

Application of Symmetry to Magnetism and its Consequences for Crystallography

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The microscopic picture of magnetism developed by Néel required extensions to be made to the description of symmetry in crystalline solids. Historically, the first of these was the application of the so-called “coloured” groups or Shubnikov groups, created by the addition to the conventional symmetry elements of crystallography of an operation that reverses magnetic moments. Whilst these are conventionally tabulated for simple commensurate periodicities defined by the Lifshits condition they can be used to describe both commensurate and incommensurate symmetries. There are, however, fundamental restrictions to the types of symmetry that can be effectively characterized using the coloured groups which limits greatly their usefulness. The most general description of symmetry in crystalline solids is that developed by Wigner and is based on the use of irreducible corepresentations.

This presentation will explain the fundamentals behind Shubnikov’s space groups and Wigner’s theory, and will detail how unspecialized researchers can use corepresentation theory to determine magnetic structures from neutron diffraction data using the computer program *SARAH* (<ftp://ftp.ill.fr/pub/dif/sarah/>) in combination with the refinement programs *GSAS* or *Fullprof* [1,2].

[1] Wills A.S., *Physica B*, 2000, **276**, 680. [2] Wills A.S., Lappas A., *J. Phys. Chem. Solids*, 2004, **65**, 65.

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