Crystal Unbending

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1 Theoretical Background

Biological crystals are seldom perfect, they present distortions and stretching, are limited in extent and disordered. These imperfections degrade the Fourier Transform (FT) and reduce high resolution information. The degradation of the FT produces a broadening of the peaks at the reciprocal lattice (i.e., they are no longer a delta function but a Gaussian) plus an attenuation of the high frequency terms. As filtering (in Fourier space) is equivalent to averaging all the unit cells in the crystal (in real space), this degradation makes the average unit cell blurred. In other words, crystal imperfections translate into small misalignments of the different unit cells and the final average then turns out blurred. Lattice unbending was developed by Henderson et al. (1986), to correct these distortions and recover high resolution information.

2 Calculation

2D crystals should be corrected, termed unbending, by identifying the displacement of the unit cells compared with the ideal lattice by cross-correlation Fourier analysis by using a reference area from the center of the crystal itself.

The method requires:

- Create a reference image (center of the crystal itself)
- Fourier transform both the crystal and the reference
- Croscorrelate both images
- Calcualte the the relative translations of the unit cells compared with a reference image.
- Create (by interpolation) a perfect crystal from the original image

3 Objetive

Using Matlab implemented 2D crystal Unbending

4 Bibliography

Henderson, R., Baldwin, J.M., Downing, K.H., Lepault, J., Zemlin, F., 1986. Structure of purple membrane from Halobacterium halobium: recording, mea-

surement and evaluation of electron micrographs at 3.5 Åresolution. Ultramicroscopy 19, 147–178.