σ — standard deviance;
I_k – peaks intensuities with $I_k \geq 10 \cdot \sigma_k$
k — a number of peaks with intensities $I_k \geq 10 \cdot \sigma_k$
I_k' – a highest peak intensity;
w_k – weight, $w_k = 1/\sigma_k+1$

The second set of R-factors and goodness of fit are calcuated only for $|I_{obs}-I_{calc}|- \sigma_i$., i.e.,

$R'_1= \Sigma((| I_{obs}-I_{calc}|-\sigma)/I_{obs})/N$ $R'_{1w}= \Sigma w((| I_{obs}-I_{calc}|-\sigma)/I_{obs})/N$
$R'_2= (\Sigma((| I_{obs}-I_{calc}|-\sigma))/N)/(\Sigma I_k/k_h)$ $R'_{2w}= \Sigma(w(| I_{obs}-I_{calc}|-\sigma)/N)/(\Sigma w I_k/k_h)$
$R'_3= (\Sigma(| I_{obs}-I_{calc}|-\sigma))/N)/ I_k'$ $R'_{3w}= \Sigma(w(|I_{obs}-I_{calc}|-\sigma))/N)/(I_k'))$

Keywords: powder diffraction, Rietvld method, R-factors

FA5-MS44-P16

Multialiquot cell approach for the SDPD of high-symmetry compounds. O.A. Smirnova. *Institute for Chemical Research, Kyoto University, Uji, Kyoto-fu 611-0011, Japan.*

Recently mentioned [1] inconsistency of figures of merit [2,3] when indexing high symmetry lattices turned to a conclusion the smaller cells of lower symmetry can be applied as building units when solving a structure by direct space methods. The approach is expected to decrease time necessary for simulated annealing of one structure solution and may appear particularly useful for large organic structures. The poster illustrates the approach based of example compounds with a small pyrochlore structure. The indexing program suggest several possible solutions and the correct solution of highest symmetry among them. The repetition of the same lattice described by different cells should be considered as an indication of the correct indexing solution. From the other hand, that might be random and unfruitful indexing solution if the lattice is non-primitive but is not observed among proposed cells with its primitive representation. The extension to indexing algorithms, eliminating lower symmetry cells for the same lattice described by high-symmetry cell, and the corrected figures of merit taking into account the number of equal proposal cells might be drawn as follows:

$$M'(20) = M(20)_h \cdot N_{ep}$$
$$F'(20) = F(20)_h \cdot N_{ep}$$

where $M(20)_h$ and $F(20)_h$ are M(20) and F(20) for the ***h***ighest symmetry cell

N_{ep} is the number of ***e***qual ***p***roposal cells

Then, one may start to search for the structural model applying a cell of lower/volume symmetry providing it may represent a building unit for the larger cell of higher symmetry or may asssist to find a sublattice..

[1] O.A. Smirnova, in Abstracts, Denver X-ray conference 2009, Colorado Springs 2009, USA. [2] De Wolff, P.M., J. APPL. CRYST. 5, 108-113 (1968). [3] Smith, G. S. & Snyder, R. L., J. APPL. CRYST. 12, 60-65 (1979).

Keywords: powder diffraction, indexing, figures of merit

FA5-MS44-P17

***DDMSuite* – a powder diffraction full-profile analysis system.** Yaroslav I. Yakimov[a], Leonid A. Solovyov[b], Alexander N. Zaloga[a], Igor S. Yakimov[a]. [a]*Siberian Federal University, Krasnoyarsk, Russia.* [b]*Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia.* E-mail: yar_yakimov@mail.ru

In this presentation we describe a new freeware program package *DDMSuite* designed for crystal structure analysis from powder diffraction data. The program is based on the recently proposed derivative difference minimization (DDM) method of whole-profile fitting [1] as a background-independent alternative to the conventional Rietveld refinement procedure. In this method the refinement is aimed not at minimizing the absolute difference between the observed and calculated patterns, but at minimizing the oscillations (or curvature) of the difference curve. The difference curve is considered as an estimation of background which, in the absence of crystalline admixtures, usually varies much less rapidly along the powder profile than does the diffraction pattern. The main advantage of this method is that it does not involve background line modelling thus avoiding the background-related systematic errors and allowing structure refinement with higher stability and accuracy [2]. Newly developed software implementation *DDMSuite* is intended to provide a free comprehensive use of the DDM method by means of an easy-to-use graphical user interface (GUI). The program includes both DDM and Rietveld refinement procedures for X-ray and neutron powder diffraction data, profile decomposition routines, the quantitative phase analysis and the size-strain calculations. Great effort has been made to design a versatile tree-type phases/atoms hierarchy navigation. It gives convenient means for macro-editing parameters of multiple selected phases and atoms. A dedicated dialog allows controlling the refinement process facilitated by a number of graphical tools: structure 3D-view; powder pattern plot; Fourier and Patterson mapper. The GUI has interfaces to a number of widely used crystallographic software packages (Diamond, CCDC Mercury etc.) and CIF import-export routines. Applications to various types of powder diffraction data including semi-crystalline substances such as mesostructured materials and complicated multi-phase samples will be demonstrated. The program (to date, a Microsoft Windows version) can be freely downloaded from:
http://www.icct.ru/eng/content/persons/Sol_LA/ddm.html.

[1] Solovyov L.A., *J. Appl. Crystallogr.*, 2004, 37, 743. [2] Solovyov L.A., in *Powder Diffraction Theory and Practice,* ed. Dinnebier R.E., Billinge S.J.L., 2008, 282.

Keywords: powder diffraction software, full-profile refinement, derivative difference minimization

FA5-MS44-P18

On execution of Pawley method without requiring intensity constraints on overlapping reflections. R. Oishi-Tomiyasu[a], M. Yonemura[a], A. Hoshikawa[b], S. Torii[a], T. Ishigaki[b], T. Kamiyama[a]. [a]*High Energy Accelerator Research Organization, Tsukuba, Ibaraki, Japan.* [b]*Ibaraki University, Hitachi, Ibaraki, Japan.* E-mail: ryoko.tomiyasu@kek.jp

The Pawley method and the Le Bail method are two major methods for extraction of integrated intensities from powder diffraction patterns. The advantage of the Pawley method to the Le Bail method is that it can directly obtain the intensity covariance matrix. In both methods, it is considered to be necessary to group overlapping reflections and impose linear