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Ultrafast X-ray fluorescence for Serial Femtosecond Crystallography and Incoherent Diffractive Imaging

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Coherent diffractive imaging with X-ray lasers opened a bright avenue for determining atomic structure of biomolecules. It uses ultrashort and intense X-ray pulses to take snapshot pictures of biological samples, single particles or protein crystals, before these turn into a plasma due to the extreme radiation dose, aka *diffraction before destruction.* During destruction the atoms will ionize and emit X-ray fluorescence and this fluorescence can be used to gain further information. In Serial Femtosecond Crystallography (SFX), it can be used to quickly determine successful crystal hits and mitigate a high-rate diffractive data deluge expected at the coming high-repetition X-ray Free-Electron Lasers. X-ray emission may also be used to gain further structural information, through a novel method called Incoherent Diffractive Imaging (IDI) that measure correlation of fluorescent photons from transient metals. Here we study X-ray fluorescence in a plasma environment driven by ultrafast X-ray pulses. We simulate X-ray lasers interacting with biological materials and study the feasibility for hit-finding of protein crystals in SFX experiments, as well as the requirements for a successful IDI experiment.

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