

Dose efficient Compton X-ray microscopy: supplementary material

P. VILLANUEVA-PEREZ^{1,*}, S. BAJT², AND H. N. CHAPMAN^{1,3,4}

¹Center for Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany

²Photon Science, DESY, Notkestraße 85, 22607 Hamburg, Germany

³Department of Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

⁴Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

*Corresponding author: pablo.villanueva-perez@cfel.de

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1. REQUIRED IMAGING FLUENCE AND DOSE FOR SCANNING COMPTON X-RAY MICROSCOPY

In this section we present the details of the calculation for the required imaging fluence and dose for scanning Compton X-ray microscopy (SCXM). Let's assume a focused beam to a square transverse shape of side dimension d' , which propagates through a sample with thickness L . If the depth-of-focus of the lens producing such focal spot is larger than L and the sample is positioned on the focal spot, it can be assumed that the illuminated area by the direct beam is unaltered through the material. For this scenario, the illuminated volume of the sample is given by $L \times d'^2$ and the flux for non-absorbing materials remains constant over the sample length. The aforementioned approximations are realistic for the focusing schemes and the size and composition of the samples considered in the main text.

In order to evaluate the minimum required imaging fluence Φ' we compare two scenarios: (a) the beam traverses only a uniform material thickness L or (b) the beam illuminates a thickness $L - d$ of background material and a thickness d of a certain material of interest. These two situations are depicted in Fig. (S1). For

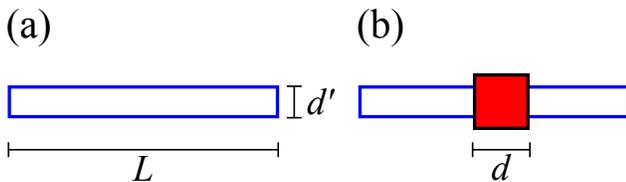


Fig. S1. The two scenarios used to determine the minimum required imaging dose and fluence having only background material (a) or embedding a voxel of size d of a certain material of interest (b).

the samples studied in the main article, the background homogeneous material is water (w) and the materials of interest (m) are PMMA, a biomolecule [1], and DNA [2]. As SCXM is a scanning technique, its resolution is correlated to the focal spot size. Thus, it is required that the beam is smaller or equal than the size of the voxel to be reconstructed, i.e. $d' \leq d$. The detectability criterion used to determine the minimum imaging fluence is the Rose criterion [3], i.e. the voxel d can be reconstructed only if the contrast between the scenarios a and b is at least five times the noise level. Assuming that the only noise contribution is Poisson photon-counting statistics, it is required that

$$5 \leq \frac{|N_S^a - N_S^b|}{\sqrt{N_S^a + N_S^b}}, \quad (\text{S1})$$

where $N_S^{a,b}$ are the number of scattered photon for each scenario. For example, the total number of scattered photons over a detected solid angle (Ω_{det}) when imaging at a given fluence Φ a certain material (i) is given by

$$N_S^i = \Phi \sigma_{\Omega_{\text{det}}}^i \rho_i V, \quad (\text{S2})$$

where $\sigma_{\Omega_{\text{det}}}^i$ is the total scattering cross section over a detected solid angle Ω_{det} for a material i per unit of mass, ρ is the density of the material, and V is the illuminated volume. Therefore, for the scenarios a and b the number of scattered photons is given by:

$$\begin{aligned} N_S^a &= \Phi \sigma_{\Omega_{\text{det}}}^w \rho_w L d'^2 \\ N_S^b &= N_S^a + \Phi (\sigma_{\Omega_{\text{det}}}^m \rho_m - \sigma_{\Omega_{\text{det}}}^w \rho_w) d d'^2. \end{aligned} \quad (\text{S3})$$

Thus, the Rose criterion imposes that

$$\begin{aligned}\Phi &\geq 25 \frac{2L\sigma_{\Omega_{\text{det}}}^{\text{w}}\rho_{\text{w}} + d\sigma_{\Omega_{\text{det}}}^{\text{m}}\rho_{\text{m}}}{d'^2 d^2 (\sigma_{\Omega_{\text{det}}}^{\text{m}}\rho_{\text{m}} - \sigma_{\Omega_{\text{det}}}^{\text{w}}\rho_{\text{w}})^2} \\ &\approx 25 \frac{2L\sigma_{\Omega_{\text{det}}}^{\text{w}}\rho_{\text{w}}}{d'^2 d^2 (\sigma_{\Omega_{\text{det}}}^{\text{m}}\rho_{\text{m}} - \sigma_{\Omega_{\text{det}}}^{\text{w}}\rho_{\text{w}})^2},\end{aligned}\quad (\text{S4})$$

where we have taken into consideration that $\sigma_{\Omega_{\text{det}}}^{\text{m}} \sim \sigma_{\Omega_{\text{det}}}^{\text{w}}$, $\rho_{\text{w}} \sim \rho_{\text{m}}$, and $L \gg d$. The equality defines the minimum required fluence Φ' . For the case that the focal spot size and the material voxel are equal ($d = d'$), the required imaging fluence is proportional to L/d^4 as reported in the main text.

The imaging deposited dose on the sample is derived from the minimum required fluence

$$D \geq \Phi' E \left[\sigma_{\text{ph}}^{\text{m}} + \int_{\Omega} \frac{d\sigma_{\text{inc}}^{\text{m}}}{d\Omega} \left(1 - \frac{1}{1 + \frac{E}{m_e c^2} (1 - \cos\theta)} \right) d\Omega \right], \quad (\text{S5})$$

where E is the energy of the incoming X-ray photon beam, $\sigma_{\text{ph}}^{\text{m}}$ and $\sigma_{\text{inc}}^{\text{m}}$ are the photoabsorption and incoherent scattering or Compton cross sections per unit of mass for the material of interest m , m_e is the rest mass of the electron, and c is the speed of light.

2. REQUIRED FLUENCE STUDY FOR SCXM

In this section we report the results of the studies performed to validate the minimum required imaging fluence and dose. We performed two computations.

First, we estimated the retrieved resolution for the simulation experiments at different fluences for 34 nm features of PMMA, a biomolecule, and DNA, embedded in 5 μm of water thickness ($L = 5 \mu\text{m}$ and $d = 34 \text{ nm}$). The resolution is estimated by comparing the ground truth with the simulated data using Fourier ring correlation with half bit criterion [4]. The results of this simulations are shown in Fig. S2(a). The horizontal red-dashed line represents the desired resolution of 34 nm and the vertical red-dashed line the minimum fluence to retrieve that resolution for the different materials. It can be observed that the simulations and theoretical limits are in good agreement, as larger fluences than the computed limit result in better resolutions than the 34 nm aim, while for smaller values the resolution is worse than the feature size.

Second, we evaluate the signal contrast between a thickness of 5 μm water with and without a 34 nm voxel of the studied materials as a function of the fluence (Fig. S1). The results of this study for PMMA, a biomolecule, and DNA are presented in Fig. S2(b). For this calculation Poisson photon-counting noise has been assumed. The horizontal dashed red line represents the five standard deviations (std) limit imposed by the Rose criterion [3] and the vertical line represent the minimum fluence to observe that exact contrast. It should be noticed that the theoretical calculation predicts systematically a higher contrast than the simulated one. This effect is due to the fact that the theoretical model does not include the point spread function of the focal spot.

Both validations show good agreement with the calculations introduced in the main text and with more detail in the previous section of the supplementary material.

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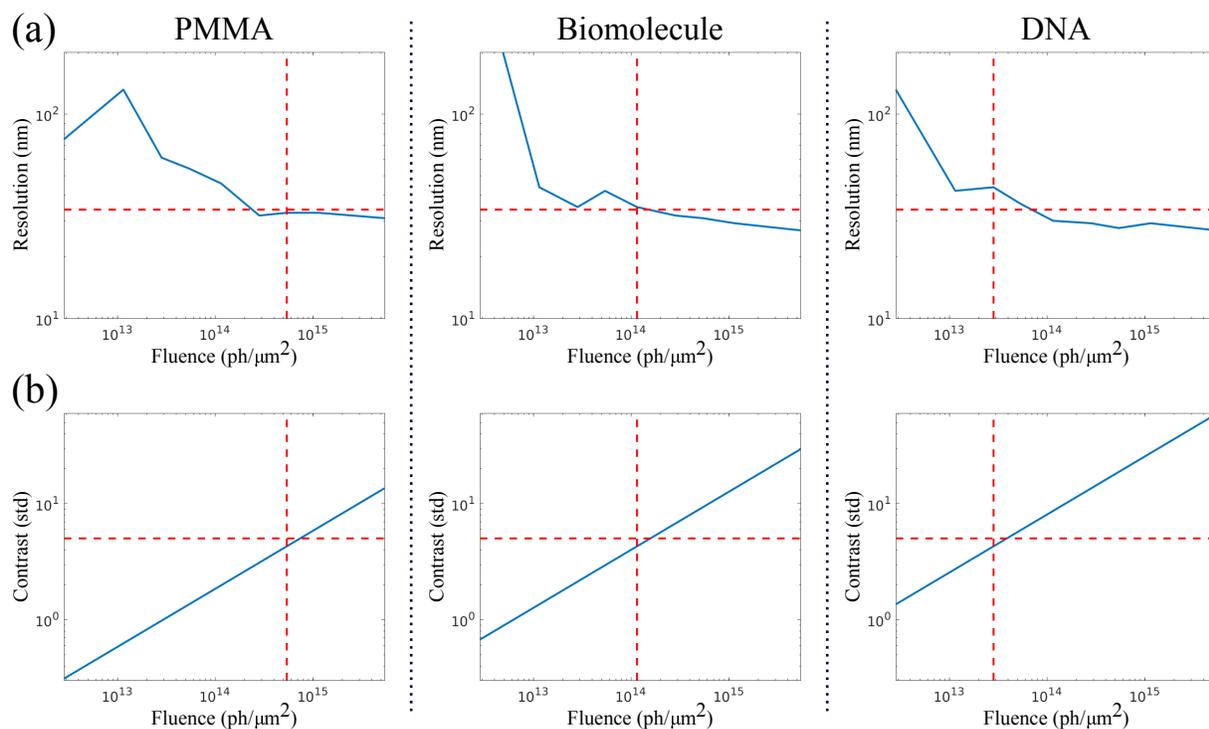


Fig. S2. (a) Resolution evaluation for PMMA, a biomolecule, and DNA as a function of the fluence using Fourier Ring Correlation with half bit criterion (blue continuous curve). The horizontal dashed red line represents the simulated feature size of 34 nm. (b) Contrast evaluation between $5 \mu\text{m}$ of water with and without a 34 nm feature embedded. The horizontal red dashed line represents the 5 standard deviation (std) criterion. The vertical dashed red line, in both subplots, represents the minimum fluence to retrieve the targeted resolution and contrast for the different materials computed assuming the Rose criterion [3].