Oral Contributions

[MS10-05] The Long-wavelength Macromolecular Crystallography Beamline at Diamond Light Source

Ramona Duman, Vitaliy Mykhaylyk and Armin Wagner

Beamline I23 at Diamond Light Source will be the first dedicated beamline for long-wavelength phasing experiments from macromolecular crystals. It is currently under construction and scheduled to receive its first users early 2014. By exploiting the weak anomalous differences from sulfur or phosphorous present in proteins or RNA/DNA molecules the crystallographic phase problem can be experimentally solved by anomalous diffraction methods based on their intrinsic signal without labelling the crystals with additional anomalous scatterers. Additionally, anomalous contrast can be used to unambiguously identify biologically important ions such as Ca^{2+}, K+ or Cl^{-}. The beamline will operate in a core wavelength range from 1.5 to 4 Å, offering a complementary setup to the suite of already five existing MX beamlines at Diamond. To minimize absorption effects, the complete beamline including sample, goniometer and detector will be operated in vacuum (10^{-6} mbar). Cooling is realized by a conductive path from a pulse tube cryo-cooler through the kappa goniometer to the sample. A large curved Pilatus 12M detector will allow access to diffraction data up to 2theta = ±90º. To enable analytical absorption correction, an X-ray tomography setup will be integrated into the experimental end station to determine the crystal shape and size. The challenges of in-vacuum long-wavelength macromolecular crystallography and the opportunities by extending the wavelength range towards the sulfur and phosphorous K absorption edges will be discussed and an overview on the current status of the project will be given.

Keywords: anomalous diffraction, macromolecular crystallography, synchrotron X-ray instrumentation