

[s10.m1.p17] **Application of Rietveld method for studying the structural characteristics of substituted copper ferrite compound.** I.S. Ahmed Farag and A.M. Moustafa, *Physics Department National Research Centre, Dokki, Giza, Egypt.*

Keywords: ferrites, structure refinement, crystals microstructure.

A series of ferrite samples of the chemical composition $\text{Cu}_{0.7}(\text{Zn}_{0.3-x}\text{Mg}_x)\text{Al}_{0.3}\text{Fe}_{1.7}\text{O}_4$ [$x=0.05, 0.1, 0.15$ and 0.2], prepared by ceramic technique at 1000°C , were found to have cubic spinel structure. On applying the full pattern fitting of Rietveld method using FullProf program, the exact coordinates of atoms, the unit cell dimensions, the atom occupation factors, isotropic temperature factors, the profile shape parameters as well as the interatomic distances have been determined.

It was found that the lattice parameter decreases with increasing the Mg content, this may be attributed to the influence of the difference between the ionic radius of Mg and Zn cations. Also the variations of the cation distribution has been discussed on the basis of site preference, size and valence of the substituting cations. The low isotropic microstrain values obtained during the refinement process may be attributed to the method of the preparation in which the samples after last sintering were subjected to a coarse of annealing

[s10.m1.p18] **Identification of small amounts of foreign phases in biomaterials containing calcium carbonate.** B. Hasse¹, J.C. Marxen², W. Becker², H. Ehrenberg³, M. Eppe^{1,*}. ¹*Solid State Chemistry, Faculty of Chemistry, University of Bochum, D-44780 Bochum.* ²*Department of Zoology, University of Hamburg, Martin-Luther-King-Platz 3, D-20146 Hamburg.* ³*Hamburger Synchrotronstrahlungslabor (HASYLAB) at Deutsches Elektronensynchrotron (DESY), Notkestraße 85, D-22603 Hamburg and Institute of Materials Science, University of Darmstadt, Petersenstrasse 23, D-64287 Darmstadt*

Keywords: powder diffraction, advanced methods, structure determination.

Calcium carbonate is the most important inorganic material found in living organisms. The biological formation of minerals (e.g. as shell or skeleton) is called biomineralization.

Shells of the tropical freshwater snail *Biomphalaria glabrata* were examined with high-resolution X-ray powder diffractometry for foreign phases. During this examination, we found up to 1.6% of vaterite besides the main phase aragonite.

The samples were measured at the high-resolution powder diffractometer at HASYLAB/DESY (beamline B2). We used the setup for flat samples in transmission geometry with secondary monochromator. The diffraction patterns were fitted with FULLPROF^[1], and the phase analyses was done by the method of Hill and Howard^[2].

Acknowledgements: We thank HASYLAB at DESY for generous allocation of beamtime. Financial support by the Deutsche Forschungsgemeinschaft (DFG) and the Fonds der Chemischen Industrie (FCI) is also gratefully acknowledged.

[1] J. Rodriguez-Cavajal, Abstract of the Satellite Meeting on Powder Diffraction of the XV. Congress of the IUCr, Toulouse, France (1990) 127.

[2] R. J. Hill, C. J. Howard: Quantitative phase analysis from neutron diffraction data using the Rietveld method. *J. Appl. Cryst.* 20 (1987) 467-474.