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Spatial beam profile-induced effects in x-ray scattering pattern at high intensity

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Synopsis Simulation of high-intensity x-ray scattering from a crystal that is larger than the transverse x-ray beam profile is presented. We consider a crystal with a size of a micron, when irradiated by an x-ray beam having a focus of 100 nm. We discuss the methodological challenges that had to be overcome in order to calculate the x-ray scattering pattern. Our calculations enable us to identify the characteristic features of the spatial beam profile imprinted in the scattering pattern.

X-ray free-electron lasers (XFEL) deliver intense femtosecond pulses that promise to yield high-resolution diffraction data of nanocrystals before the destruction of the sample by radiation damage. The characteristics of XFEL radiation and associated sample environments have triggered the development of new data collection methods, such as serial femtosecond crystallography (SFX). In SFX, a complete data-set can be obtained by exposing thousands of randomly oriented, individual crystals of proteins (Figure 1) to the x-ray beam. A bottleneck for x-ray structure determination in biology is radiation damage manifested by ionization and sample deterioration during irradiation. From the reconstruction aspect, that means the changes of scattering form factors [1] and atomic positions are strongly fluence dependent. A crystal with a size of a micron is large as compared to the 100 nm focus of an XFEL pulse. Thus it is not valid to consider a homogeneous fluence distribution throughout the whole crystal under the influence of such a focused beam. As a consequence of different fluence regions in the crystal, one might see the characteristics of the beam imprinted in the scattering pattern.

In realistic simulations of SFX experiments, it is mandatory to take into account the fluence dependent dynamics of different crystal regions as well as their different contributions to the scattering pattern. In our theoretical study we consider a micron-size protein crystal in a 100 nm focus beam. The number of atoms under the influence of the beam is, thus, of the order of 10^9. To follow the time evolution of the crystal we developed an extension of XMDYN [2], which is a complex simulation tool for modeling dynamics of molecular systems (e.g. biological molecules) irradiated by an intense hard x-ray pulse. Using the original XMDYN code, simulation of that many particles is too expensive. We present a model, employing our extension of XMDYN, that is capable of describing this challenging situation. We use, XATOM [3] toolkit to calculate all atomic x-ray scattering form factors required. To this end, we extend XATOM in order to enable the calculation of x-ray scattering form factors for many fluences for a large number of particles. Based on the sample dynamics and the scattering parameters we construct realistic scattering patterns for an inhomogeneous spatial pulse profile and compare them with the ideal ones. Moreover, we also investigate the effect of the shape of the beam profile by considering Gaussian and trapezoidal envelopes.

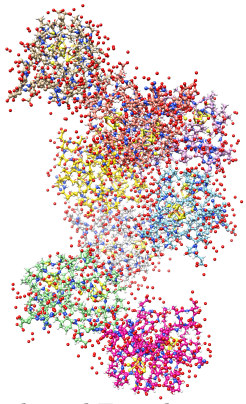

Figure 1. Unsolvated Ferredoxin unit-cell, containing 8 Ferredoxin molecules with a total of 9500 atoms.

References

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