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.

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