

FA4-MS12-P06**Improving the S-FFT Algorithm for Positive and Negative Density-function Peaks.**

Jordi Rius^a, Carles Frontera^a. ^a*Institut de Ciència de Materials de Barcelona (CSIC), Campus de la UAB, 08193-Bellaterra, Catalunya, Spain.*

E-mail: jordi.rius@icmab.es

Some years ago the direct-methods origin-free modulus sum function (S) [1] was adapted to the processing of intensity data from density functions with positive and negative peaks [2]. That implementation used phase relationships explicitly. Although successfully applied to different situations where the number of reflections was small, its generalization to larger problems required avoiding the time-consuming manipulation of quartet terms. To circumvent this limitation, a modification of the more recent S-FFT algorithm [3] (that maximizes S with only Fourier transforms) was investigated. The resulting S₂-FFT algorithm proved highly effective for crystal structures with positive and negative scatterers in the presence of at least one moderate scatterer in the unit cell [4]. To increase its versatility, the S-FFT algorithm has been adapted now to density functions formed exclusively by positive and negative peaks of similar strength. The results are very promising and some examples describing different situations are analysed in detail.

[1] Rius, J., *Acta Cryst. A*, **1993**, 49, 406. [2] Rius, J.; Miravittles; C.; Allmann, R., *Acta Cryst. A*, **1996**, 52, 634. [3] Rius, J.; Crespi, A.; Torrelles, X., *Acta Cryst. A*, **2007**, 63, 131. [4] Rius, J.; Frontera, C., *Acta Cryst. A*, **2008**, 64, 670.

Keywords: direct methods; phase refinement method; ab-initio structure determination

FA4-MS12-P07**New Modelling for Disordered Atoms in Free-form Based Hybrid Refinement and Visual Representation.**

Mustapha Sadki. *Inorganic Chemistry Department, University of Oxford, OX1 3QR, UK.*

E-mail: mustapha.sadki@chem.ox.ac.uk

The number of structures flagged in the CSD as disordered has doubled over the last 25 years, so that the treatment of disorder has become a significant hindrance to fully automatic structure determination.

In a disordered structure, the classical partially occupied anisotropic displacement parameter model is not always appropriate [1]. A new treatment has been devised which integrates a free-form refinement of the disorder together with traditional refinement of other parameters. The method optimises and illustrates the free-form, as well as quantifies and refines related parameters.

We investigate a free form disorder refinement method to optimally combine classic refinement with an iterative process between object and diffraction pattern, overwriting known information in each space.

To optimise the region of interest (ROI) boundaries (in our case, a disordered region), the ROI is modelled after each

iteration as a free form with *deformable models*, where a surface is defined within the density domain, able to move under the influence of internal forces coming from within the model itself and external forces computed from the density values. We use the *gradient vector flow* (GVF) field [2] for the external force, computed as a diffusion of the gradient vectors of a density-value. The GVF was preferred to other forces because of its large capture range and its ability to move a deformable model into boundary concavities.

Given the results obtained from a classic refinement which indicated a potential disorder, the initial free-form configuration is defined within the ROI, in the real space where the optimisation process of a deformable model will operate. Thus the main loop of the refinement process consists of two parts of residuals: one computed as known with all non-disordered sites; the other using the structure factors, obtained by inverse- transform of the optimised ROI. Other parts can be included as usual, such as restraints. The resulting refined parameters and phases produce a new density which when added to the current ROI define a domain where a new ROI optimisation operates. At the final iteration, the refined form represented as *2-simplex meshes* is then visualised, jointly with the refined non-disordered sites, using a volumetric visualisation method, instead of a surfacic one based on iso-surface.

We will discuss how this method leads to improved parameter estimates and a more favourable and comprehensive 3D representation. Notwithstanding, a new specification for a CIF file is required to support the free-form representation.

[1] P. v. d. Sluis and A. L. Spek. BYPASS, **1990**, *Acta Cryst. A* 46, 194-201. [2] C. Xu and J. L. Prince. Snakes, shapes, and gradient vector flow. *IEEE Trans. on Image, Processing*, 7(3):359-369, March **1998**.

Keywords: refinement disorder; computational modelling methods; computational crystallography

FA4-MS12-P08**Olex2: Workflow and User Experience.**

Horst Puschmann^a, Luc Bourhis^a, Richard Gildea^a, Oleg Dolomanov^a. ^a*Department of Chemistry, Durham University, Durham, UK.*

E-mail: horst.puschmann@durham.ac.uk

Olex2 [1] is an analysis and visualisation program for small-molecule crystal structures. It integrates seamlessly with the SHELX [2] package as well as our own cctbx/smtbx-based structure solution and refinement utilities [3,4]. All aspects of the structure determination and publication process are presented in a single, workflow-driven package – from structure solution, refinement and CIF preparation through to the final step of generating publication reports and tables.

While Olex2 combines a wide variety of sophisticated crystallographic tools (space-group determination, symmetry tools, charge-flipping structure solution, smtbx-based refinement routines, tools to deal with disorder efficiently, void calculation, electron density viewer, polyhedral volume calculation and many more), this presentation will focus on workflow aspect of this software: