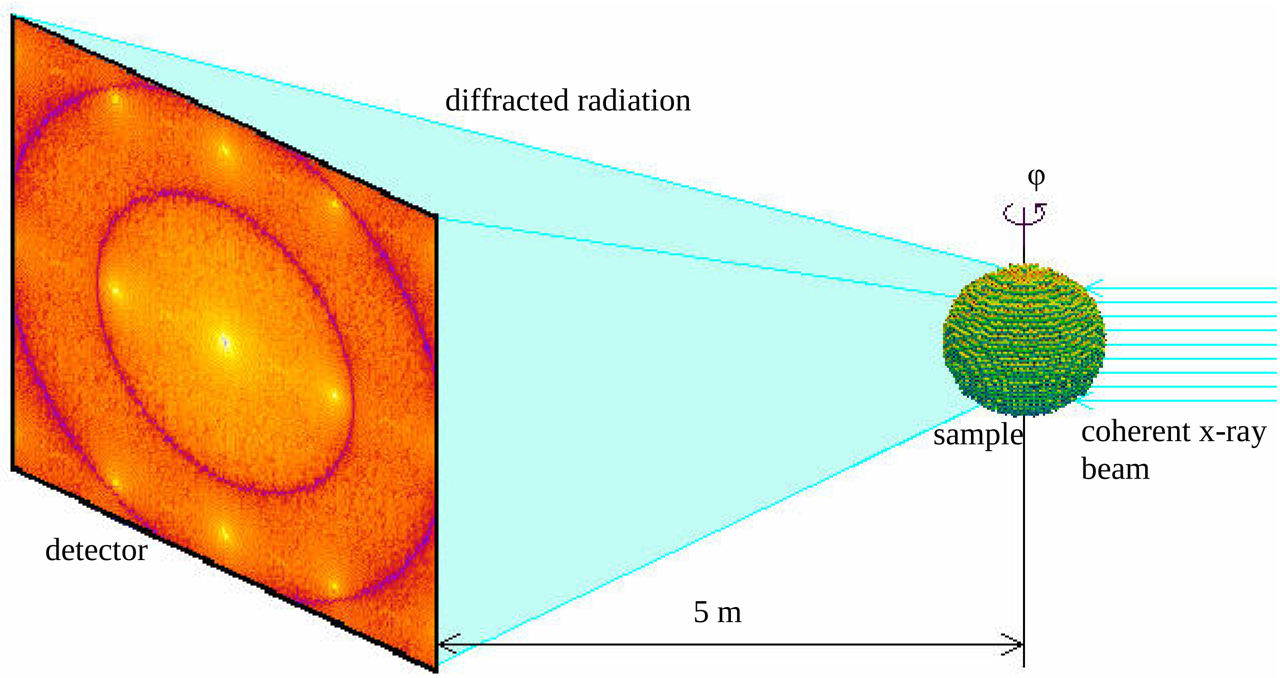

FIG. 1: Schema of CXDI experiment.

To better understand the measured results we simulated diffraction patterns with the corresponding experimental parameters. Initial model for our reconstruction consisted of 200 nm colloidal balls and contained a stacking fault. Its total size was 5x6x7 μm. The 3D model of a sample in Fig. 2 (a) is shown. We first simulated diffraction patterns by the program MOLTRANS. Rotation of the sample enabled us to simulate different diffraction planes of the sample for different angels with several Bragg peaks [Fig. 2 (b) – (d)].

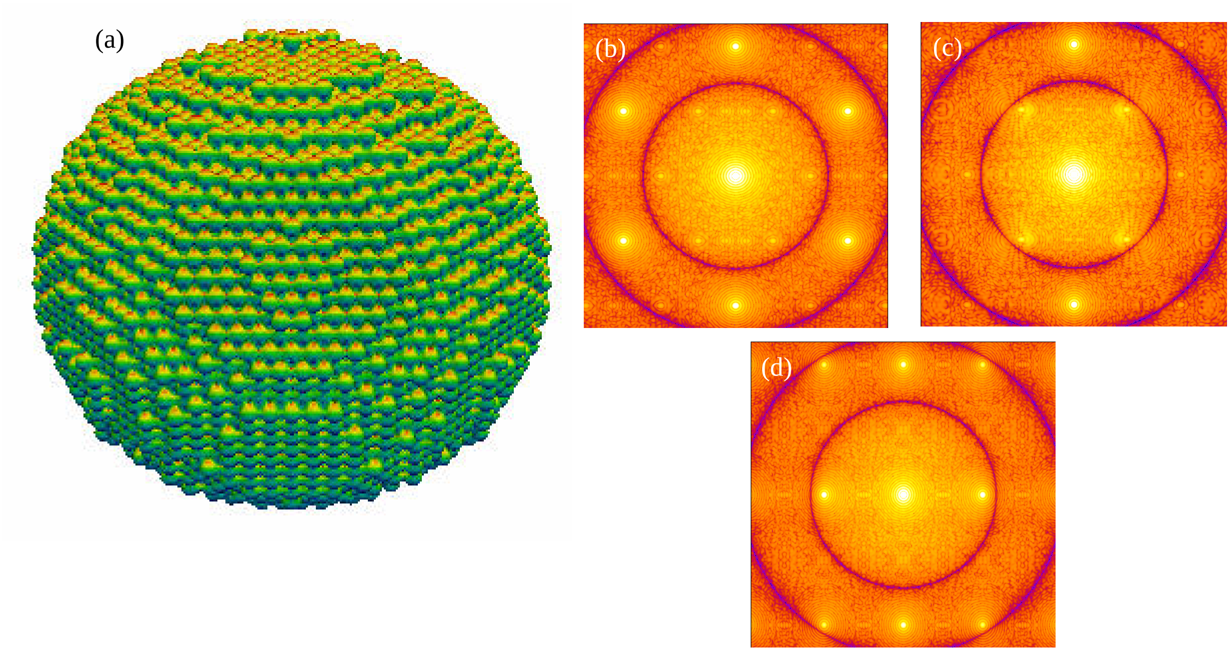

FIG. 2: (a) – initial model for reconstructions. Simulated diffraction patterns for different angles: (b) φ = 0, (c) φ = 90°, (d) φ = 180°.

The simulated diffraction patterns were used to identify which conditions are necessary to reconstruct the object.

RESULTS AND DISCUSSION

The diffraction data were used to reconstruct the object with the error reduction (ER) and the hybrid input-output (HIO) algorithm [5]. We found a tight rectangular support which was used as the real space constraint. The first reconstructions (see Fig. 3) of the sample did not show the desired result, because the reconstruction strongly depends on the choice of the support and the first chosen support turned out to be too loose (see Fig. 4). This problem was finally overcome by using the Shrink-Wrap method. The second problem was to find a convenient number of iterations of the ER and HIO algorithm and the constraint by Shrink-Wrap. By these procedures we achieved success and reconstructed a 3D model of the colloidal sample presented in Fig. 5.

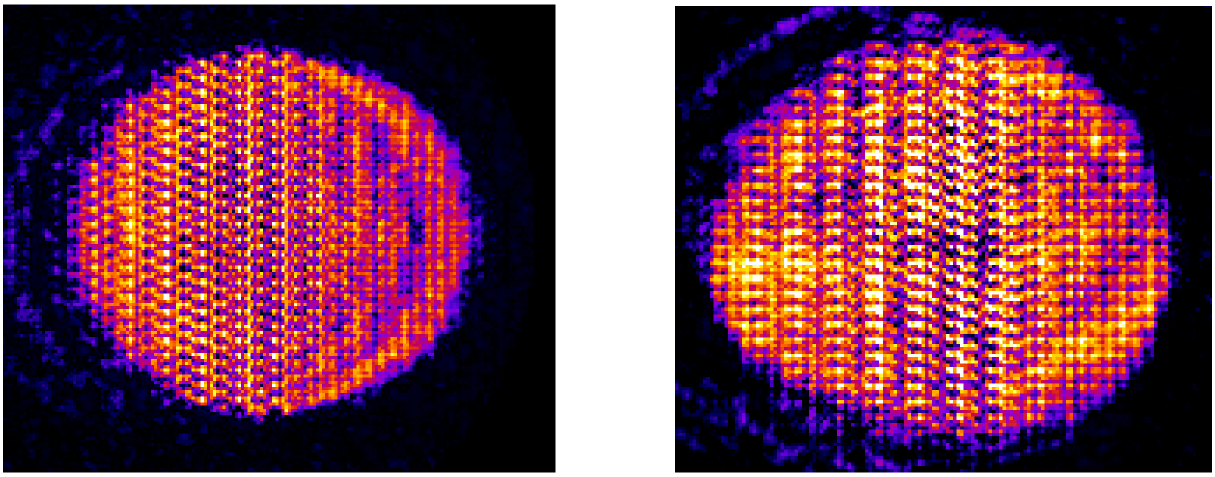

FIG. 3: Real images of wrong reconstructions for different parameters of algorithm. We can see only blurred lines and bounds.

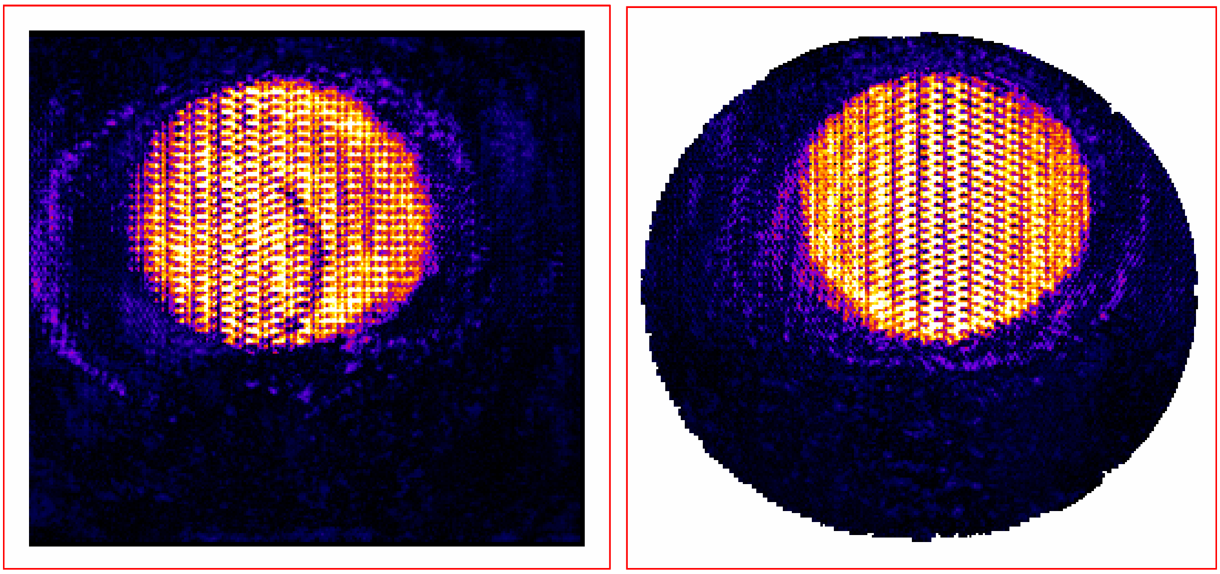

FIG. 4: The support about real space images which was far too big.

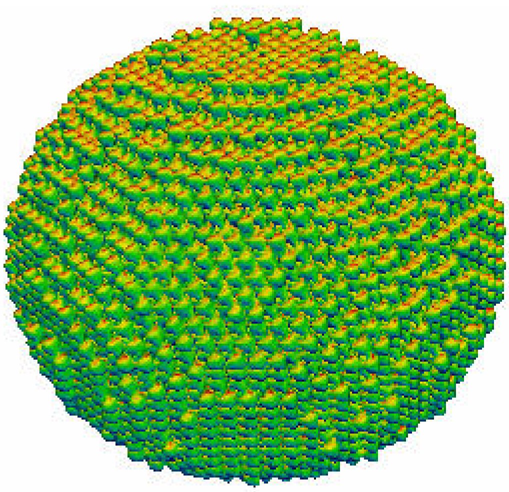

FIG. 5: Reconstructed 3D electron density of the ellipsoid crystal.

The best result (see Fig. 6) we achieved by applying 3 cycles of 6 runs with 100 iterations of HIO, 50 iterations of the ER algorithm. The Shrink-Wrap method was applied at the end of each cycle.

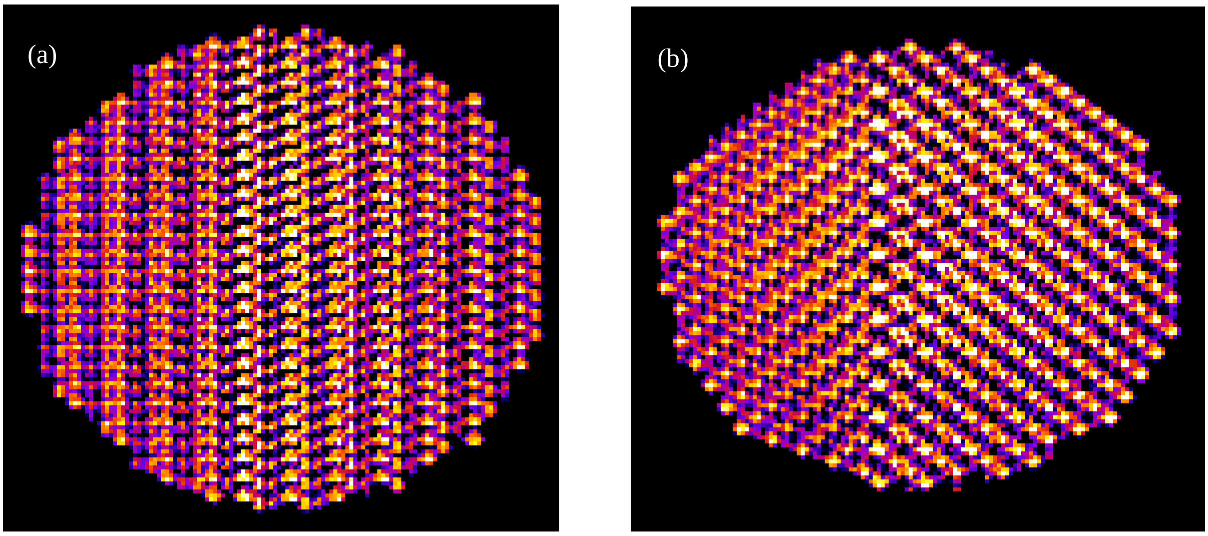

FIG. 6: The best reconstruction – (a) and (b) real space images – cuts through the 3D reconstructed volume. On fig. (b) we can see stacking fault in the crystal.

We can compare the achieved 3D image of our reconstruction (Fig. 5) with 3D initial model. The reconstructed result corresponds very well with our model.

CONCLUSION AND OUTLOOK

The result presented in this report show that it is possible to reconstruct the electron density of a colloidal ball from its diffraction patterns. In future work the influence of a beamstop has to be investigated, and finally the obtained knowledge has to be applied to the measured data. I would also like to use my present and new achievements for Student Scientific Conference at my home university.

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