

MS1-O2 The long-wavelength
macromolecular crystallography beamline
I23 at Diamond Light Source

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The Long-Wavelength MX Beamline I23 at Diamond Light Source will be the first dedicated beamline for long-wavelength phasing experiments from macromolecular crystals. By exploiting the weak anomalous differences from sulfur or phosphorus 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 labeling the crystals with additional anomalous scatterers. Additionally, anomalous contrast can be used to unambiguously identify biologically important ions such as Ca²⁺, K⁺ or Cl⁻. The beamline operates 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 and scattering effects, the complete beamline including sample, goniometer and detector is operated in vacuum. A large curved Pilatus 12M detector allows access to diffraction data up to $2\theta = \pm 100^\circ$. Sample cooling is realized by a conductive path from a pulse tube cryo-cooler through the kappa goniometer.

The challenges of in-vacuum long-wavelength macromolecular crystallography and the opportunities by extending the wavelength range towards the sulfur and phosphorus K-absorption edges will be discussed and first results from the beamline will be presented.

Keywords: long-wavelength crystallography, native SAD, synchrotron beamline

MS1-O3 *In vacuo* X-ray data collection
from graphene-wrapped protein crystals

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The focus in macromolecular crystallography is moving towards more challenging target proteins, often leading to smaller crystals and more challenging data collection conditions. Sources of X-ray background start to become more of an issue with a decrease in crystal volume as this is accompanied by a reduction in diffraction intensity. One method of reducing X-ray background is to place samples in an evacuated environment; however crystals are prone to dehydration. A series of experiments have been run on test crystals in which it has been possible to collect room temperature data on graphene-wrapped crystals in a rough vacuum. Further tests were also carried out on graphene-wrapped crystals exposed to different relative humidities and to a chemically harsh environment to confirm the effectiveness of graphene as a protective layer against dehydration.

Keywords: graphene, crystal mounting, microcrystallography