Poster

Spherical Crystals: Laser Shaping of Biological and Chemical Materials

Christian Orr

Diamond Light Source

christian.orr@diamond.ac.uk

For many experimental techniques, sample morphology is a critical factor for success. For example, in the case of low energy diffraction experiments, a spherical crystal can mitigate and potentially remove the need for absorption corrections of the diffracted X-rays [1]. We have developed a laser system to shape crystals or other materials into spheres (Figure 1), or any shape required to optimise samples under both cryogenic conditions and at room temperature.

A previously described system to shape protein crystals utilises a deep UV laser, relying on the absorption of the peptide bonds in proteins to cut samples [2]. Our system utilises non-linear optical effects with a femtosecond laser to ablate material, removing the laser wavelength and material dependence. We demonstrate that damage to the surrounding material from the footprint of the laser does not impair diffraction quality.

Using data collected from shaped protein crystals, we can significantly boost the anomalous signal obtained from diffraction experiments in comparison to non-shaped crystals. This can aid in phasing experiments for difficult cases and allow anomalous difference Fourier map generation for localisation and identification of light elements in crystal structures, including Na (Figure 2) and Mg [3].

We also predict that this technique can be used to increase the signal to noise ratio of reflections for standard data collections. This can be especially useful for crystals with large unit cells, where the overall intensity is distributed among a high number of reflections [4]. By removing surrounding solvent, loop and ice from the crystal, scatter from these constituents is eliminated, resulting in reduced background from non-crystal sources on the detector. When coupled with the in-vacuum end station at beamline I23 at Diamond Light Source, the resulting signal to noise ratio can be significantly improved.

In the field of chemical crystallography, strong sample absorption often deteriorates data quality. Our laser shaping technique offers a solution to alleviate these effects by minimising the absorption correction required. Additionally, high-resolution imaging techniques can profit from precisely sized and shaped samples. Initial experiments have proven effective, enabling the generation of bespoke sample geometries, such as 20 um cylinders for X-ray ptychography.