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

MS.88.5

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

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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

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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?

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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

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Space groups G are the fundamental tool to describe the symmetry

of crystals. As important as the space groups themselves are their subgroups. Here, we review how they have improved our understanding of the space groups themselves, how they have proved useful in solving various problems of crystallography and how they have been used to define new groups. Furthermore we give an outlook of what still has to be done. One of the most important subgroups is the group T of lattice translations, which we can use to construct the quotient group P=G/T, which is better known under the name point group. We start our presentation by reviewing the work of E. Ascher and A. Janner, who have shown how to view space groups as extensions of P by T. We pass on to more general subgroups and discuss coset and double coset decompositions and how they have been applied to phase transitions and twins in crystals. Closely connected to coset decompositions are colour groups, which have been studied among others by J.J. Burckhardt. A special kind of colorings are Bravais colorings, which leads us to similar sublattices and the group of similarity rotations, which is a supergroup of the point group. In between these two groups is the group of coincidence rotations, thus we arrive at coincidence site lattices (CSLs) and grain boundaries and return to twins. Last but not least we discuss the connections between colorings and CSLs, thus arriving at current research topics.

Keywords: space groups, colourings, coincidence site lattices

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J.J. Burckhardt's contributions to crystallography

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Johan Jakob Burckhardt, who died in 2006 at the age of 103, was deeply interested in crystallography all of his life and made invaluable contributions to the mathematical foundations of space group theory. After first studying mathematics in Basel and Munich, he was so impressed by Andreas Speiser's *Die Theorie der Gruppen von endlicher Ordnung* that he moved to Zurich to study with Speiser the year after its publication. There he also attended lectures of Paul Niggli and (explicitly recommended by Speiser) Leonhard Weber.
On the basis of his acquired mathematical background, Burckhardt developed a new derivation of the 230 space group types which placed the earlier work of Schoenflies and Fedorov in the modern algebraic context of cohomology theory. His approach via Frobenius congruences in particular freed space group theory from dimensional constraints. For example, he determined the space groups for cyclic, symmetric and alternating permutation groups (in their natural permutation representation) for arbitrary degree. Burckhardt's work on space groups culminated in the publication of *Die Bewegungsgruppen der Kristallographie* in 1947 which is still a standard reference in mathematical crystallography. Together with Bartel Leenert van der Waerden he published a short but crystal clear article about colour symmetry which clarified the somewhat obscured ideas around that topic and influenced a generation of researchers. Burckhardt also became a historian of mathematical crystallography, and helped to illuminate its long and multi-lingual, multi-disciplinary path. Perhaps most important of all, Burckhardt corresponded widely with mathematicians and crystallographers all over the world, helping to create the community that this symposium implicitly celebrates.

Keywords: J.J. Burckhardt, space group theory, colour symmetry

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Heterogeneous cylinder packing: Space group on periodic structures with <110> six directions

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Several cylinder packing structures were found by authors around 1995. We gave equations of structures and calculated packing density. But we have left their space group undetermined for many years.
In this talk, we report space group on periodic structures of cylinder packing with <110> six directions. All the cylinders are congruent and the length of the cylinders is infinite and their directions are restricted to only six directions of <110>. Each cylinder is fixed by cylinders of other directions, so that the whole structure sustains mechanical stability. The space group tell us each structure is not homogeneous. But they have ingenious feature: parallel cylinders in six directions form equivalent two-dimensional rhombic lattice respectively.

Keywords: cylinder packing, rod packing, space group

MS.90.1

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Life sciences at Diamond Light Source and prospects with new light sources

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Diamond Light Source was commissioned for users in 2007. The machine consists of a 100 MeV linear accelerator, a 3 GeV booster synchrotron and a 3 GeV storage ring, together with interconnecting beam transfer lines. The storage ring (circumference 562 m) based on 24 cells is run at 300 mA. The electron beam emittance is 2.7 nm rad with bunch length (FWHM) 25.6 ps. The accelerating voltage is provided by two superconducting cavities based on inductive output tubes (IOTs) each capable of delivering a maximum total output power of 300 kW. In Phase I, 7 insertion devices were installed: 5 in-vacuum undulators, one variable polarisation device and one superconducting wiggler. At the end of Phase II (2011) Diamond will have 22 experimental stations for research in both the life sciences and physical sciences, 7 beam lines in Phase I (completed 2007) and 15 beam lines in Phase II. This talk will consider the impact of synchrotron radiation on life sciences research and will attempt to assess the future demand for new X-ray sources. Diamond will have 8 beam lines dedicated to life sciences research: 5 macromolecular crystallography beam lines, a non-crystalline diffraction and solution scattering beam line, a circular dichroism beam line and an infrared microspectroscopy beam line. These will provide for exciting and