Potential Implications of Time-resolved Diffuse Scattering Measurements

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The departure of a crystal structure from perfect periodicity gives rise to diffuse or non-Bragg scattering, which is normally measured as an average both over time and over the illuminated crystal volume. Diffuse scattering contains enormous amounts of information. For example, for typical protein crystal more than half the photons are scattered outside the Bragg peaks at resolutions of 3 Å or higher. However, extracting this information has proved to be a formidable problem, with difficulties both in inverting the patterns, and in establishing uniqueness. The advent of x-ray lasers provides a potential pathway for undoing the spatial and temporal averages in normal diffuse scattering measurements, and thus for sharpening our ability to extract useful information. Imagine illuminating a small crystalline volume with a coherent, femtosecond x-ray pulse. The resulting diffraction pattern will have no temporal averaging because atomic motion is frozen on this short timescale. It will have no spatial averaging because the coherence of the beam means that every atom in the illuminated volume is scattering coherently, so that we are seeing scattering from a fully asymmetric object. In such an experiment the distinction between Bragg and non-Bragg scattering disappears. The entire scattering pattern observed in such an experiment has a defined phase, which is anchored by the phase of the diffraction pattern at the Bragg peaks. In principle, the full scattering pattern, Bragg and non-Bragg alike, can be calculated by using the structure factor equation for all the atoms in the illuminated volume, and not just for those atoms in a single unit cell.

Obviously grave experimental difficulties lie in the path of measuring and phasing this pattern. Yet, much less than a fully phased pattern might still be very useful. The talk will leave time for beginning a dialogue about how this topic might be further explored. For example, do time-resolved patterns actually look different from time-averaged ones?