Multi-wavelength anomalous diffraction phasing method at high intensity

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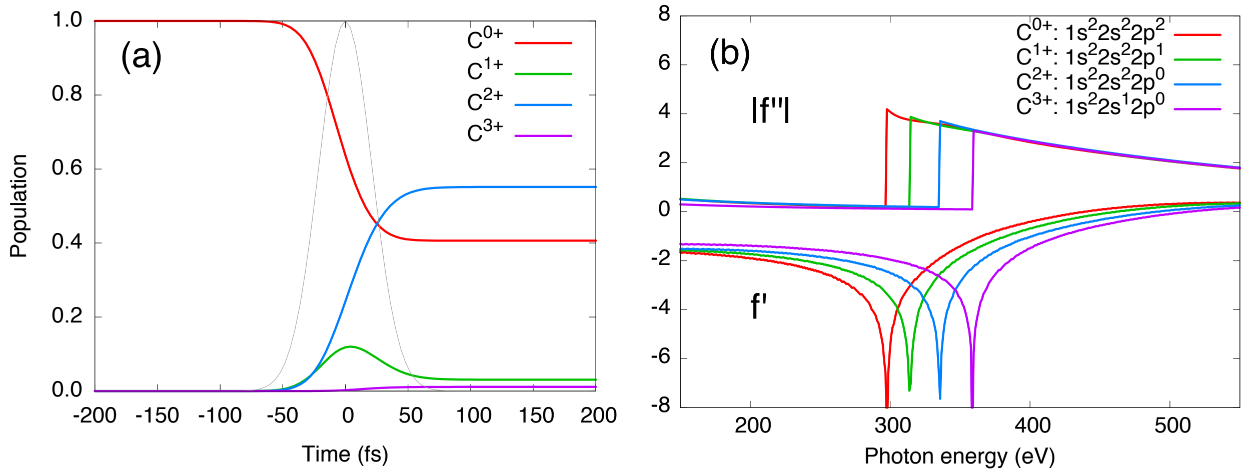
Multi-wavelength anomalous diffraction (MAD) is widely used in x-ray crystallography with synchrotron radiation to determine phase information by employing dispersion corrections from heavy atoms. It has been extended to the XUV and soft-x-ray regime with light atoms for nanoscale imaging of noncrystalline materials [1]. X-ray free-electron lasers (FELs) show promise for revealing the structure of single molecules or nanocrystals within femtoseconds [2], but the phase problem at high intensity of FEL remains largely unsolved. Due to an extremely high fluence of FEL, samples experience severe and unavoidable electronic radiation damage, which hinders direct implementation of the MAD method with FELs. We propose a generalized version of the MAD phasing method at high intensity [3]. The essential equation for the MAD method is reformulated and relevant coefficients are calculated with damage dynamics and accompanying changes of the dispersion correction. Here we present the XATOM toolkit to simulate detailed electronic damage dynamics [4] and discuss how the proposed method is applicable to the phase problem in molecular or nanoscale imaging with FELs.



Figures: (a) Population dynamics of several charge states of carbon during a 10^{10} photons / μm^2, 300 eV and 50 fs FWHM pulse. (b) Dispersion corrections of atomic form factors for several configurations of carbon.

References

[1] A. Scherz et al., Nanoscale Imaging with Resonant Coherent X Rays: Extension of Multiple-Wavelength Anomalous Diffraction to Nonperiodic Structures, Phys. Rev. Lett. **101**, 076101 (2008).

[2] H. N. Chapman et al., Femtosecond diffractive imaging with a soft-X-ray free-electron laser, Nature Phys. **2**, 839 (2006).

[3] S.-K. Son, H. N. Chapman, and R. Santra, Multi-wavelength anomalous diffraction at high x-ray intensity, (submitted).

[4] S.-K. Son, L. Young, and R. Santra, Impact of hollow-atom formation on coherent x-ray scattering at high intensity, Phys. Rev. A **83**, 033402 (2011).