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Symmetry Studies of Ferroic Structures with the Bilbao Crystallographic Server. Moisés I. Aroyo^a, J. Manuel Perez-Mato^a, Daniel Orobengoa^a. ^a*Department of Solid State Physics, University of the Basque Country, Bilbao, Spain.*

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The Bilbao Crystallographic Server [1] is a free web site with crystallographic databases and programs available at <http://www.cryst.ehu.es>. The server is built on a core of databases that contains data of the *International Tables for Crystallography*, Vol. A (*Space-group Symmetry*), Vol. A1 (*Symmetry Relations between Space Groups*) and Vol. E (*Subperiodic Groups*). More specialized crystallographic software is also available and distributed in shells according to different topics: group-subgroup relations of space groups, solid-state physics and crystal chemistry applications or representation theory.

The aim of the contribution is to report on the databases and tools available on the server facilitating the symmetry-mode analysis of distorted structures of displacive type, the ferroic structures being a particular case. Starting from the experimental structures of the high- and low symmetry phases, it is possible to determine the global structural distortion that relates the two phases. The symmetry-modes compatible with the studied symmetry break are calculated, their orthonormalization permits the decomposition of the global distortion into symmetry-mode contributions, and the determination of the corresponding polarization vectors. This type of analysis allows the determination of the correlated atomic displacements that correspond to the structural instabilities at the origin of the ferroic distortion, *i.e.* the so-called *primary modes*, and to distinguish them from *secondary ones*, weaker distortions of limited relevance for the transition mechanism.

The server also offers online tools for the evaluation of the pseudosymmetry of a given structure with respect to a supergroup of its space group [2]. The detection of structural pseudosymmetry as the consequence of a small distortion of a higher symmetry, described by a supergroup of the crystal space group, is a powerful method for the prediction of new ferroelectric and ferroelastic materials. For example, polar structures with pseudosymmetry related to a hypothetical non-polar configuration can be considered as good candidates for ferroelectrics.

There are also computer tools for systematic studies of the possible transition paths of phase transitions with no group-subgroup relation between their phases [3]. The method is based on the assumption that the transformation involves, at least locally, an intermediate “hypothetical” configuration corresponding to a common space subgroup of the two end phases. The structure-dependent characterization of the proposed mechanisms and an evaluation of their plausibility is achieved by the analysis of lattice strains and atomic displacements involved in the transition. The procedure proves to be very useful for the study of structural relationships between different phases of ferroic materials with no group-subgroup relation between the symmetries.

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Compositional Heterogeneities in Relaxor Ferroelectric Oxides. Karim Z. Baba-Kishi. *Department of Applied Physics, The Hong Kong Polytechnic University, Kowloon, Hong Kong.*

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Pb-based complex perovskite-structured relaxor oxides are a special class of ferroelectric compounds that exhibit outstanding pyroelectric properties, characterized by broad dielectric permittivity peak and diffuse phase transition. The structure of these compounds conform to the nominal chemical formula $A(B'_{1/2}B''_{1/2})O_3$, where the Pb atom is positioned on the A-site and the iso-valent or off-valent cations, occupy the crystallographically equivalent B' and B'' positions. Examples include $Pb(Sc_{1/2}Ta_{1/2})O_3$ and $Pb(Sc_{1/2}Nb_{1/2})O_3$. There are also the compounds with B'^{1/3} and B''^{2/3} that include $Pb(Mg_{1/3}Nb_{2/3})O_3$ and $Pb(Zn_{1/3}Nb_{2/3})O_3$. The relaxor ferroelectric state is confined to the disordered compounds in this group. As the degree of 1:1 long-range order (LRO) on the {111} planes increases, the relaxor state dissipates. Using various advanced microscopy techniques, e.g. HAADF, EELS and XEDS, including results recorded in a Cs-corrected STEM, it will be illustrated that the disorder in relaxors involve various forms of structural characteristics that include: 1:1 long-range order; mixed occupancy on the B-site positions [1]; development of superstructures related to higher chemical order (disparate from the 1:1 LRO); Pb displacement on the {110} planes that result in diffuse streaking along the <110> directions, and random occupational clustering of the Pb atoms on the A-site positions. It will be shown that a combination of these various forms of disorder may assist in establishing a unified approach to compositional heterogeneities in relaxors.

[1] K.Z. Baba-Kishi, C.W. Tai and X. Meng, *Philosophical Magazine*, 86, No.32, **2006**, 5031-5051.

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Beyond the Landau Theory: Unusual Phase Transitions in Some $R_aSb_bX_{(3b+a)}$ Salts (where R: Organic Cation; M:Sb, Br; X: Br, Cl). Anna Gagor^a, Ryszard Jakubas^b, Anna Piecha^b, Adam Pietraszko^a, Maciej Wojtaś^b. ^a*Institute of Low Temperature and Structure Research Polish Academy of Sciences, Okólna 2, 50-950 Wrocław, Poland.* ^b*Faculty of*