pI7 Femtosecond imaging of biomolecules by X-rays.
R. Neutze[1], R. Wouts[1], D. van der Spoel[1], E. Weckert[2,3], J. Hajdu[1], *(1)Department of Biochemistry, Biomedical Centre, Box 576, Uppsala, University, S-75123 Uppsala, Sweden, (2) Institut fr Kristallographie, Universitt Karlsruhe, Kaiserstrasse 12, D-76128 Karlsruhe, Germany, (3) Present address: HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germanys.*
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The structural information that can be recovered from scattering of intense femtosecond X-ray pulses by single protein molecules and small assemblies is analysed using computer simulations. We present an estimate of radiation damage to a sample as a function of photon energy, pulse length, integrated pulse intensity and sample size based on a classical model describing sample dynamics. The results show that experiments using very high X-ray dose rates and ultra short exposures may provide useful structural information before radiation damage destroys the sample. The predicted radiation tolerance to hard X-rays in the femtosecond time-domain is several orders of magnitude higher than theoretical limits in conventional X-ray experiments. Under these conditions, scattering to atomic resolution may be recorded from single macromolecular structures like large proteins, viral capsids or nanoclusters. We foresee that such ultrashort, high-intensity X-ray pulses, in combination with novel container-free sample handling methods based on spraying techniques, will open up new horizons for structural determinations with X-rays.

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