in the chimney ladders, the blocks are separated by planar interfaces, the interfaces in $NaCd_2$ form a minimal surface, the P surface.
Keywords: intermetallic structures, electronic structure calculations, aperiodicity

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Ordering as Occupational Modulations, and their Superspace Description
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A new perspective in the field of modulated structures has emerged with the use of so-called *crenel* occupational functions in one-dimensional modulations. These functions limit the atomic occupation to a certain interval along the internal space and, as in quasicrystals, we can talk of atomic domains. The concept of average structure becomes ambiguous and, in general, it is possible to define alternative average periodicities, the division of diffraction peaks between main and satellite reflections being not unique. Also, a clear borderline between composite and single modulated structure disappears. The use of crenel functions allows a very efficient unified description of homologous series of mixed layered compounds. Their composition dependent layer stacking sequences can be understood as *uniform* sequences, which order a minority motif as uniformly as possible. This uniform orderings are reflected in superspace into a so-called *closeness* condition of the corresponding atomic domains, forcing a direct relation between the modulation wave vector and the size of the domains, and therefore, composition. This *closeness* condition, earlier proposed in another context for quasicrystals, is a universal feature of these mixed layered compounds. We will show that it can also be used in (3+2)d superspace to obtain and describe uniform ordering schemes within two-dimensional lattices. Two-dimensional ordered patterns of vacancies observed in various materials can be explained within this framework.
Keywords: superspace, ordering, modulated structures

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Flexible Local Crystal Chemistry and its (modulated) Consequences
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There exists an extraordinarily broad range of compositionally and/or displacively flexible "modulated" crystalline materials (displacively flexible framework structures, materials susceptible to Fermi surface driven structural instabilities, substitutionally disordered solid solutions *etc*) whose reciprocal spaces at one temperature or the other exhibit either sharp satellite reflections and/or highly structured diffuse intensity distributions accompanying the strong Bragg reflections of an underlying, well-defined average structure. The existence of such additional scattering reflects strong local crystal chemical "rules" underlying, for example, the correlated rotations of neighbouring polyhedra in flexible framework structures, the local distribution of dopant ions in substitutionally disordered systems or the correlated displacements of neighbouring ions induced by temperature-dependent, charge density wave (CDW) type structural instabilities. The local crystal chemistry as well as the associated physico-chemical properties of such flexible phases can not be understood until such modulations are recognized and properly taken into account. The results of recent structural investigations of some flexible framework structures [1], of O/F ordering in transition metal oxyfluorides [2] and of the low temperature Kondo effect in ThAsSe [3] will be used to highlight these different types of local flexibility and their structural consequences.

[1] Liu Y., Withers R.L., *J. Solid State Chem.*, 2003, **172**, 431. [2] Brink F.J., Norén L., Withers R.L., *J. Solid State Chem.*, 2004, **177**, 2177. [3] Withers R.L., Vincent R., Schoenes J., *J. Solid State Chem.*, 2004, **177**, 701.

Keywords: modulated structures, adaptive systems, order-disorder

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Incommensurate Crystallographic Shear Structure of $Ba_xBi_{2-2x}Ti_{4-x}O_{11-4x}$ (x=0.275)
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The 4d structure of the title compound consists of atoms with sawtooth-like modulation functions and step-like occupation functions (occupation domains, OD). Most of the structural parameters defining OD are concerned with γ (=0.36693), the **c*** component of the modulation wavevector. The 3d structure is closely related to the β-$Bi_2Ti_4O_{11}$ structure, where the linkage of TiO_6 coordination octahedra constructs the host framework providing the one-dimensional tunnel-like space for the accommodation of Bi ions. Domain boundaries are introduced by a kind of the crystallographic shear (CS) operation in the present structure. Namely, the layer unit consisting of $Bi_2Ti_2O_8^{2-}$ is removed from the β-$Bi_2Ti_4O_{11}$ structure, and remained blocks are displaced to fill the gap. The negative charge of the removed unit is compensated by the substitution of Ba^{2+} ions for Bi^{3+} ions in tunnels.

The unique character of this incommensurate structure is the aperiodic insertion of domain boundaries in contrast to usual (*i.e.* commensurate) CS structures. To the best of our knowledge, the present study is the first example of the quantitative analysis of the incommensurate CS structure.
Keywords: incommensurate structures, higher-dimensional structure analysis, crystallographic shear structures

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Solving Modulated Crystals of Profilin:Actin
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Cellular motility, regulated through cytoplasmic profilin:actin (PA) interactions, is intrinsic to many cellular functions. Profilin both sequesters actin monomers and delivers it to filamentous assemblies. Detailed structural information on monomeric actin in complexes with various actin binding proteins have been provided by X-ray crystallography, but currently no atomic structures for filamentous actin have been determined, although several hypothetical models have been proposed. PA crystals retain the dynamic nature of actin and provide an excellent way to study the protein-protein interactions involved in filament formation. When exposed to conditions known to promote actin filament formation, PA crystals can be transformed into a modulated state characterized by unusual off-lattice satellite reflections. Evidence suggests the presence of a modulated or periodic structure that is occupied by metastable actin filaments. Methods to determine modulated structures are known to "chemical" crystallographers, yet macromolecular crystallographers have, to date, mostly avoided this class of crystal structures. The biological importance of these challenging modulated crystals of PA has prompted the development of methods to solve the underlying atomic structure(s). Progress on this structure determination will be presented.
Keywords: macromolecule, incommensurate, modulation