JOURNAL OF APPLIED CRYSTALLOGRAPHY

Volume 56 (2023)

Supporting information for article:

Bragg coherent modulation imaging for highly strained nanocrystals – a numerical study

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S1. BCMI Phase Retrieval Algorithm

Following the BCMI propagation models, a dedicated phase retrieval algorithm was composed and its pseudocode is given in Fig. S1. The inputs of this algorithm are diffraction intensity measurements $\{I_j\}_{j=1}^{J}$, the prior knowledge of the modulator function $Modu$, the support function $supp$ and the object estimate $S^0(\boldsymbol{r})$. To speed up the iterations, the Q_z^j-related phase term $\{\phi_j\}_{j=1}^{J}$ [in equation (3)] can also be calculated in advance for use. In the main iteration cycle, all the recorded diffraction intensity slices, I_j, will be looped through to update the running estimate of real-space object representation $S(\boldsymbol{r})$. For each slice, the corresponding object projection is propagated to the detector plane using the forward propagation model of equations (6)-(10) (steps 2-5 in Fig. S1). The diffraction wave estimate E_j is then updated by applying the modulus constraint defined as

$$\hat{E}_j = \sqrt{I_j}\frac{E_j}{|E_j|}. \tag{20}$$

Using $\hat{E}_j$, the real-space object component $S_j(\boldsymbol{r})$ can be obtained using the BCMI backward propagation model described by equations (11)-(14), and the updated object $\hat{S}(\boldsymbol{r})$ is then calculated by summing all the $S_j(\boldsymbol{r})$ with equation (5) (steps 6-8 in Fig. S1). After getting $\hat{S}(\boldsymbol{r})$ in one loop, the real-space support constraint is applied (step 9 in Fig. S1). If necessary, the support function can be refined using the shrink-wrap algorithm after a certain number of iterations (step 10 in Fig. S1).

// Given quantities

$\{I_j\}_{j=1}^{J}$ (intensity measurements); *Modu* (modulator function); *supp* (support function); S^0 (initial object estimate); $\{\phi_j\}_{j=1}^{J}$ (the Q_z^j-related phase term)

for $k = 1 \ldots$ do // The main iteration

// ① Give the current estimate

$S^k = S^{k-1}$

$\hat{S}^k = 0$

for $j = 1 \ldots J$ //loop each 2D diffraction pattern

// ② Generate the object projection along *z*-axis

$S_j^k = \int S^k \cdot \phi_j dz$

// ③ Propagate the object projection to modulator plane

$E_j^k(m) = \mathcal{P}\{S_j^k\}$

// ④ Apply modulation

$E_j^k(M) = Modu \cdot E_j^k\,(m)$

// ⑤ Propagate to detector plane

$E_j^k(D) = \mathcal{F}\{E_j^k(M)\}$

// ⑥Apply the modulus constraint and propagate back to the modulator plane

$\hat{E}_j^k(M) = \mathcal{F}^{-1}\left\{\sqrt{I_j} \cdot \frac{E_j^k(D)}{\left|E_j^k(D)\right|}\right\}$

// ⑦ Undo modulation

$\hat{E}_j^k(m) = E_j^k(m) + \frac{Modu^*}{\max(|Modu|^2)} \cdot \left(\hat{E}_j^k(M) - E_j^k(M)\right)$

// ⑧ Propagate back to the object plane to update the object

$\hat{S}^k \mathrel{+}= \phi_j^* \cdot \mathcal{P}^{-1}\left\{\hat{E}_j^k(m)\right\}$

end

// ⑨ Do support constraint

if ER type

$S^k = \hat{S}^k \cdot supp$

elseif HIO type

$S^k = \hat{S}^k \cdot supp + \beta(S^k - \hat{S}^k) \cdot (1 - supp)$

end

// ⑩ Update the support in each N^{th} iteration

if k is a multiple of *N*; $supp = Shrink\_wrap(S^k)$; end

end

Figure S1 Pseudocode of the BCMI phase retrieval algorithm. The pair $\mathcal{P}\{\cdot\}$ and $\mathcal{P}^{-1}\{\cdot\}$ are the forward and backward propagation operators between the object and modulator plane. The pair $\mathcal{F}\{\cdot\}$ and $\mathcal{F}^{-1}\{\cdot\}$ are the direct and inverse 2D Fourier transforms. The waves in the front and rear plane of the modulator, and in the detector plane, are marked by m, M, and D, respectively.

S2. BCMI Reconstruction Results of *model-1* and *model-2* Crystals under Different Acquisition Diffraction Intensities

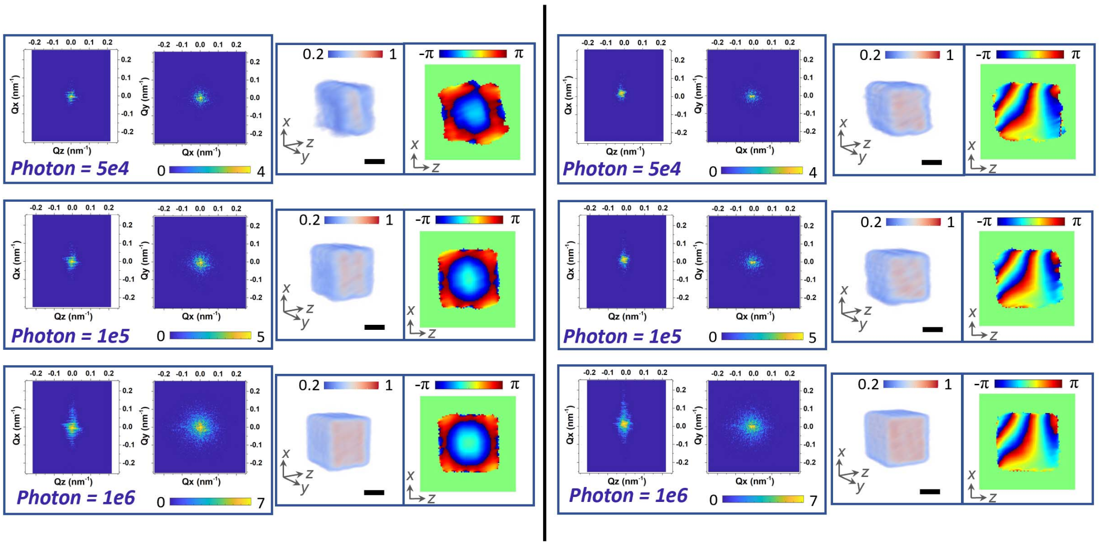

Figure S2 The central diffraction slices and the BCMI reconstruction results of *model-1* (left) and *model-2* (right) crystals when acquisition diffraction photons are 5×10^4, 1×10^5 and 1×10^6. The BCMI diffraction data generation and phase retrieval use the same way as in the text. The scale bar is 200 nm and only the reconstructed central xz phase cross sections are shown.

S3. Overall BCDI and BCMI Reconstruction Results of *model-1* and *model-2* Crystals

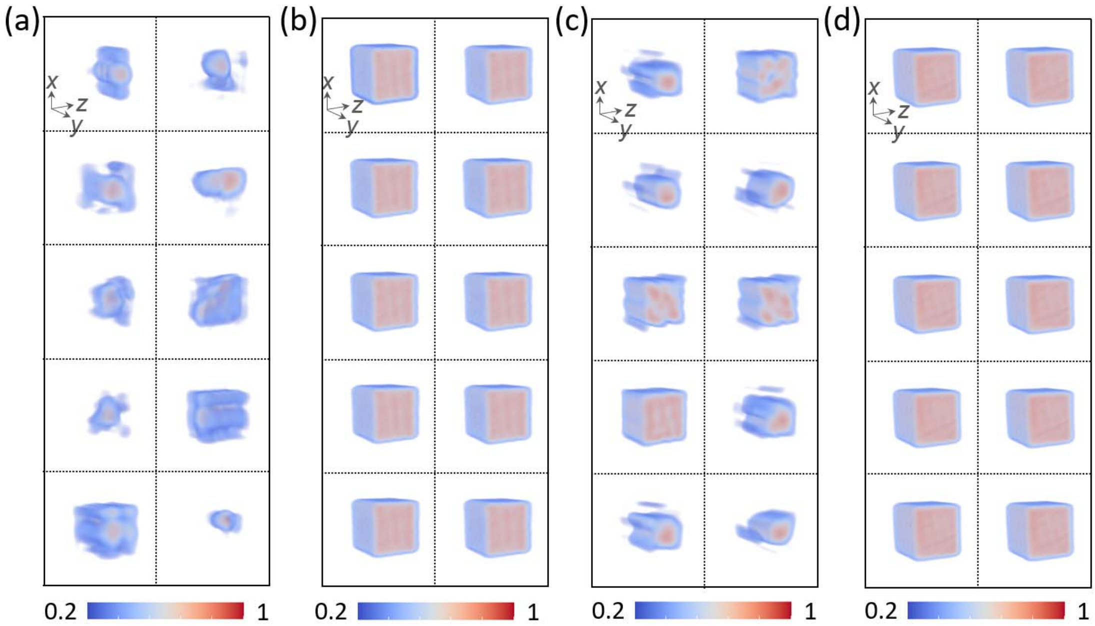

Figure S3 (a), (b) 10 BCDI and 10 BCMI reconstruction results of crystal *model-1*. (c), (d) 10 BCDI and 10 BCMI reconstruction results of crystal *model-2*. Only the 3D amplitudes are shown.