FA5-MS01-O1
Resolution Bias Correction in EXPO2009. Angela Altomare1, Corrado Cuocci1, Carmelo Giacovazzo2, Sabino Maggi3, Anna Moliterni3, Rosanna Rizzi3.
1CNR-Institute of Crystallography (IC), via Amendola 122o, Bari 70126, Italy. 2Dept. of Geomineralogy, University of Bari, via Orabona 4, Bari 70125, Italy. E-mail: angela.altomare@ic.cnr.it

Fourier syntheses providing electron density maps always show series-termination errors due to the limited experimental resolution. The worse the resolution, the worse the quality of the map: peaks are misplaced with respect to the true positions, positive and negative peaks occur, the peak profile is deformed. Two new algorithms have been developed aimed at reducing the resolution bias. The first one works in direct space [1,2], the second one in reciprocal space [3]. They are able to improve both peak positions and peak form in such a way that the map better fits the real atomic electron density. The new procedures have been introduced in EXPO2009, the strengthened and updated version of EXPO [4] and applied to the electron density maps provided by Direct Methods. Organic as well as metalorganic powder structures with non-rionic resolution experimental data have been tested. In spite of the difficulties in structure solution by powder data, the new approaches succeeded in several cases which could not be solved without the resolution bias correction. The theory of the resolution bias correction and its application by EXPO2009 will be presented.


Keywords: ab-initio powder structure determination; resolution; electronic density

FA5-MS01-O2
New Frontiers in Powder Diffraction Pattern Indexing: the Program N-TREOR09. Anna Moliterni2, Angela Altomare3, Gaetano Campi3, Corrado Cuocci3, Lars Eriksson3, Carmelo Giacovazzo2, Rosanna Rizzi3, Per-Erik Werner4. 1IC, Sede di Bari, via Amendola 122/o, 70126 Bari, Italy. 2Dipartimento Geomineralogico, Università di Bari, Campus Universitario, Via Orabona 4, 70125 Bari, Italy. 3Department of Structural Chemistry, Arrehnus Laboratory, University of Stockholm, S-106 91 Stockholm, Sweden. 4Laboratory of Crystallography, University of Geneva, Quai E.-Ansermet 24, CH-1211 Geneva, Switzerland. Email: annagrzia.moliterni@ic.cnr.it

Despite its long history and the recent advances in theoretical methods, computer speed and experimental devices, powder pattern indexing can still be a challenge. More plausible different unit cells are often suggested, among which the identification of the correct cell can be difficult. The cell reliability is generally assessed via historical figures of merit (i.e., $M_\infty$ by De Wolff [1] and $F_\infty$ by Smith & Snyder [2]) that sometimes fail. Usually the space group identification follows the indexing. We propose a new approach which simultaneously determines the unit cell and the extinction symbol by N-TREOR09 (the evolved version of the indexing package N-TREOR [3]). A new figure of merit has been also introduced in N-TREOR09. It has been proved to be more powerful than $M_\infty$ and combines the contribution by $M_\infty$ with additional parameters like the number of unindexed lines, the agreement between the calculated and observed profiles, the degree of overlap in the pattern, the symmetry suggested by the automatic evaluation of the extinction group. N-TREOR09 has been also enriched by an improved indexing procedure in the triclinic system and integrated into EXPO2009, the updated version of EXPO2004 [4]. The main features of N-TREOR09 and its applications to a large set of test structures will be described.


Keywords: powder indexing; space-group determination from powders; crystallographic computing

FA5-MS01-O3
Avarage and Local Structure of Laves Phase Deuterides YFe2Dx, Joanna Ropka4, Radovan Černý4, Valerie Paul-Boncour5, Michel Latroche6, Thomas Proffit. 4Laboratory of Crystallography, University of Geneva, quai E.-Ansermet 24, CH-1211 Geneva, Switzerland. 5CMTR, ICMPE, CNRS, 2 rue H. Dunant, 94320 Thiais Cedex, France. 6Lujan neutron Scattering Center, LANL, Los Alamos, NM 87545, USA. Email: Joanna.Ropka@unige.ch

Beetwen all cubic (C15) Laves phases, widely investigated for years, the YFe2Dx system is especially interesting because of its magnetic properties. The structure of particular YFe2Dx deuteride depends on deuterium content, likewise deuterium and magnetic ordering temperatures [1].

The most rich phase of this system under ambient condition - YFe2D1.42 - is formed as a cubic (Fd\bar{3}m) and monoclinic (Pc) above and below deuterium ordering temperature, respectively. The deuteriums in disordered (cubic) structure partially occupies 3 sites, while occupancies in fully ordered monoclinic structure equal to 1 for almost all of 18 deuterium sites. Deuterium atoms make polyhedras (1 tetrahedron, 7 trigonal bipyramids – fig.1) around iron with distances Fe-D between 1.62-1.83 Å. [2]