

from X-ray, synchrotron and neutron diffraction can be combined regardless of the powder or single crystal nature of samples and refined jointly in order to get a structure model profiting from unique features of various experimental techniques. The most obvious and widely used case is combination of neutron powder data yielding good resolution for light atoms with carefully measured X-ray single crystal data in order to improve the overall quality of the structure model. The joint refinement is also very useful for magnetic structure determination which is often done from limited neutron powder data set at very low temperature. Joint refinement with complete low temperature X-ray data opens possibility to investigate relationship between magnetic and conventional structure. As a special case refinement of multiphase single crystal data should be mentioned. In this contribution we shall summarize our experience with joint refinement gathered during the last two years. Several practical examples will be presented as well as technical aspects of the joint refinement.

Keywords: structure refinement, joint diffraction data, Jana software

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FIDDLE: A method for simultaneous indexing and structure solution from powder diffraction data

Rene De Gelder, Carmen Guguta, Jan M.M. Smits

Radboud University Nijmegen, Molecular Materials, Heyendaalseweg 135, Nijmegen, Gelderland, 6525 AJ, The Netherlands, E-mail : r.degelder@science.ru.nl

The complexity of crystal structures determined from powder diffraction data has steadily increased through further development of traditional methods for structure determination in reciprocal space and application of global optimization algorithms in direct space. The usual process for structure determination from powder diffraction data consists of the following steps: (1) indexing of the pattern, (2) space group determination, (3) structure solution, (4) structure refinement. The currently available powder methods rely on successfully passing the first step, powder indexing. Due to a number of fundamental and experimental problems, like peak broadening, the presence of impurity phases, dominant zones and geometrical ambiguities, powder indexing will remain difficult in many cases, thereby hampering the next steps in structure determination. There is no fundamental reason to separate, as is usual today, the process of unit cell determination and the process of structure solution. Structure determination from powder diffraction data can be seen as a process of global optimization of all model parameters, including the unit cell parameters. This strategy is applied in the FIDDLE program. For the simultaneous optimization of the parameters that describe a crystal structure genetic algorithms together with a pattern matching technique based on auto and cross correlation functions are used. This one-pot strategy for indexing and structure solution, as applied in FIDDLE, was successfully used for determining the unknown crystal structures of Ethinyl Estradiol anhydrate, Naloxone monohydrate and Creatine anhydrate, cases for which indexing was problematic.

Keywords: indexing, crystal structure determination X-ray powder data, optimization algorithms

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Experiencing space groups

Aloysio Janner

Radboud University Nijmegen, Theoretical Physics, Heyendaalseweg 135, Nijmegen, Nederland, NL-6525 AJ, The Netherlands, E-mail : A.Janner@science.ru.nl

Presented are highlights of fifty years of personal experience with space groups, enriched by their many different aspects (algebraic, geometric, arithmetic, crystallographic, computational, material oriented) and interwoven with friendly human relations, started in 1958 with Edgar Ascher at the Battelle Institute, Geneva, and kept on later from the University of Nijmegen leading eventually to higher-dimensional space groups acting on a lower-dimensional space.

Keywords: space groups, group cohomology, superspace crystallography

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Space groups resulting from 3D sections of (3+1)D superspace groups. Can all 3D groups be generated?

Ivan Orlov, Lukas Palatinus, Gervais Chapuis

Ecole Polytechnique Federale de Lausanne, Laboratoire de Cristallographie, EPFL, BSP - Dorigny, Lausanne, Vaud, 1015, Switzerland, E-mail: ivan.orlov@epfl.ch

Using the superspace formalism for the unified description of sets of commensurate structures requires an unambiguous understanding of how symmetry of a 3-dimensional structure may be inherited from the symmetry of a higher-dimensional one. Although reducing 3D groups to 2D groups has been thoroughly described [1], the similar research for (3+1)D and 3D groups was missing. Further research on space-superspace symmetry relations is needed for the extension of the International Tables for Crystallography towards incommensurately modulated crystals and quasicrystals. We studied the hyperplane t cuts of (3+1)D symmetry elements and constructed a complete network relating (3+1)- and the corresponding 3-dimensional space groups derived by rational cuts. A complete set of data for (3+1) to 3D group relations has been obtained for the first time. The corresponding database has been established and is available via Web interface at <http://superspace.epfl.ch/finder>. It is particularly useful in finding common superspace 'denominators' for series of 'composition-flexible' structures and analysis of possible or forbidden space group sequences for phase transitions. The results answer among other questions like: can all space groups be obtained as sections of superspace groups?

Keywords: superspace approach, symmetry groups, commensurate modulation

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Space groups, subgroups and a lot more

Peter Zeiner

Bielefeld University, Faculty of Mathematics, Postfach 100131, Bielefeld, NRW, 33501, Germany, E-mail: pzeiner@math.uni-bielefeld.de

Space groups G are the fundamental tool to describe the symmetry