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Abstract for an Invited Paper
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Serial Crystallography¹

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To solve proteins which cannot be crystallized we have devised an aerodynamic focussing, monodispered droplet beam, which runs in single file across a synchrotron X-ray beam (LBNL Advanced Light Source) as it freezes in vacuum. The aim is to obtain a charge-density map of the protein at 0.7nm resolution, sufficient to locate alpha-helices. Water is removed before the proteins, coated by a thin ice-jacket, are aligned by the dipole moment induced by a 100 W NIR polarized fiber laser. All three orthogonal beams (proteins, X-rays, laser) intersect in a 10 micron diameter volume, and run continuously without synchronization. Elliptical polarization aligns molecular axes in direction but not sense. Data is collected continuously until adequate statistics are achieved before rotating the polarization to a new orientation. Details of the adiabatic laser-alignment and damping processes will be given. Misalignment is shown to be proportional to temperature and inversely to laser power and molecular volume. Polarizability tensor calculations for proteins will be discussed. Preliminary X-ray results (without laser) will be shown. Iterative methods for solving the phase problem will be demonstrated using experimental soft X-ray diffraction patterns from non-crystalline particles. Detailed simulations of the continuous diffraction patterns from a moving stream of partially aligned large hydrated molecules will be shown, and inverted to density maps using the Fienup-Gerchberg-Saxton algorithm. From this the exposure time and resolution may be estimated for tomographic reconstruction. Experimental comparisons of Rayleigh, electrospray and aerodynamic focussing droplet beam sources will also be described. The research team includes B.Doak, U. Weierstall, D. Shapiro (LBNL), D. Deponte, P. Fromme, D. Starodub, G. Hembree and H. Chapman (LLNL).

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