

**MS4-P3** Experimental phase determination of the structure factorGyula Faigel<sup>1</sup>, Gabor Bortel<sup>1</sup>, Miklos Tegze<sup>1</sup>

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Structure determination of crystalline substances is mostly done by x-ray diffraction. In these experiments an almost parallel probe beam is scattered by the sample, which is rotated to many orientations to fulfill Bragg condition and to measure enough reflections. This arrangement makes the study of time dependent structural changes, and experiments at non-ambient conditions very difficult, especially in the short time scale. In addition, in these traditional diffraction experiments the phase of the scattered wave is lost, which makes structure solution non trivial. These difficulties could be overcome by using point like inside x-ray sources within the sample. In this case a so called Kossel line pattern is formed [1]. Theoretical description of this pattern was worked out by Max von Laue [2]. Later, more detailed studies showed that not only the position and magnitude of Bragg reflections, but also their phase can be determined by measuring the fine structure of Kossel lines [3,4].

Although this was known for a long time, experimental realization of measuring the fine structure of several lines in parallel has not been presented. In this work we demonstrate experimentally for GaAs that phases can be directly determined from the profile of the Kossel lines [5,6]. These measurements are interesting not only theoretically, but they would facilitate structure solution of samples within extreme conditions, such as high pressure, high and low temperatures, high magnetic fields and extremely short times. The parallel measurement of many diffraction lines on a stationary sample will allow a more efficient use of the new generation of x-ray sources the X-ray free electron lasers (XFELs).

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**MS4-P4** BioMEX Solutions: An expert facility for structure solution in macromolecular X-ray crystallographyRonan Keegan<sup>1</sup>, Karen McIntyre<sup>1</sup>, Eugene Krissinel<sup>1</sup>

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Macromolecular crystallography is an indispensable tool for researchers in many different fields of science. Much effort has been put into automating the procedure but more often than not the structure solution process requires manual effort and some degree of experience with the software techniques. Even with manual intervention, the process of eliciting a structural model from a set of X-ray images can be far from trivial. Problems such as twinning, pseudo symmetry and anisotropic data can all complicate the procedure and often frustrate the efforts of the researcher.

In sharp contrast to the situation 10-15 years ago, most structural biologists consider crystallography as a black-box tool designed to produce the structural information required for an understanding of the biological process being studied. However, solving a structure can take several months of valuable research time if the quality of the X-ray data is not sufficient for straightforward computational protocols. In such cases, structure solution becomes a burdensome routine, consuming effort to the disadvantage of project's main goals. BioMEX Solutions is a new service being established in the UK by the Science and Technology Facilities Council. It is designed to act like a facility giving access to a network of experts with many years of experience working with difficult X-ray data sets and a depth of knowledge that is hard to find elsewhere.

BioMEX offers a range of services from the initial data processing to structure completion and analysis/validation. There are many benefits to using our service and it optimizes the chances of successfully deciphering a solution from the X-ray data. Our experts have the skills to produce the best model that the data will allow for and in the quickest possible time. It frees up the valuable time of research staff to concentrate on the more important questions that the structural information is being used for. All of the processing done by our experts is documented and provided to the user in a form suitable for writing a publication or report, and may also be treated as a useful educational resource.

**Keywords:** Structure solution, data processing, phasing, refinement