s1.m1.o1 **Superspace Description of Incommensurate and Commensurate Structures beyond the Perturbative /Modulation Approach**. J.M. Perez-Mato, *Departamento de Fisica de la Materia Condensada, Universidad del Pais Vasco, Apdo. 644, E48080 Bilbao, Spain.*
Keywords: aperiodic, incommensurate.

Superspace formalism was in principle developed for modulated structures where the modulation (displacive or occupational) constitutes a perturbation with respect to a so-called average conventional structure. Even modulated composite structures are usually considered as a set of conventional periodic average substructures with small modulations resulting from their reciprocal interaction. Typical examples are temperature stabilized modulated phases, inclusion compounds and misfit materials. Under this perspective, the structural analysis of modulated phases has been usually considered a *refinement* problem with the average structure(s) as starting model.

In the last few years, however, it has become clear that the superspace approach can also be extraordinarily efficient when dealing with structures outside the above picture. In general, any structure, which can be approximately considered as the stacking of atomic layers, can in principle be described as a modulated structure with an average periodicity related with the layer thickness. The modulation associated with the layer sequence is then described by step (crenel) occupational functions, which are beyond a perturbative approach. In this sense, these structures are close to the quasicrystals, since a starting structural model requires the definition of discrete atomic occupation domains along the internal space. This includes the quite trivial fcc or hcp layer models, but is valid for more general situations. The power of the superspace description becomes obvious when the layer sequence is either long period and/or is variable within an homologous series of compounds or a solid solution. Typical examples are polytypoids, polytypes and intergrowth layer compounds. The implementation of crenel (step) occupational functions in the JANA98 package by Petricek et al. allows efficient analyses of these structures, provided a starting realistic model of atomic occupational domains is known, for instance through an approximate layer model. Also, long-period layered structures taken from the literature can be «transposed» into a superspace description with spectacular results. Several examples will be presented[1,2], stressing common features as the linear composition-dependence of the wave vectors, Farey-tree rules governing the layer sequences, the typical approximate saw-tooth form of the displacive modulations, and the existence of equivalent descriptions as either single modulated structures or composites.

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s1.m1.o2 **Aperiodicities in 2201 and 2212 cuprates, ferrites and cobaltites: differences and similarities.** D. Grebille, O. Pérez, N. Jakubowicz, H. Leligny, *Lab. CRISMAT (UMR CNRS 6508), ISMRA, 14050 Caen Cedex,France.*
Keywords: incommensurate, oxides, superconductors.

High Tc superconductors oxides are well known for their physical properties. Among them, Bi-based cuprates are also known for their complex modulated structure. Their structural study is particularly difficult first because of experimental reasons (synthesis, anisotropy, absorption), and second because of the existence of different types of modulations, and of structural defects or disorder related to these modulations and implying simultaneously atomic displacements, substitutional modulations, non stoichiometry and pseudosymmetry.

In order to give a better insight in this family, the general system (Bi,Pb)-Sr-Ca-M-O with M=Cu,Fe or Co has been extensively studied.[1,2,3] As a matter of fact, the diffraction patterns of these different compounds show very strong analogies (symmetry, diffracted intensities, modulation vectors, centering conditions...).

The most frequent structural model can be described with an orthorhombic symmetry, on the basis of the stacking of structural slabs along c, with a modulation vector $\beta b^* + c^*$, with β varying between 0.12 and 0.25. Ferrite and cuprate compounds show isotopical analogies of the modulated configuration of the rock-salt type layers. In particular, one systematically observes the periodic alternation along b of modulated and of disordered regions which are probably responsible for non stoichiometry phenomena.

Cobaltite compounds are characterized by apparently analogous diffraction patterns but by shorter modulation periods. The structural study shows that the structural model is in fact quite different concerning the configuration of the rock-salt type layers. A disordered model for the non substituted compound can be solved using a partly Pb substituted compound, involving a new modulation type for the [BiO] layers.[3]

The main structural characteristics of these different phases can also be compared with structural configurations of original phases in the same systems (collapsed phases, misfit layer compounds)[4,5] pointing out the intrinsic character of some local Bi-O arrangements. The different modulated configurations are then the results of the accomodation of these structural blocks in long range order agencements.

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