MS.20.2

Acta Cryst. (2011) A**67**, C59

Symmetry considerations in commensurate and incommensurate multiferroic materials

J.M. Perez-Mato,[a] J.L. Ribeiro,[b] V. Petricek[c] and M. I. Aroyo,[a] [a]*Dpto. de Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco UPV/EHU, Bilbao (Spain).* [b]*Centro de Física da Universidade do Minho, 4710-057 Braga (Portugal).* [c]*Institute of Physics, Academy of Sciences of the Czech Republic v.v.i., Na Slovance 2, 18221 Praha 8, (Czech Republic).* E-mail: jm.perez-mato@ehu.es.

Magnetic symmetry (expressed in terms of Shubnikov space groups for the case of commensurate magnetic structures, or in terms of magnetic superspace groups for the case of incommensurate structures) is at present seldom applied in the analysis and description of magnetic structures. In most cases, magnetic structures are determined, described and analyzed using the so-called representation analysis. In this methodology (as it is presently applied) the magnetic symmetry group of the configuration does not play any relevant role. Magnetic structures are described by a nuclear structure with symmetry given by a normal space group, plus a set of static waves of atomic magnetic moments with symmetries described by irreducible representations (irreps) of this space group. It is then not rare to find reports of new magnetic structures without the identification of their magnetic symmetry, not even their magnetic point group. This is an unfortunate situation especially in the case of multiferroic materials, for which the identification of the magnetic point groups of the parent and ferroic phases (the so-called ferroic species) is fundamental to rationalize their ferroic/switching properties. As many multiferroics have incommensurate magnetic ordering, the lack of symmetry characterization has been often justified by the lack of lattice periodicity.

In this talk we pretend to convey by means of several examples two basic messages: i) incommensurate magnetic phases have a magnetic symmetry that can be described by a group defined within the superspace formalism, similarly as it is done for non-magnetic incommensurate structures; and ii) the most efficient approach to the analysis and description of magnetic structures (both commensurate and incommensurate) is a combined use of magnetic symmetry and representation analysis. The relation between the two approaches and their combined use will be discussed. In the simplest cases, to assign some irrep to the magnetic arrangement is equivalent to the identification of its magnetic symmetry (a space group or superspace group depending on the propagation vector being commensurate or incommensurate). But in most cases the two concepts are inequivalent and, contrary to what is usually assumed, the assignment of a specific magnetic symmetry can be much more restrictive. In general, for a given irrep, several possible magnetic space (or superspace) groups can be realized, depending on how the irrep basis functions are combined. A systematic controlled exploration of the different alternative magnetic symmetries for a given irrep (or set of irreps) is bound to give more robust results during the refinements. By means of some examples, the practical application of these concepts to the analysis of multiferroics will be shown.

Keywords: magnetic structures, representation analysis, magnetic symmetry.

MS.20.3

Acta Cryst. (2011) A**67**, C59

Affine extensions of noncrystallographic groups and quasi-lattices

Reidun Twarock, Tom Keef, Jess Wardman, *York Centre for Complex Systems Analysis, University of York (UK).* E-mail: reidun.twarock@york.ac.uk

In his seminal work, Janner has demonstrated that techniques from crystallography can be used to characterise the layouts of biomolecules, and in particular those of viruses [1]. Since viruses display icosahedral symmetry, a noncrystallographic symmetry, quasi-lattices are appropriate tools for the modeling of their architectures [2]. We show here that via an affine extension of the icosahedral group a library of point arrays can be generated, that by construction is related to the vertex sets of quasi-lattices, and can be used to predict the material boundaries in viruses [3]. In particular, this theory is able to predict the genome organization in simple RNA viruses, and reveals geometric constraints on the capsid proteins that could not be predicted with previous theories.

We moreover show that this approach also applies to nested carbon cage structures called carbon onions [4].

[1] A. Janner, *Acta Crystallogr A* **2010,** *66,* 301-11. [2] R. Twarock, T. Keef, *Micobiology Today* **2010,** *37,* 24-27. [3] T. Keef, R. Twarock, *J. Math. Biol.* **2009,** *59,* 287-313. [4] J. Wardman, T. Keef, R. Twarock, Affine extensions of the icosahedral group with applications to nested carbon cage structures, *in preparation*

Keywords: noncrystallographic coxeter group, quasi-lattice, virus

MS.20.4

Acta Cryst. (2011) A**67**, C59

The Lie group of translations: a unified way for describing structures, modulated or not

Philippe Kocian, Kurt Schenk, Gervais Chapuis *Laboratoire de Cristallographie, FSB – IPSB, EPFL, Lausanne (Switzerland).* E-mail: gervais.chapuis@epfl.ch

The appropriate tool for describing the concept of repetition of a brick in three (or $n \in \mathbf{N}\backslash\{0\}$) dimensions is the so-called group of translations and its action on the points of a metric space.

When the metric space corresponds to the Euclidean space (that is the so-called point space), the action of a translation on a point consists in adding one real number to each of its coordinates. If this holds in the case of the Euclidean space, it certainly does not for a general metric space, for instance a curved surface or a curved space. Thus, in order to have a definition of the concept of translation taking into account the geometry of the considered space, a more general framework is required; the point space has to be replaced by the concept of manifold and the group of translations must be treated as a Lie group.

From this point of view, we show that the electron density of a crystal on a manifold (*i.e.* modulated or not), can be obtained by applying to the electron density of one unit cell the exponential of a finite free **Z**-module of the Lie algebra associated with the group of translations of the considered manifold. This illustrates that an electron density, as well as its Fourier transform, can be split into two parts, the first one in which appears the geometry of the space in which the crystal exists, and the other which contains the elements of the group of translations. The geometry of a space, *i.e.* the parameterisation of this latter, and the group of translations are two different objects which, when blended together, generate pictures like those obtained from diffraction.

Keywords: modulated structures, lie groups, translations