Mater. Chem., **2007**, 17, 3696. [3] E. Fernández-Zapico, L. Roces, S. García-Granda, J.R. García, F. Liu, J. Rocha, *Acta Cryst.,* **2007**, A63, s183.

Financial support from Spanish Ministery of Science and Technology (MAT2006-01997 and 'Factoría de Cristalización' Consolider Ingenio 2010) and FEDER founding is acknowledged.

Keywords: lanthanides; phosphonates; singlecrystal; powder diffraction; structural characterization; rietveld

FA5-MS01-P09

Polytypism, Polymorphism and Compositional Faults in Layered Ternary and Quaternary Compounds. Mahmud Kyazumov[a], Lale Rustamova[a], Mahbub Kazimov[a]. [a]*Institute of Physics of the National Academy of Sciences of Azerbaijan, Baku, Azerbaijan.*
E-mail: elmira@physics.ab.az, el_max63@yahoo.com

It has been determined that on depend on various growth conditions in crystals and type of their synthesis the multicomponent layered crystals have a big variety of polytypic and polymorphic modifications. Not only separate crystal's bits taken from various places of the same ampoule may distinguish by their structures but many other polytypic phases can also exist in the same crystal. It is naturally that the presence of one phase on the basis of another one is connecting with packing defects of sulphur atoms and formation of cation's base of a new phase. Deficit of sulphur atoms as a rule is leading to change the cation's valency in crystals as a result of which the ionic radiūs of cations are also changed and element's base of a new phase is forming. An increase of octahedral (O) position's shares due to decrease of tetrahedral (T) ones in ÒÒÎÒÒE, ÒÎÒÒE, ÒÎÒE, ÒÎÒE2ÒÎÒE1ÎÎE1, ÒÎE, ÒÎÒEÎE, ÒÎÒE1ÎÎE1 types of structural units stimulates creation of such a phases. In these structures the shares of octahedral position in common tetrahedral and octahedral share's positions are as followed: 20%, 25%, 33%, 50%, 50%, 50%, 60%. In case when cations have a permanent valences a creation of a new phase becomes impossible and for packing defects of sulphur atoms only compositional faults are coming up.

Keywords: polytypism; polymorphism; layered compounds

FA5-MS01-P10

Two-Level Genetic Algorithm for Direct-Space Structure Solution and Refinement. Yaroslav I. Yakimov[a], Eugene S. Semenkin[a], Igor S. Yakimov[a]. [a]*Siberian Federal University, Krasnoyarsk, Russian Federation.*
E-mail: yar_yakimov@mail.ru

Genetic algorithms (GA) have been used to generate crystal structure models from the knowledge of only the unit cell and constituent elements by powder diffraction data in the direct space [1]. This work is dedicated to GA spread-out to Rietveld method including full-profile fitting and refinement of crystal structure models. A two-level genetic algorithm has been developed for this purpose. The two-level genetic algorithm is based on a combination of conventional GA similar to [2] with a new Rietveld-like derivative difference minimization (DDM) method [3]. First-level GA chromosomes comprise values of profile and structure parameters used in the Rietveld method. Since initial population is generated randomly, a priori known parameter values are not required. GA fitness function is based on the weighted profile R-factor of DDM (R_{DDM}). Second-level GA chromosomes are bit strings containing one bit per parameter of first-level parameter string, where bit values specify parameters to be refined with the DDM on a current iteration. In whole, a path of local descent on R_{DDM} - hypersurface is defined by second-level GA. Both levels are executed alternately with transferring better found parameter values to another level.
The algorithm was tested on some powder patterns of single and multi-phase samples with known crystal structures. As an example, the crystal structure of $Pd(NH_3)_2(NO_2)_2$ which initially had been solved from powder diffraction data by the Patterson method [4] was found from X-ray powder diffraction data by applying the proposed GA method. All general atomic coordinates and thermal factors including coordinates of hydrogen atoms were searched and refined successfully in a fully automatic way (26 structural parameters in total). The GA was applied for quantitative phase analysis of three- and four-phase samples CPD1 and CPD2 from Round Robin on QPA [5] as well. All profile parameters, general atomic coordinates and thermal factors (20 profile and 9 structural parameters in total in case of CPD1 sample) were searched with the GA simultaneously and then phase concentrations were calculated as usual for QPA by Rietveld method with mean error about 0.3% mass.

[1] Rizzi, R. (Ed.), *CPD IUCr Newsletter*, **2007**, 35. [2] Turner, G.W., Tedesco, E., Harris, K.D.M., Johnston, R.L., Kariuki, B.M., *Chem. Phys. Lett.*, **2000**, 321, 183. [3] Solovyov, L.A., *J. Appl. Cryst.*, **2004**, 37, 743. [4] Blokhin, A.I., Solovyov, L.A., Blokhina, M.L., Yakimov, I.S., Kirik, S.D., *Rus. J. Coord. Chem.*, **1996**, 22, 185. [5] Scarlett, N.V.Y., Madsen, I.C., Cranswick, L.M.D., Lwin, T., Groleau, E., Stephenson, G., Aylmore, M., Agron-Olshina, N., *J. Appl. Cryst.*, **2002**, 35, 383.

Keywords: genetic algorithm; structure solution; powder diffraction

FA5-MS01-P11

Successful Cryocooling of Protein Microcrystalline Samples for Powder Diffraction. Yves Watier[a*], Irene Margiolaki[a], Jonathan Wright[a], Andrew Fitch[a], Mathias Norrman[b], Gerd Schluckebier[b]. [a]*European Synchrotron Radiation Facility (ESRF), Grenoble, France.* [b]*Novo Nordisk A/S, Copenhagen.*
E-mail: watier@esrf.fr