Developments in FullProf for magnetic structures determination in superspace

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In the last three years, a series of developments within the *FullProf Suite* [1], concerned with magnetic structures (both commensurate and incommensurate), have been performed. From the the first publication describing shortly the program *FullProf* [2] in 1993 many changes and re-writing of the code were done. In particular, the phase convention in the expression of the magnetic structure factor were changed. In 1993, we introduced for the first time the Simulated Annealing (*SAnn*) procedure for solving magnetic structures in a program called *MagSan* [2] that was later developed for incommensurate structures and embedded within *FullProf*. The method to make a symmetry analysis during many years was based in the Bertaut's and Izyumov proposals [3-5] and we developed the program *BasIreps* to help the *a priori* construction of magnetic models to be refined. The use of magnetic space groups (MSG) was possible but, in the absence of appropriate tables or computing tools, the user had to construct the symmetry operators by hand. The treatment of incommensurate magnetic structures either was only possible by using basis vectors of irreducible representations or by constructing a series of 3D operators accompanied by a phase factor that was done by looking at the output of *BasIreps* and completing the information if the user was able to understand group theory.

The availability of new tools on the Web [6-8] and the creation of the *Commission on Magnetic Structures* of the IUCr has allowed the development of precise and unambiguous ways of describing magnetic structures using MSG and magnetic superspace groups (MSSG) [8, 9] by mean of magnetic CIF files. The team working in the *FullProf Suite* has accompanied these developments and created new tools to import these CIF files and convert them to input control files for *FullProf*. We have now the possibility of treating MSSG within *FullProf* with up to three independent modulation wave vectors, both for powders and single crystals, with automatic symmetry constraints determination for the amplitudes of modulations [10]. The displacement and thermal amplitudes are implemented but, for the moment, the calculation of structure factors using integration in internal coordinates is not yet available.

One important feature of *FullProf* is the use of *SAnn*, using the full powder diffraction pattern in which the components of the magnetic amplitudes are free parameters, in either crystallographic or spherical settings. This is very important for the powder case in which the loss of information may give rise to ambiguous or degenerate solutions. Moreover, the *SAnn* method may be used as an alternative to refinement because in such cases the least squares refinement procedure diverges of it is unable to arrive to convergence.

In this talk, after summarizing the full set of changes performed during the last years (interoperability with the *Bilbao Crystallographic Server* [6, 7] and *ISODISTORT* [8], the use of magnetic Hall symbols [11], magnetic symmetry modes, etc.) I will present few recent examples of the use of *FullProf* in the magnetic structure determination of magneto-electric and multiferroic materials.

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