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Magnetic Option in Jana2006: A Unified Approach by Shubnikov (Super)space Groups

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The concept of Shubnikov (magnetic) symmetry becomes frequently used for description, solution and refinement of magnetic structures. Its growing importance is connected with the ease of application to various classes of magnetic structures having the translation periodicity identical, commensurate or incommensurate with the nuclear one. Recently generalized superspace approach [1] for incommensurately modulated magnetic structures allows for combination of nuclear and magnetic modulations. This unified description helps fully understand e.g. multiferroic phases. The program Jana2006 (http://jana.fzu.cz) combines the concept of Shubnikov (super)space groups with the representational analysis based on the decomposition of the magnetic configuration space into basis modes, which transform according to different physically irreducible representations (irreps) of the space group of the paramagnetic phase [2]. Moreover, Jana2006 can launch the recently developed program ISODISTORT [3] to obtain similar but more general analysis. The generalized symmetry concept facilitates data processing where symmetry related reflections for single crystal data can be merged and the list of generated reflections for powder data can be reduced to independent ones. Another benefit concerns calculation of magnetic structure factors, stability of refinement and logical way to describe twin domains. Unlike in the Fullproff program [6], Jana2006 can combine the nuclear and magnetic scattering internally without necessity to introduce two phases. It can also calculate magnetic structures with modulated parent phase where the modulation appears before the magnetic phase transition. The lecture shows manifold possibilities how to refine modulated magnetic structures from various experiments. Several recently solved magnetic structures will be presented.

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