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?

T1

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.

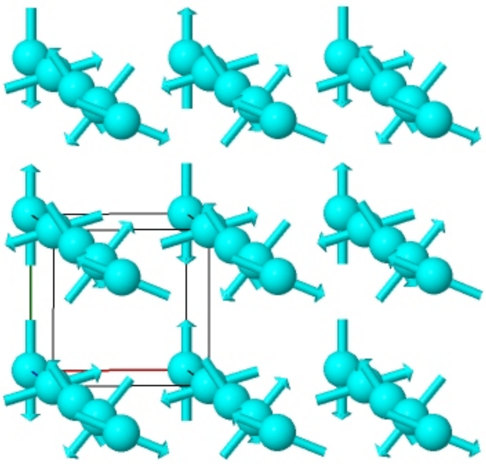

Figure 1. Helical arrangement of Ce atoms in $CeRhIn_5$. Magnetic superspace group: P4221'(1/2,1/2,)q00s (MAGNDATA entry #1.1.16).

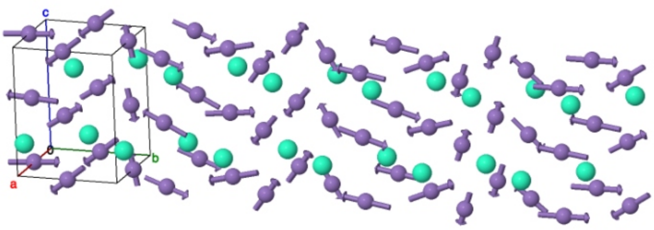

Figure 2. Cycloidal arrangement of Mn atoms in $TbMnO_3$. Magnetic superspace group: Pbn$2_1$1'(0, ,0)s00s (MAGNDATA entry #1.1.8)

1. J. M. Perez-Mato, J. L. Ribeiro, V. Petricek, M. I. Aroyo, *J. Phys. Condens. Matter.* **24**, (2012), 163201.

I am especially indebted to Robert Hanson for his rapid "immersion in superspace" and his adaptation of Jmol to magnetic superspace symmetry, making this visualization tool (used here and in our Bilbao server) unique. I should also express my deep recognition to Vaclav Petricek, Branton Campbell, Harold Stokes and Juan Rodriguez-Carvajal, plus the whole team of the Bilbao Server for their constant efforts to achieve, through new or improved computer tools, an efficient application of magnetic superHspace symmetry. This work has been supported by the Spanish Ministry of Science and Innovation (project MAT2012-34740) and by the Government of Baskland (project IT779-13).

T2

STRUCTURE MODELS OF ICOSAHEDRAL QUASICRYSTALS

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The discovery of the binary icosahedral (i) quasicrystal (QC) $YbCd_{5.7}$ brought a breakthrough in the field of QCs [1]. An established atomic model for this Tsai type i-QC based on its characteristic atomic cluster is now available [2] and is being used as the basis of describing its related i-QCs, such as i-YbCdMg [3] and i-*R*Cd (*R*=rare earths) [4]. The Tsai type i-QCs are described by the three building units: rhombic triacontahedron (RTH, located on the 12 fold vertices of a 3D Penrose tiling), acute rhombohedron and obtuse rhombohedron. A RTH unit corresponds to icosahedral atomic cluster, and other two units with atomic decorations fill the gap in between the clusters. No established models for Al-transition metal type and Frank-Kasper type i-QCs have been obtained yet. However, a similar structural description with the three building units is also applicable to these types of i-QCs. A key is to choose a suitable length scale for the building units. The remaining question is to give an appropriate atomic decoration to each building unit for these types of i-QCs. Note that the model of Tsai type i-QCs has no ambiguity in terms of the atomic decorations. Some features for the structure models of i-QCs which belong to the different structure types and the difference between them will be discussed.

1. A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura, T. J. Sato, *Nature*, **408**, (2000), 537.
2. H. Takakura, C. P. Gómez, A. Yamamoto, M. de Boissieu, A. P. Tsai, *Nature Materials*, **6**, (2007), 58.
3. J. Q. Guo, E. Abe, A. P. Tsai, *Philos. Mag. Lett.*, **81**, (2002), 27.
4. A. I. Goldman, T. Kong, A. Kreyssig, A. Jesche, M. Ramazanoglu, K. W. Dennis, S. L. Bud'ko, P. C. Canfield, *Nature materials*, **12**, (2013), 714.

T3

GENERAL MEYER SETS AND THEIR DIFFRACTION SPECTRUM

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We start by reviewing the definition and properties of Meyer sets. Next we look at the diffraction pattern of an arbitrary Meyer set: we see that every Meyer set has a relatively dense set of Bragg peaks, which are highly ordered. We complete the talk by observing that Meyer sets have many similar properties to subsets of lattices.