Micron X-ray Protein Crystallography Beamline Design Calculated in Phase Space Analysis

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X-ray crystallography is a powerful method to define the arrangement of atoms. This technique enables us to observe protein structures and their interaction with other molecules or enzymes. Moreover, it can help to develop the new cures for diseases and the designs of novel drugs. Hence, it is importance to develop the micron x-ray protein crystallography beamline. Phase space analysis (PSA) is a useful approximate method to estimate the performance of beamline designs in synchrotron radiation x-ray optics. This analytic method in position-angle-wavelength space concisely represents widths, angular divergences, and intensities of the x-ray beam. All acceptance functions of the optical components are based on the approximation of Gaussian distribution. The parameters of an x-ray beam can be defined simultaneously in the horizontal and vertical plane by matrix algebra. The intensity of an x-ray source is represented by its brilliance [1-3] and the mathematical form is given by $I(x, x´, z, z´, \lambda) = I(0, 0, 0, 0, \lambda) \, I_x(x, x´) \, I_z(z, z´) \, I_\lambda(\Delta\lambda/\lambda)$, where $I_x(x, x´) = exp\{-(1/2) [x^2/\sigma_x^2 + x´^2/\sigma_{x´}^2]\}$, $I_z(z, z´) = exp\{-(1/2)[z^2/\sigma_z^2 + (z´-\Gamma z)^2/\sigma_{z´}^2]\}$, and $I_\lambda(\Delta\lambda/\lambda) = exp\{-(1/2) [(\Delta\lambda/\lambda)^2/\sigma_\lambda^2]\}$. $I(0, 0, 0, 0, \lambda)$ is the brilliance at the center of the beamline source. The parameters of σ_x, $\sigma_{x´}$, σ_z, and $\sigma_{z´}$ are the standard deviations of the source size and the divergence in both perpendicular to the optical axis, and λ is the x-ray wavelength. The parameter of Γ is zero and σ_λ depends on the use of beamlines for an undulator source. The coordinate transformation in the phase space from source to sample is described by $M_{soure}(x, x´, \Delta\lambda/\lambda) = T_1 T_2 \dots T_N M_{sample}(x, x´, \Delta\lambda/\lambda)$ [1-3], where T_i is the inverse of the transformation matrix of the ith optical component. Here, the parameters of $\sigma_x, \sigma_{x´}, \sigma_z, \sigma_{z´}$, and σ_λ are 0.12 mm, 18 μrad, 4.92×10^{-3} mm, 8.59 μrad, and 3.94×10^{-3}, respectively. In this study PSA is used to calculate the parameters of the micron x-ray protein crystallography beamline and the beam size (HxV, FWHM) and divergence (HxV, FWHM) in the sample position are 51.9x3.9 μm^2 and 68x250 μrad^2, respectively.

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