

# Multiwavelength anomalous diffraction at high x-ray intensity

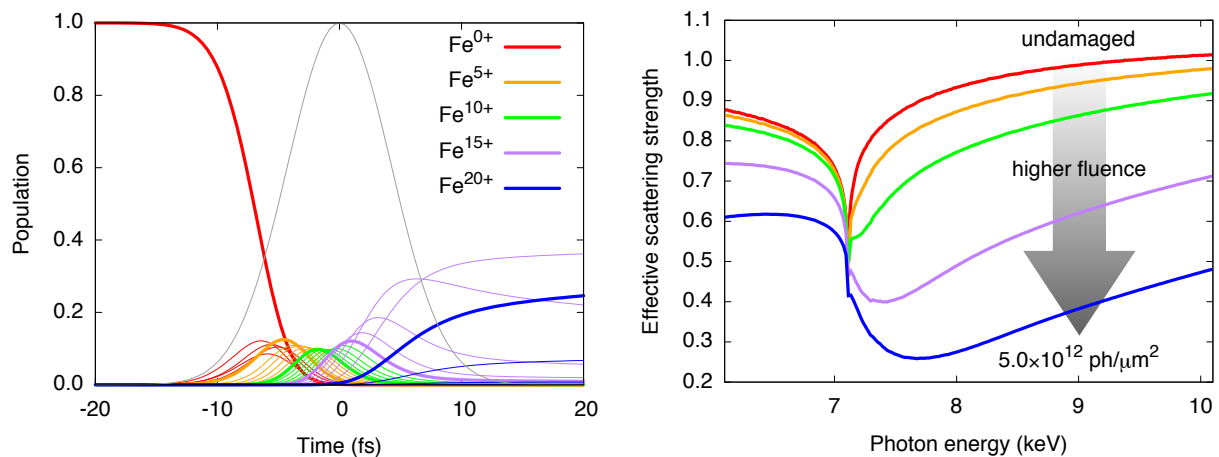
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The determination of the atomically resolved 3D structure of proteins is a central goal of structural biology. X-ray crystallography has been widely used for structural determination, but it suffers from two bottlenecks: the phase problem and growing high-quality crystals. The multiwavelength anomalous diffraction (MAD) method with synchrotron radiation is used to determine phase information by employing anomalous scattering from heavy atoms. X-ray free-electron lasers (XFELs) show promise for revealing molecular structure using nanocrystallography [1], but the associated phase problem remains largely unsolved. Because of the extremely high fluence of XFELs, samples experience severe and unavoidable electronic radiation damage, especially to heavy atoms, which hinders direct implementation of MAD with XFELs.

We propose a high-intensity version of the MAD phasing method [2]. Our work combines ultrafast electronic response at the atomic level and molecular imaging during intense x-ray pulses. We demonstrate the existence, in spite of the high degree of ionization, of a key equation for MAD. The XATOM toolkit [3] is used to calculate the relevant coefficients with detailed electronic damage dynamics as shown in the Figures. We discuss how the proposed method provides a new path to phasing in femtosecond x-ray nanocrystallography.



Figures: (Left) Population dynamics of Fe charge states during an ultrashort high-intensity x-ray pulse. (Right) Dramatic changes in effective scattering strength of Fe as the fluence is increased.

## References

- [1] H. N. Chapman *et al.*, Femtosecond X-ray protein nanocrystallography, *Nature* **470**, 73 (2011).
- [2] S.-K. Son, H. N. Chapman, and R. Santra, Multiwavelength anomalous diffraction at high x-ray intensity, *Phys. Rev. Lett.* **107**, 218102 (2011).
- [3] 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).