Main Plenary Lecture

USEFULNESS AND UNUSEFULNESS OF THE SUPERSPACE APPROACH TO APERIODIC CRYSTALS

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The superspace approach to the analysis of aperiodic crystals has been quite successful. An overview will be given of its development for various classes of aperiodic crystals, such as modulated phases, magnetic phases, composite systems and quasicrystals. There remain, however, several open questions.

The approach has mainly been successful in structure determination. For the study of physical properties one meets severe problems. These problems will be discussed, as well as some techniques used to circumvent them.

Also there are limitations to the types of structures that may be described. What can one do if one wants to go further?

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SUPERSPACE SYMMETRY OF MAGNETICALLY MODULATED CRYSTALS

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Although the articles of A. Janner and T. Janssen, which started the development of the superspace symmetry formalism, already stressed its possible application to magnetically ordered systems, the community investigating incommensurate magnetic structures has remained during decades rather alien to this methodology. The drawbacks of this situation became particularly patent when dealing with magneto-structural properties, like multiferroicity, where symmetry arguments are especially powerful. Only in the last years the development of specially adapted computer tools, and in particular, the extension of JANA options to magnetic structures is changing this situation. Steadily, through the use of these tools, the advantages of applying superspace symmetry are becoming known in the realm of modulated magnetic structures research [1]. In this same direction, we have started in the Bilbao Crystallographic Server a small database (www.cryst.ehu.es/magndata), where the magnetic superspace groups of some of these structures have been identified and the structures are described accordingly (see Figures 1, 2)

In this talk I will review the concepts of magnetic superspace symmetry and its application, with special emphasis on its peculiarities. The relation with the traditional representation method will be discussed, stressing the differences. Some examples will help to show how representation analysis and superspace symmetry can be combined to achieve an optimal approach to the characterization of magnetically modulated structures and the exploration of possible incommensurate magnetic orderings.

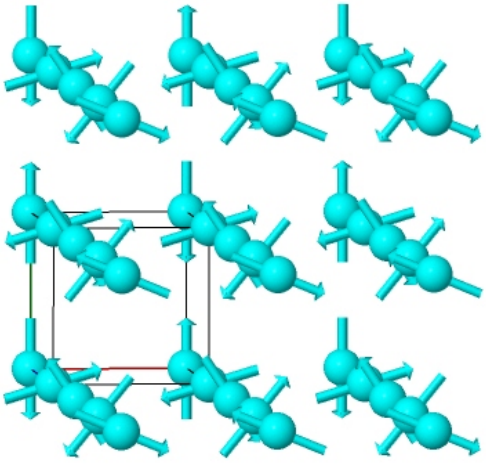

Figure 1. Helical arrangement of Ce atoms in $CeRhIn_5$. Magnetic superspace group: P4221'(1/2,1/2,)q00s (MAGNDATA entry #1.1.16).

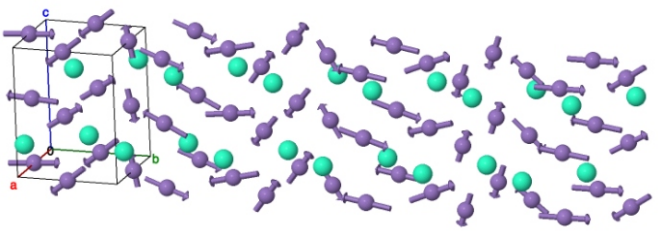

Figure 2. Cycloidal arrangement of Mn atoms in $TbMnO_3$. Magnetic superspace group: $Pbn2_11'(0, ,0)s00s$ (MAGNDATA entry #1.1.8)