P02.02.06

Acta Cryst. (2008). A**64**, C202

Direct space and simultaneous direct-reciprocal space optimization models for phasing structures

Alexander B. Smith[1], Nikolaos V. Sahinidis[2]
[1]University of Illinois at Urbana-Champaign, Chemical and Biomolecular Engineering, 620 Whitney Ave, Pittsburgh, PA, 15221, USA, [2]Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh, PA, 15213, USA, E-mail：absmith2@uiuc.edu

The phase problem has recently been approached via combinatorial optimization techniques and the resulting Sieve method has been demonstrated to be effective for phasing centrosymmetric structures [1]. The purpose of the current work is to develop a more robust model for accurate phasing in the presence of odd triplets, and more important, to provide a combinatorial optimization approach to phasing non-centrosymmetric crystals. Two mixed-integer linear programming models for phasing are proposed; both of which include the introduction of specific direct space constraints with one additionally operating in reciprocal space. Direct space is constrained through sampling of electron density on a grid. Structure factors are calculated at these points in terms of the integer variables, which describe the phases. Bounds are then formulated using experimental data. Computational results are presented for a variety of structures.
References
[1] A. B. Smith, H. Xu, and N. V. Sahinidis. An integer minimal principle and triplet sieve method for phasing centrosymmetric structures. Acta Crystallographica A, 63(2):164 − 171, 2007.

Keywords: phasing methods, algorithms, direct methods

P02.02.07

Acta Cryst. (2008). A**64**, C202

Macromolecular structure solution by charge flipping

Arie Van Der Lee[1], Christian Dumas[2]
[1]Institut Europeen des Membranes, cc047 Universite de Montpellier II, Montpellier, Herault, 34000, France, [2]Centre de Biochimie Structurale, CNRS UMR5048, INSERM U554, F-34090 Montpellier, France, E-mail：avderlee@univ-montp2.fr

The solution of the crystallographic phase problem continues to be a challenge for the development of new and robust approaches. The recently discovered charge flipping phasing algorithm has received a growing interest in small-molecule crystallography and powder diffraction. This computational methodology radically differs from the classical direct methods as it neither requires a priori knowledge of space-group symmetry nor chemical composition and does not rely on probabilistic phase relations or a statistical framework. We show here that the charge flipping algorithm is capable to solve ab initio large macromolecular structures, up to ~4,000 atoms in the asymmetric unit, using suitable normalized intensity data at atomic resolution (1.1 Å or better). Moreover, we demonstrate that this algorithm also provides a very efficient tool for the determination of complex anomalously-scattering heavy-atom substructures at medium to low resolution (down to 5 Å). With the present extension to macromolecular crystallography charge flipping proves to be a very performing and general phase recovery algorithm in all fields of kinematical diffraction.

Keywords: charge flipping, macromolecular structure determination, sub-structure determination

P02.02.08

Acta Cryst. (2008). A**64**, C202

Direct observation of structural phase in CBED patterns - applications to structure determination

Joanne Etheridge, Philip N Nakashima, Alexander F Moodie
Monash University, Monash Centre for Electron Microscopy, Monash Centre for Electron Microscopy, Monash University, Victoria, 3800, Australia, E-mail：joanne.etheridge@mcem.monash.edu.au

It has been shown that the signs of three-phase invariants of a centrosymmetric structure can be observed directly by inspection of 3-beam convergent beam electron diffraction (CBED) patterns [1-5]. This ability to read-off phases directly and quickly from diffraction patterns suggests a new approach to the determination of structures that begins with knowledge of structure factor phases, rather than magnitudes. As demonstrated by Lonsdale [6], almost 80 years ago, knowledge of structure factor phases alone can be sufficient to determine outline structures. However, the difficulty in measuring phase has traditionally meant that structure determinations start from a knowledge of measured magnitudes, not phases. In this paper, we demonstrate practically how the signs of three-phase invariants can be observed directly from 3 beam CBED patterns using corundum as an example. (We will also describe how the corresponding structure factor magnitudes can be determined from the measurement of distances in the same 3 beam patterns.) We demonstrate how these observations of three-phase invariants alone can be applied using Lonsdale's simple, powerful and unambiguous approach to structure solution [6], to determine an outline of the structure of corundum.
[1] J. Gjonnes and R. Hoier A25 (1969) 595.
[2] A.F. Moodie, Chem. Scripta 14 (1978-79), 21
[3] A.F. Moodie, J. Etheridge and C.J. Humphreys, Acta Cryst. A52 (1996), 596.
[4] P.N.H. Nakashima, A.F. Moodie and J. Etheridge, Acta Cryst. A63 (2007), 387.
[5] P.N.H. Nakashima, A.F. Moodie and J. Etheridge, Ultramicroscopy (2008), in press.
[6] K. Lonsdale, Proc. R. Soc. 123A (1929), 494.
[7] The authors thank the Australian Research Council (ARC DP0346828).

Keywords: phase problem, structure solution, electron diffraction

P02.04.09

Acta Cryst. (2008). A**64**, C202−203

Studies for S-SAD method using various wavelength at SPring-8 and SAGA-LS

Masahide Kawamoto[1], Nobutaka Shimizu[2,3], Seiki Baba[2], Kunio Hirata[3], Koutaro Ishiji[1], Kazushi Sumitani[1], Toshihiro Okajima[1], Hiroyuki Motoshima[4], Keiichi Watanabe[4], Takashi Kumasaka[2,3], Masaki Yamamoto[3]
[1]Kyushu Synchrotron Light Research Center, Beamline Group, 8-7 Yayoigaoka, Tosu-shi, Saga, 841-0005, Japan, [2]Japan Synchrotron Radiation Research Institute, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan, [3]RIKEN SPring-8 Center, Harima Institute, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5198, Japan, [4]Department of Applied Biochemistry and Food Science, Faculty of Agriculture, Saga University, 1 Honjo-machi, Saga-city, Saga 840-8502, Japan, E-mail：kawamoto@saga-ls.jp

Single-wavelength anomalous dispersion (SAD) method using sulfur atoms as an anomalous dispersion atom (S-SAD) is a powerful tool for the phase determination in protein crystallography. There are two