[MS43-02] SUPERSPACE FORMALISM: THE SWISS ARMY KNIFE OF THE CRYSTALLOGRAPHER, Olivier Pérez,

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The superspace formalism has been developed by PM de Wolff, T Jansen and A Janner at the beginning of the 70's [1] for solving the incommensurate modulated structures, materials belonging to the class of aperiodic crystals. Aperiodic crystals are characterized by the loss of the 3d periodicity and the principle of the superspace formalism is to recover a periodicity by introducing additional dimensions (up to 3) perpendicular to the real space; the classical tools of the crystallographer (symmetry, atoms, structure factor, …) can be then generalized to the (3+d) dimensions space. These last years, owing to the improvement of the diffraction technics (X-rays sources, detectors), the number of observed modulated structures has significantly increased and this formalism is less and less confidential. Moreover, some intrinsic properties of this approach make it useful for the structure solution of a large range of more or less classical crystalline materials (superstructures, disordered materials). After "classical" uses of the superspace for the structure solution of an incommensurate modulated structure, more exotic studies will be proposed. Thus the efficiency of the formalism for solving or just for describing long period commensurate phases will be shown; the tricky problem of the sections of the superspace and the resulting symmetry will be explored. Finally, the application of the multidimensional approach to disordered materials will be proposed. This part will be devoted to compounds exhibiting diffraction patterns where both Bragg reflections and diffuse scattering coexist. Classical approach considers only the long range order coherent part of the diffraction pattern and leads to an average structure of the material often characterized by atoms split over different too close positions. Thereafter, the disorder must be elucidated thanks to the vivid imagination of the crystallographer. But diffuse scattering phenomena are related to short range order. The real structure of the material is then somewhere in between the average structure and an ideal perfectly ordered structure. Then, the description of this ideal ordered structure gives an insight of the local order of the real structure. The CaTeO4, NH4Fe2(PO4)2 [2] and Sr2Fe3O6.5 phases show a diffraction pattern where both punctual reflections and diffuse lines coexist; the disorder prevents the determination of the local atomic environments. To obtain an ideal ordered structure, an ideal diffraction pattern is designed by replacing the diffuse scattering, observed in the real reciprocal space, by punctual reflections resulting from the partial integration of the diffuse lines. Superspace formalism is then very useful for a modeling of this pseudo long range order; it allows the building of a model, step by step, and improves the convergence by reducing the number of refinement parameters; a perfectly ordered structure is then obtained. A with comparison the average structure provides an accurate description of the real local structure.

[1] P.M. de Wolff, T. Janssen and A. Janner Acta Cryst. (1981), A37, 625-636.
[2] Pérez O, Adam L, Guesdon A, Daturi, M., Raveau B, Acta Cryst. B63 (2007), 521-531

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