MS30-05 **Facilities for Handling Twins in CRYSTALS.** Simon Parsons,[a] Richard I. Cooper,[b] *[a]EaStCHEM School of Chemistry and Centre for Science at Extreme Conditions, The University of Edinburgh, UK [b] Department of Chemistry, University of Oxford, UK*
E-mail: S.Parsons@ed.ac.uk

A twinned crystal is an aggregate in which different domains are joined together according to a specific symmetry operation, the twin law. The diffraction patterns derived from different domains are rotated, reflected or inverted with respect to one another, depending on the nature of the relationship between the different domains, and weighted according to the quantity of a particular domain present in the crystal.[1] The diffraction pattern measured during data collection is a superposition of all of these. Reflections from different domains may overlap and different refinement programs differ in the way this is specified. The aim of this talk is to describe how twins are handled in the refinement program CRYSTALS.[2]

In CRYSTALS the user provides up to nine twin law matrices, and each reflection carries a flag indicating which domains contribute to an intensity observation. This format can handle situations where all observations contain contributions from all domains (e.g. merohedral twins) or where only some reflections are affected by twinning (e.g. in non-merohedral twinning). If twinning has been taken into account during integration an HKLF5 format reflection file can be imported into the program. Once a set of twin laws has been defined domain scale factors can be refined with a constraint that their sum is equal to unity.

CRYSTALS also has a facility called ROTAX[3] which is able to assist in identification of twin laws. It is most useful for non-merohedral twins where only certain zones of data contain contributions from more than one domain. If the crystal structure is refined without taking twinning into account F_{calc} these reflections is systematically lower than F_{obs}. Matrices which transform the indices of these reflections to integers are possible twin laws.

CRYSTALS can be downloaded from: http://www.xtl.ox.ac.uk/tag/crystals-release.html

[1] Herbst-Irmer, R. & Sheldrick, G. M. (1998) *Acta Cryst.* **B54**, 443-449.
[2] Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003) *J. Appl. Cryst.* **36**, 1487.
[3] Cooper, R. I., Gould, R. O., Parsons, S. & Watkin, D. J. (2002) *J. Appl.Cryst.* **35**, 168-174.

Keywords: Twinning; Refinement; Software

MS31-01 **How to apply to the EC Framework Programs: Opportunities for young scientists .** S. García-Granda, [a] J. Álvarez, [b] Anne Hörlein, [c] *[a] Faculty of Chemistry, University Oviedo-CINN, Spain, [b]Cluster of Biomedicine and Health, University Oviedo, Spain, [c]European R&D Office, University Oviedo, Spain.*
E-mail: sgg@uniovi.es

The aim of this talk is to present a general overview of the opportunities offered by European Research Programs to young scientists for developing their scientific career, focused mainly on FP7 (Seventh Framework Program for Research and Technological Development). FP7,[1] is the EU's main instrument for funding research in Europe, running from 2007-2013. The last calls are envisaged for 2012-2013. This current Framework Program will be followed by HORIZON 2020, [2] covering the period 2014-2020. The European Crystallographic Association, as member of the Initiative for Science in Europe (ISE), is contributing to discuss and improve these European research initiatives.

FP7 is divided into 4 different programs: Cooperation, Ideas, People and Capacities. Each of these programs offer opportunities for young scientists, with specific calls addressed to young scientists under People and Ideas.

The characteristics of the different programs will be presented, together with a general overview of the strategic lines in Horizon 2020. Specific aspects of European research proposals will be addressed and hints for successful proposal preparation will be given.

Acknowledgements: We thank financial support from Spanish Ministerio de Economía y Competitividad (MAT2010-15094, MAT2006-01997, Factoría de Cristalización – Consolider Ingenio 2010) and FEDER.

[1] http://cordis.europa.eu/fp7/home_en.html
[2] http://ec.europa.eu/research/horizon2020/index_en.cfm?pg=home

Keywords: fp7, horizon 2020, young scientists