Commensurate and incommensurate modulations in magnetic materials

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'Magnetic material' is a broad term that generally refers to the existence of magnetic order in a material, that is, the onset of an orderly arrangement of magnetic spins below a certain critical temperature. Magnetic phases and transitions are important and modern topics in different research fields, from fundamental to applied Physics. As the number of new materials that are being currently studied for their magnetic properties, either coupled with other properties or not, is expanding, a comprehensive characterization of magnetic phases is essential.

Magnetic ordering involves symmetry breaking. Therefore, the description of a magnetic phase includes the assignment of the relevant symmetry modes for the spin configuration and its constraints consistent with the parent paramagnetic phase and the magnetic propagation vector(s) (expressed in the form of a magnetic (Shubnikov) space group for commensurate ordering, or by magnetic superspace groups if the ordering is incommensurate). Furthermore, the symmetry group of a magnetic phase also encompasses unambiguously other important features such as magneto-structural couplings.

Despite the clear advantages of a symmetry-based approach to determine and describe magnetically ordered systems, it was only recently that the scientific community has more extensively adopted it. This achievement is mostly due to the development of computation tools that are now able to directly use the symmetry operations in Shubnikov space and in superspace groups. In particular, the new magnetic option implemented in Jana2006 is capable of handling different sets of diffraction data to consistently solve and describe commensurate and incommensurate magnetic structures based on symmetry considerations [1]. The representation analysis uses the magnetic symmetry of the paramagnetic phase and its irreducible representations. Other remarkable symmetry-based computational tools in magnetic crystallography are the ones available at the Bilbao Crystallographic Server, comprising, for example, a full listing of magnetic point groups, symmetry-forced magnetic extinctions, and a database of magnetic structures [2]. The ISODISTORT program explores distortion modes in crystalline materials, including the magnetic order and magneto-structural modes [3]. Both tools are connected with the magnetic option of Jana2006.

Here we will review the fundamental concepts of magnetic symmetry and the superspace formalism, and present the working flow and the capabilities of the magnetic option of Jana2006. Several examples of magnetic ordering models will be presented for both commensurate and incommensurate types of magnetic structures.

1. V. Petricek, M.S. Henriques, M. Dusek, *Acta Phys. Pol. A* **130** (2016) 848.

2. J.M. Perez-Mato, S.V. Gallego, E.S. Tasci, L. Elcoro, G. de la Flor, M.I. Aroyo, *Annu. Rev. Mater. Res.* 45 (2015) 13.1.

3. ISOTROPY Software Suite, iso.byu.edu (03/2018).