Electronic damage for short high-power x-ray pulses: its effect on single-particle x-ray imaging for 100 as - 10 fs pulse durations.

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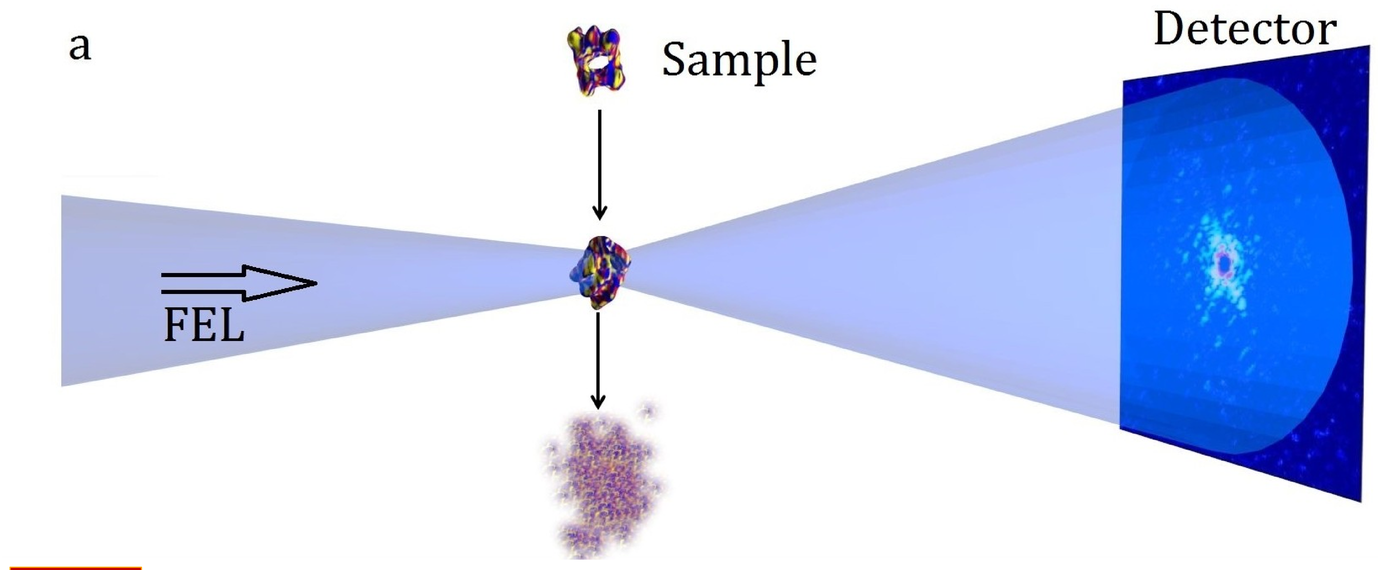
Single-particle diffraction imaging experiments at XFELs have a great potential for the structure determination of reproducible biological specimens that cannot be crystallized. In these experiments, samples are exposed to intense x-ray pulses to obtain single-shot diffraction patterns. The high intensity induces electronic dynamics on the femtosecond time scale in the system, which can reduce the contrast of the obtained diffraction patterns [1]. By going to shorter pulse durations, electronic damage can be partially avoided [2].

A. Experiment scheme and diffraction patterns

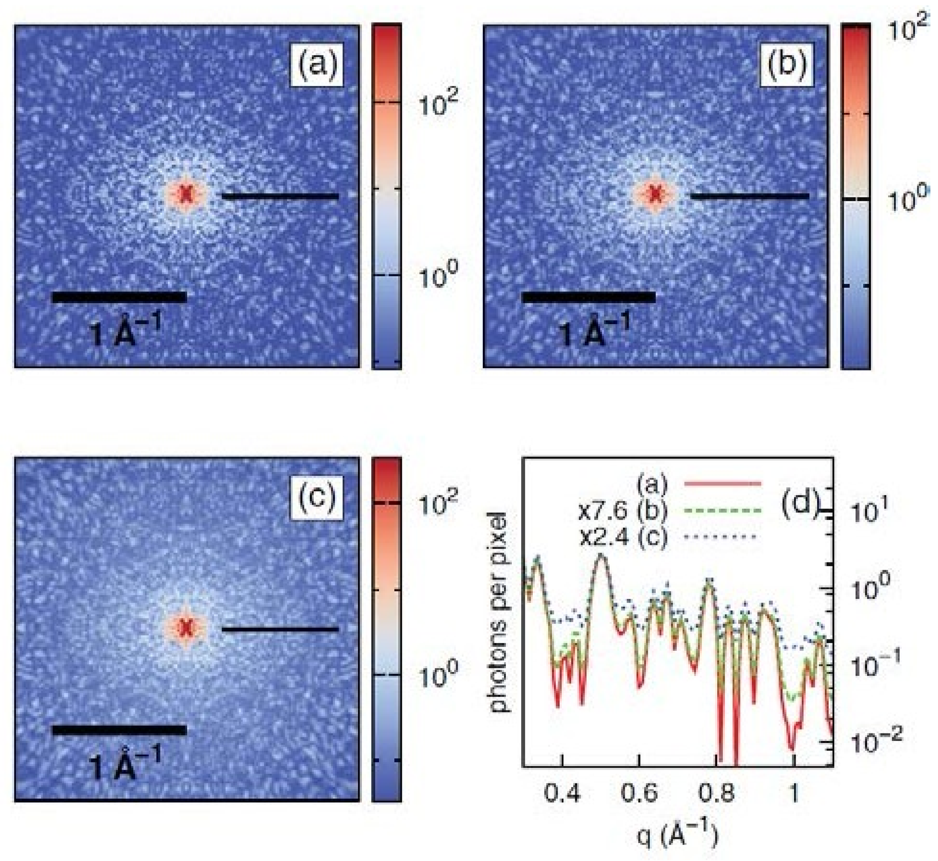


A.1 Experiment geometry

Diffraction pattern from a sample in random orientation is measured by a single FEL pulse.
After the pulse propagation the particle explodes due to Coulomb forces between ions.

A.2 Diffraction patterns

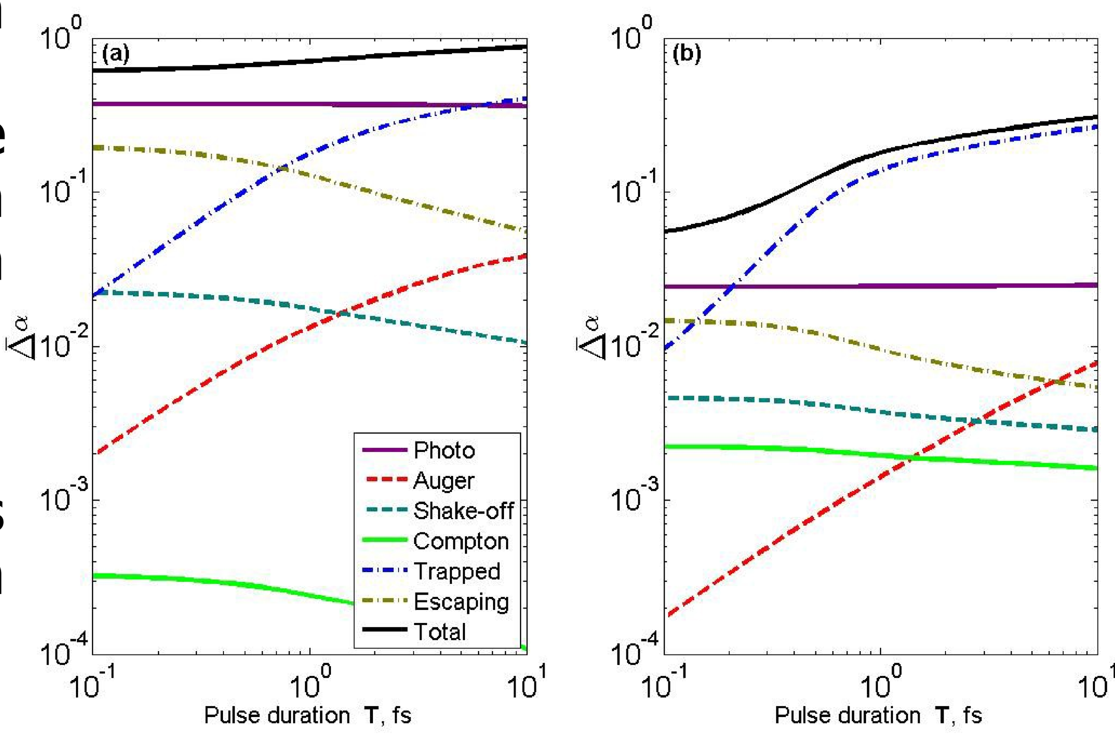
Diffraction patterns are affected by the electronic damage to the particle during pulse propagation.
Shown: averaged two-dimensional diffraction patterns of the Adenovirus shell for a 5-fs x-ray pulse and 3.1-keV photon energy. (a) No electronic damage, fluence of 1014 ph/μm2. [(b) and (c)] Ionized sample, 1014 ph/μm2 (b) and 1016 ph/μm2 (c). (d) Intensity profiles along the black lines. From Ref. [1]



B. Different processes and Compton scattering

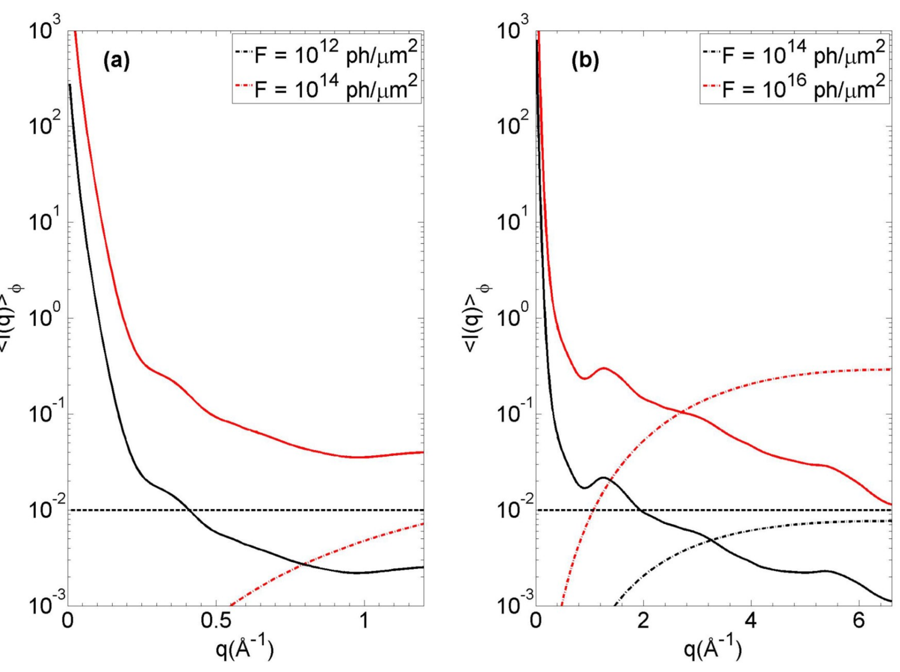
B.1 Total contribution of different processes

Different ionization channels exist.
Their importance (average ionization degree) changes with pulse duration.
Photon energies 3.1 keV (a) and 12.4 keV (b). The fluence is 1014 photons/μm2 in both cases. Ref. [2].



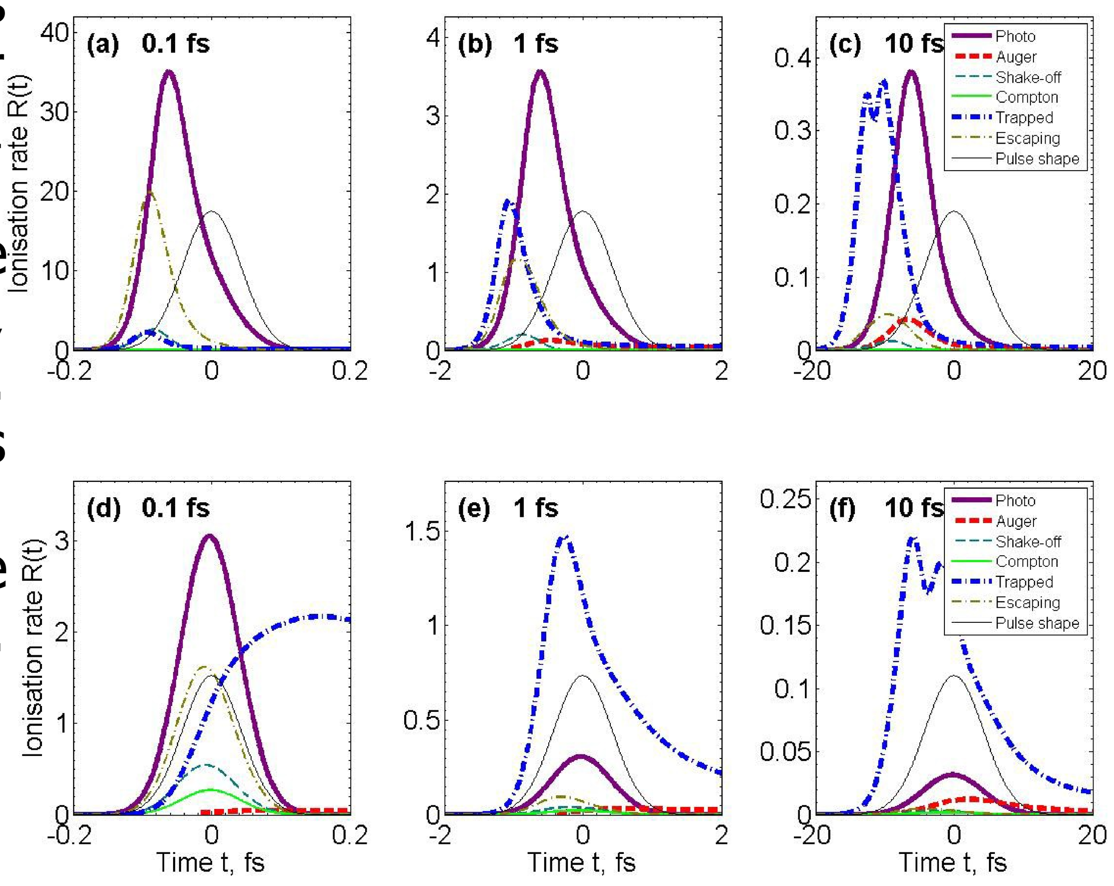
B.3 Compton background

Compton background from inelastic atomic scattering contributes to the problem. Angular averaged scattered signal (solid lines) and the Compton scattering signal (dashed lines) for photon energies of 3.1 keV (a) and 12.4 keV (b). 1 fs pulse. The horizontal dashed black line corresponds to the requirement of 10-2 photons per resolution element. [2].



B.2 Time evolution of the electronic damage

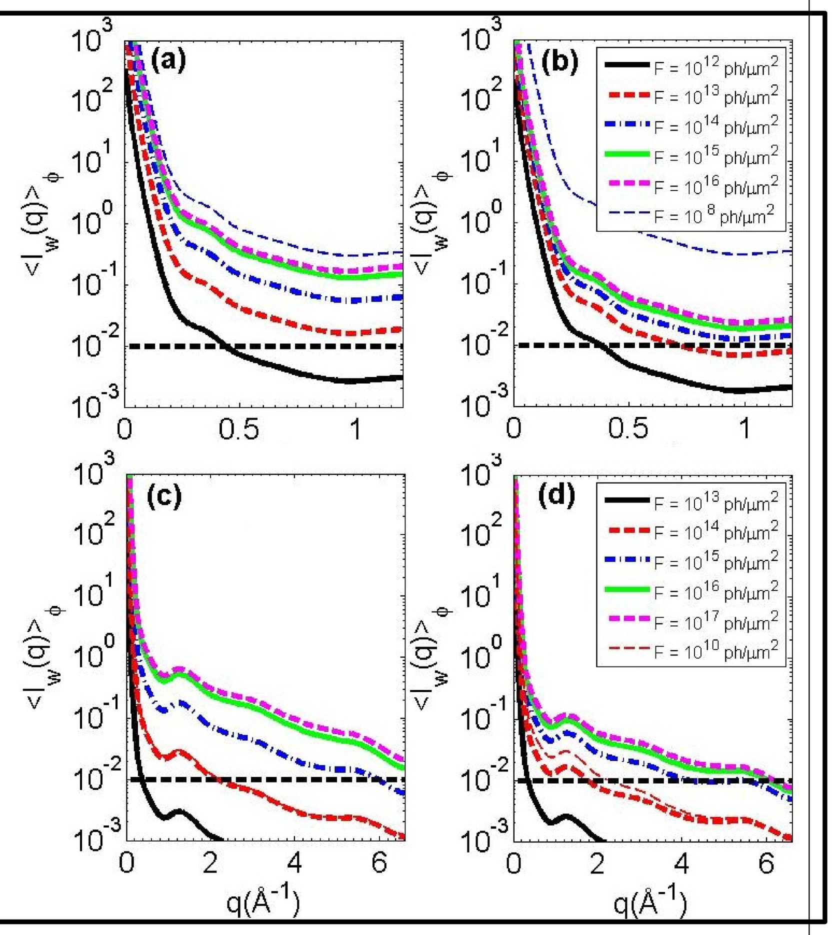
Average ionization rates during the pulse for photon energies of 3.1 keV (a-c) and 12.4 keV (d-f). The pulse durations are 0.1 fs (a,d), 1 fs (b,e), and 10 fs (c,f). The pulse fluence is 1014 ph/μm2 in all cases. The dashed line shows the pulse shape. Ref. [2].



C. Effect of electronic damage on the signal

C.1 Scattered signal

Angular averaged scattered signal stops growing with the fluence at certain power. Here it is shown for photon energies of 3.1 keV (a-b) and 12.4 keV (c-d) and different fluences. Pulse durations are 0.1 fs (a,c) and 10 fs (b,d). Ref. [2].



Summary

The simulation of ionization dynamics for different pulse parameters and quantification of the contribution of single mechanisms were performed. For sufficiently short pulses (~1 fs already), it is possible to outrun the ionization from the trapped electron gas, and thus reduce the electronic damage considerably. We also notice that Compton scattering introduces a noticeable background for higher photon energies.

References

[1] U. Lorenz, N. M. Kabachnik, E. Weckert, I. A. Vartanyants, Phys. Rev. E 86, 051911 (2012).
[2] O. Gorobtsov, U. Lorenz, N. M. Kabachnik, E. Weckert, I. A. Vartanyants, *in preparation*