A new example of the unified structural description in superspace of perovskite-related compounds of type $A_nB_nO_{3n+2}$. The case $n > 5$ with A = Na and Ca, B = Nb.

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The structures of the various members of the homologous $A_nB_nO_{3n+2}$ family composed of ABO_3 perovskite layers can be described to a first approximation in terms of the stacking of (110)-bounded perovskite slabs. Inside these single slabs the number of atomic layers varies systematically with composition. In the classical three-dimensional standard crystallographic approach, one must describe for each composition the corresponding structure with its particular cell parameters and space group separately, while the recently proposed unified higher-dimensional superspace model [1] is essentially common to the whole compound series: the layer stacking sequences, which are composition-dependent, are interpreted in terms of the structural modulation of a common underlying average structure. Applying the superspace approach, the structure is interpreted as a modulated structure with discontinuous atomic domains. These atomic domains are described by step-like (crenel) occupational functions and introduce automatically the layered configuration of the three-dimensional structure in real space. The average interlayer separation distance is directly related to the average structure periodicity along the layer stacking direction, while an inherent modulation thereof is produced by the presence of different types of layers (particularly vacant layers) along this stacking direction. The superspace group is unique and independent of the composition, while the modulation wavevector and the width of some occupation domains vary linearly with composition.

We have recently shown [3] that the structure of $NaCa_4Nb_5O_{17}$ [2] follows in general the superspace model proposed for the whole family $A_nB_nO_{3n+2}$ [1] (A = Na and Ca, B = Nb and $n = 5$). The underlying superspace group was determined and shown to be a subgroup of the maximal symmetry group defined in [1]. This superspace group is expected to be valid for the whole [Na,Ca] series. We present here the results of the investigation of another compound of this series with $n > 5$, where this unified superspace description is further checked.

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