Aligned Protein-Beam Diffraction

Spence J.C.H., Doak B., Schmidt K., Weierstall U., Starodub D., Wu J., Hembree G., Howells M.*, Shapiro D.**, Chapman H.***

Physics, Arizona State University, Tempe Az. 85287 USA., Email: spence asu.edu, *Lawrence Berkeley Lab, Berkeley, Ca. 94720 USA, **CBST, UC Davis, Sacramento, Ca 95817 USA.

Apparatus is under construction at ASU physics (electrons) and at the Advanced Light Source in Berkeley (X-rays) to obtain diffraction patterns from a single-file submicron liquid droplet stream. The aim is to solve proteins which cannot be crystallized, and help understand protein folding. Each water droplet contains, on average, one protein. The droplets freeze by evaporative cooling to from a vitreous ice jacket. The molecules are aligned by a 100 watt CW fiber laser - induced polarization generates a torque as for the laser-wrench, which depends only on the RMS value of the CW laser intensity. Each molecule receives much less than the critical damage dose during its transit across the Xray beam, but many doped droplets fall within the beam at any instant. All three beams, laser, X-rays and droplets, run continuously, and diffraction data is aquired continuously until adequate signal-to-noise is achieved. The laser polarization is then rotated into a new orientation using a quarter-wave plate, allowing tomographic diffraction data collection for three-dimensional reconstruction. The phase problem is solved by iterative Gerchberg-Saxton-Fienup methods to about 0.7nm resolution. The requirements of laser power and droplet temperature needed to achieve sub-nanometer resolution and so observe the secondary structure of proteins will be described in detail, together with damping and thermal fluctuation limits. Experimental images of our monodispersed Rayleigh droplet beam will be shown, together with the layout of the X-ray water jet diffraction camera. The project is described in detail elsewhere [1]. Supported by NSF funding.

Reference

 J.C.H.Spence, K. Schmidt, J. Wu, G. Hembree, U. Weierstall, B. Doak, P. Fromme. Acta Cryst A61, p. 237 (2005).