Oral Contributions

[MS14] Aperiodic crystals: structure, dynamics and magnetism

Co-Chairs: J. Manuel Perez-Mato (ES), Marc de Boissieu (FR)

[MS14-01] Magnetic structures determined using Shubnikov space and superspace groups: implementation in Jana2006,

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Solution and refinement of magnetic structures is usually made with help of the decomposition of the magnetic configuration space into basis modes transforming according to different physically irreducible representations (irreps) of the space group of the paramagnetic phase [1]. Recently it has been shown that a direct use of Shubnikov (magnetic) space and superspace groups facilitates work with non-modulated as well as with modulated magnetic structures. This concept can simplify algorithms for handling diffraction data of magnetic structures [2]. For incommensurately modulated magnetic structures this approach may be especially beneficial [3], for instance in analyzing multiferroic phases. The lecture explains symmetry analysis and refinement of complicated magnetic structures with the program Jana2006 [4] and gives the theoretical background used for the implementation of the presented tools. The works start with symmetry analysis, where Jana2006 provides a simple procedure for testing different irreps of the parent paramagnetic structure. It offers interactively a list of Shubnikov space or superspace groups as follows from individual irreps and visualizes the corresponding magnetic structure model in the VESTA program [5]. Simulated powder data of such model can be compared against the measured diffraction profile. Jana2006 can also call through the internet the recently developed program ISODISTORT [6] which provides similar but more detailed analysis, and use its results The basic idea behind the new option for magnetic structures in program Jana2006 lies in the application of the magnetic and nuclear symmetry not only during data processing (merging symmetry related reflections for single crystal data or reducing generated reflections to independent ones for powder) but also in calculation of magnetic structure factors.
Combination of the nuclear and magnetic diffraction can be made either by combining two independent phases as in the Fullprof [7] or preferably from a common structural description of both phases in which the combination of intensities is made internally. Jana2006 offers simultaneous refinement against different diffraction experiments including commensurate and incommensurate phases and allows for combination of powder and single crystal data. The new approach offers good stability of refinement, a logical way how to describe twin domains and manifold possibilities for refinement of modulated magnetic structures from various experiments. It has been recently applied successfully to several magnetic structures [8], [9], [10].

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