Multiwavelength anomalous diffraction at high x-ray intensity

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The multiwavelength anomalous diffraction (MAD) method is widely used in x-ray crystallography with synchrotron radiation to determine phase information by employing dispersion corrections from heavy atoms on coherent x-ray scattering. X-ray free-electron lasers (FELs) show promise for revealing the structure of single molecules or nanocrystals within femtoseconds, but the phase problem remains largely unsolved. Because of the extremely high fluence of FELs, samples experience severe and unavoidable electronic radiation damage, especially to heavy atoms, which hinders direct implementation of the MAD method with x-ray FELs.

We propose a generalized version of the MAD phasing method at high x-ray intensity [1]. We demonstrate the existence of a Karle–Hendrickson-type equation for the MAD method in the high-intensity regime and calculate relevant coefficients with electronic damage dynamics and accompanying changes of the dispersion correction. Here we present the XATOM toolkit [2] to simulate detailed electronic damage dynamics and discuss how the proposed method is applicable to the phase problem in femtosecond x-ray nanocrystallography.

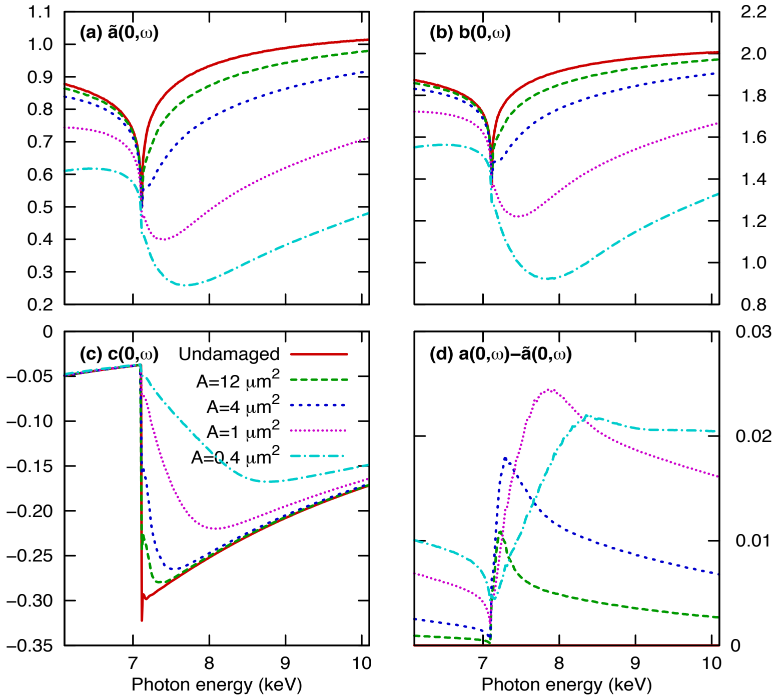

Figure 1: MAD coefficients for Fe as a function of the photon energy.
The fluence is given by $2{\times}10^{12}$ photons/*A*, where *A* is the focal spot area.

References

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