

MS31 P06

FoxGrid – multi PC execution support for powder diffraction structure solution by Fox program. Jan Rohlíček, Michal Hušák, Bohumil Kratochvíl *Department of Solid State Chemistry, Institute of Chemical Technology Prague, Czech Republic.* E-mail: rohlicej@vscht.cz

Keywords: parallel computing, powder structure determination, software

For most structures (small molecules) the existing global optimisation algorithms and programs are sufficient to find the structure solution from powder data very quickly. But there are still a number of problems for which more computing power is required: this includes complex structures (>50 independent atoms or >30 internal degrees of freedom), and problems for which a wide range of structural models (different unit cells, space groups, building blocks,...) or algorithm parameters has to be tested.

We had try to solve the performance problem by modifying the FOX[1] structure solution code for an automatic multi PC parallel run. The concept uses simple client-server architecture for distributing the computation. Any PC can be configured either as a server or a client. The data is passed as an XML file between the client and the server. Grid computing can even be used on a single computer with multiple cores or hyper-threading technology, to fully use the available computer power while gathering all the results in a single Fox instance – the one configured as a server.

All the additional code works along the existing Fox code, using cross-platform socket code from the wxWidgets library.

The current work on the code development is targeted on benchmarking, automatic analysis of the obtained results and implementation of an intelligent task generation module. This module can help the user to solve the problem by “brute force”, i.e. preparing tasks trying to solve the structure in different space groups and with different lattice parameters (and other input conditions) automatically.

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[1] V. Favre-Nicolin and R. Cerny, *J. Appl. Cryst.* 35 (2002), 734-743.

MS31 P07

Structural Characterization of Nanocrystalline Apatites Obtained by Mechanochemical Synthesis Ivonne Rosales^a, Lauro Bucio^a, Eligio Orozco^a and Carlos R. Magaña^a. ^a*Department of Physics, National Autonomous University of Mexico. Mexico City, México.* E-mail: rosales@fisica.unam.mx

Keywords: Nanocrystalline apatites, Mechanochemical synthesis, X-Ray powder diffraction.

Apatite compounds have gained recently considerable attention because their wide range of physicochemical properties such as high ionic conductivity at low temperatures and low activation energies associated with the migration of oxygen ions [1-3]; host material for the nuclear industry [4]; as ceramic pigment [5]; and so on.

The compounds considered here, were those characterized by the general formula $A_{10}(BO_4)_6X_2$ in which A: Na, Ca and Ho; B: P and Si; and X: OH^- , F^- , Cl^- or O^{2-} .

The studied systems for obtaining compounds type apatite from the systems NaCl-Ho₂O₃-SiO₂, NaF-Ho₂O₃-SiO₂ and CaCO₃-(NH₄)₂HPO₄; were treated by mean mechanochemical synthesis method with few hours of milling. This method was used since it allows us to obtain compounds of nanocrystalline size.

The structure and microstructure of apatites were characterized by X-ray powder diffraction. The Rietveld refinement in space group P 6₃/m for all the systems in study leads to lower R values. Scanning electron microscopy (SEM micrographs) of the samples in NaCl-Ho₂O₃-SiO₂ and NaF-Ho₂O₃-SiO₂ system revealed compact crystallites of ~ 60 nm.

[1] Nakayama, S., Aono, H., Sadaoka, Y. *Chem Lett*, 1995, 6, 431.

[2] Nakayama, S., Kageyama, T., Aono, H., Sadaoka, Y. *J. Mater. Chem*, 1995, 5, 1801.

[3] Marques, F. and Kharton, V. *Ionics*, 2005, 11, 321.

[4] Hidouri, M., Bouzouita, K., Kooli, F., Khattech, I. *Mater. Chem. Phys*, 2003, 80, 296.

[5] Karpo, A., Nuss, J., Jansen, M., Kazin, P., Tretyakov, Y. *Solid State Sci*, 2003, 5, 1277.

MS31 P08

Retrieval system for qualitative and standardless quantitative phase analysis Igor Yakimov, Institute of non-ferrous metals and gold, Siberian federal university, Krasnoyarsk, Russia. E-mail: I-S-Yakimov@yandex.ru

Keywords: search/match, quantitative phase analysis, standardless QPA.

A search/match retrieval system (Q&QPA Retrieve) has developed for qualitative and standardless quantitative phase analysis of complex powder patterns and their groups. The system includes itself retrieve based on high selective query language and problem oriented GUI for visualization and operating under powder patterns and reference spectrums from DB. A Boolean logic is complemented in the query language by elements of calculus predicate theory. A qualitative phase analysis is executed by programs made from sequence queries. Hidden program are created automatically during mouse manipulations on analysing pattern, searching inquiry reference spectrums and elemental table over GUI. The GUI includes two main graphical windows for comparison of patterns and reference spectrums and for model spectrum. The model spectrum is optimal line combination of matching reference spectrums in limits of analyzing powder patterns.

Two automatic standardless quantitative phase analysis (QPA) methods have incorporated into search/match system. The first is intended for QPA of individual powder patterns and based on reference intensity ratio (RIR) method modified for using of powder pattern model spectrum. Line combination coefficients are included into known variants of RIR: normalized RIR and RIR with internal standard for without and in presence amorphous phases accordingly. There is possibility to refine a model spectrum by known quantitative elements composition during QPA. The modified RIR more resistance to preferred orientations and other distortions of powder patterns but need to use reference intensity ratio values (“corundum numbers” of phases) adequately to analyzing