

ENHANCED TRIPLE-PHASE MEASUREMENTS AT $\pi/2$ SCATTERING GEOMETRY

S. Morelhao¹ S. Kycia²

¹Instituto de Física, Univ. de Sao Paulo, CP 66318, 05315-970 Sao Paulo, SP, Brazil ²Laboratorio Nacional de Luz Sincrotron/LNLS, CP 6192, 13084-971 Campinas, SP, Brazil

Physical determination of the reflection phases is a fundamental problem in X-ray crystallography. It is well known that the n-beam diffraction (n-BD) phenomenon can provide a direct solution for the 'phase problem', however, the phases extracted by the actual n-BD phasing techniques are not very precise, mainly due to the uncertainties on the kinematical diffraction present in the process. In this work, we present a simple and innovating mathematical expression -based on the second-order Born approximation- for 3-BD profile simulation, which is capable of dealing with a mixed dynamical/kinematical diffraction regime. By using the linear polarization of synchrotron radiation, a new procedure of X-ray data collection is employed to generate a polarization dependent dataset of 3-BD profiles. The fit of the dataset with the mathematical expression above mentioned has allowed triple-phase measurements with a precision better than 2° as the amount of kinematical diffraction is also determined. Examples are given for several single crystals. The effects of the incident beam divergences and energy resolution on the precision of this phasing technique is discussed as well as its efficiency for practical applications.

Keywords: SYNCHROTRON RADIATION REFLECTION PHASES DIFFRACTION

NEW ALGORITHM TO DEDUCE INDIVIDUAL STRUCTURE-FACTOR PHASES BY REFERENCE-BEAM DIFFRACTION

Q. Shen¹ J. Wang²

Cornell University Chess Department Wilson Laboratory ITHACA NEW YORK 14853 USA

By incorporating phase-sensitive three-beam interference into an oscillating-crystal setup, reference-beam diffraction (RBD) technique allows parallel measurements of a large number of triplet-phases in a crystallography experiment. In order to solve the crystal structure, however, individual structure-factor phases are needed from the measured triplet-phases. We show that due to a unique pattern of triplet-combinations in the RBD geometry, it is possible to deduce the individual structure-factor phases from a single RBD data set involving only one reference reflection. A complete algorithm based on this principle has been developed and applied to a triplet-phase data set measured on a tetragonal lysozyme crystal. We show that the method can be useful for phasing macromolecular crystal structures using only the measured triplet-phases from a RBD experiment.

Keywords: PHASE PROBLEM REFERENCE BEAM DIFFRACTION DIRECT METHOD

PHASE PROBLEM IN CRYSTALLOGRAPHY AS THE ANGULAR MOMENTUM EIGENVALUE PROBLEM

P. Bhanumoorthy

Purdue University Department of Biological Sciences Room#B202, LILLY WEST LAFAYETTE INDIANA 47907 USA

The quantum theoretic solution to crystallographic phase problem in which the dynamics of the crystal is described by Schrodinger wave equation is presented. The term 'space quantization' is used in Stern-Gerlach experiment due to the discrete directions in space the intrinsic magnetic moment vector can assume. The discrete nature of diffraction pattern is the proof for similar space quantization of orbital magnetic moment vector. The phase problem in crystallography is realized as angular momentum eigenvalue problem in quantum mechanics. A relation for diffraction pattern ($2\pi r \sin\theta = m\lambda$, where m is the magnetic quantum number), similar to Bragg's law, is derived in terms of atomic radius as the direct consequence of quantization of total orbital angular momentum. The diffraction pattern as a function of unit cell dimensions manifests as the direct consequence of constraints on propagation vector in box normalization of electron density wavefunction. The expansion of electron density wavefunction in terms of spherical harmonics in accord with Fuchian algebra as applied to wave equation provides a means of direct phase determination through Condon-Shortley phase. The advantages of Schrodinger wave equation as the equation of motion for the crystal in the viewpoint of phase problem will be described. The need for the inclusion of isobaric spin as a new degree of freedom i.e., charge conjugation of electron under reflection to restore Friedel's law and thus the Extended Euclidean principle of relativity of quantum dynamics will be discussed. Such a representation only can ensure the conservation of probability and thus a non-subjective abstract phase solution for macromolecular crystallography.

Keywords: QUANTUM CRYSTALLOGRAPHY, QUANTIZATION OF ORBITAL ANGULAR MOMENTUM, EXTENDED EUCLIDEAN PRINCIPLE OF RELATIVITY

INTEGRATING DIRECT METHODS INTO A SEMI-AUTOMATED, PROTEIN-PHASING PACKAGE

C. M. Weeks¹ R. H. Blessing¹ R. Miller^{1,2} R. Mungee¹ S. A. Potter¹ J. Rappleye² G. D. Smith³ H. Xu¹ W. Furey^{4,5}

¹Hauptman-Woodward Institute & Dept. of Structural Biol., SUNY at Buffalo, 73 High Street, Buffalo, NY 14203, USA ²Center for Computational Research, Norton Hall Rm. 9, SUNY at Buffalo, Buffalo, NY 14260, USA ³Structural Biol. & Biochem., Hospital for Sick Children, 555 University Avenue, Toronto M5G 1X8, Ontario, Canada ⁴Biocrystallography Lab., VA Medical Center, University Drive C, Pittsburgh, PA 15240, USA ⁵Dept. of Pharmacology, University of Pittsburgh, Pittsburgh, PA 15261, USA

The dual-space direct-methods program SnB provides an efficient means for solving protein substructures containing many heavy-atom sites (current record: 160). In order to meet the high throughput requirements of structural genomics projects, substructure determination needs to be tightly integrated with other aspects of the protein-phasing process. This has been accomplished through the design of a common Java interface, BnP, for SnB and the PHASES program suite. BnP facilitates inter-program communication, and it creates scripts for executing the components of PHASES required to proceed from heavy-atom positions through substructure refinement, protein phasing, and solvent flattening to a skeleton and map ready for examination using O. The user can choose between two operating modes that differ in the degree of automation provided. A new scoring criterion based on the improvement in the minimal function and crystallographic R values during the course of SnB phase refinement permits automated detection of most substructure solutions. Selection of the correct heavy-atom sites is facilitated by a trial-structure comparison option that identifies sites present in multiple independent solutions. In all cases examined so far (SeMet MAD data), the correct hand could be determined automatically prior to substructure refinement in PHASES. A beta version of the BnP package is available from <http://www.hwi.buffalo.edu/bnP/>.

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