

Detection of protein crystals frozen in loop-shape holders

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With an increasing use of modern robotics equipment, macromolecular crystallography is now aiming at a full-fledged software and hardware pipeline from protein samples to their atomic models. The fully automated data collection at synchrotron beamline is a key component of such a pipeline. Since a crystal, typically flash-frozen in a loop, is mounted onto a beamline goniostat, one of the important tasks is to automatically centre the crystal with respect to the beam. This has already been addressed by, e.g. Karain *et al.* (2002) and Philippe *et al.*, (2004) with the use of optical and X-ray (scattering and fluorescence) techniques, edge detection as well as sophisticated image processing. In both approaches the loop holding a crystal is first looked for. Here we present a computational approach for automatic detection of a crystal in a loop using image-processing techniques with an emphasis on the use of algorithms related to crystal structure determination. No prior knowledge about the size, location and orientation of the loop or the crystal is needed. The centre of the crystal can be accurately detected with either visible or ultra violet illuminating light and with the presence of background noise. Two complementary algorithms have been designed: MoRCI (Molecular Replacement in Crystal Imaging) and FuChi (Fuzzy Categorisation of image Histogram). The first algorithm resembles a 2-dimensional analogue of molecular replacement in crystallography. In the current implementation a circular object (rolling disk) with variable radius is matched to the image so that the rotational component vanishes. The translation function becomes equivalent to an evaluation of a local variance that is efficiently implemented in reciprocal space (e.g. Terwilliger, 1999). The latter algorithm uses the fuzziness of the image gray levels that is achieved through an activation function. For images that contain light reflections and occlusions it has a higher performance. Application of the detection algorithms for crystals with different morphology will be discussed and the implementation of the software for high-throughput data collection will be presented.

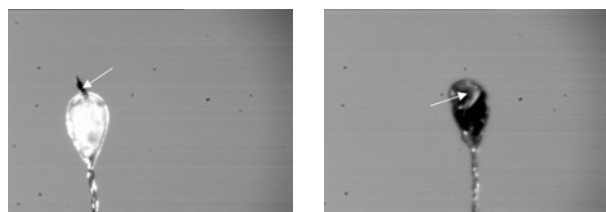


Figure: Examples of crystal detection in the loops

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