s3.m11.p9 **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.** Andreas Schönleber[a], F. Javier Zúniga[a], J. Manuel Perez-Mato[a], Tomasz Breczewski[b] and Jacques Darriet[c], [a]*Departamento de Física de la Materia Condensada, Universidad del País Vasco, Apto. 644, 48080 Bilbao, Spain,* [b]*Departamento de Física Aplicada II, Universidad del País Vasco, Apto. 644, 48080 Bilbao, Spain, and* [c]*Institut de Chimie de la Matiere Condensée de Bordeaux, 87 Avenue du Dr A. Schweitzer, 33608 Pessac Cedex, France. E-mail: wmxscxxa@lg.ehu.es*

Keywords: Superspace approach; Modulated structure; Perovskite-related compounds

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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s3.m11.p10 **From harmonic modulations to quasicrystals.** Grzegorz Urban and Janusz Wolny, *Faculty of Physics and Nuclear Techniques, AGH University of Science and Technology, Poland. E-mail: urban@novell.ftj.agh.edu.pl*

Keywords: Modulated structures; Quasicrystals; Fibonacci chain

Quasicrystals belong to the incommensurately modulated structures. The most famous in 1D is the Fibonacci chain, which consists of quasiperiodic tiling of two bounds (*L* and *S*) and can be also obtained by the cut and projection of the quadratic 2D structure onto physical space. Diffraction pattern of the Fibonacci chain consists of main reflections and their satellites only. The modulation vector is $\tau \approx 1.618$ (the golden mean value) times shorter then the average distance between the nodes.

In one dimension, the positions of an n-th atom in higher-harmonic modulated structure is given by:

$$x_n = na + A_1 \sin(qna) + A_3 \sin(3qna) + ... + A_m \sin(mqna),$$

where q is the modulation vector and A_m - the amplitude of the m-th component of the modulation. The diffraction pattern of such structure can be easily calculated in an average unit cell approach [1,2], leading to universal probability distribution $P(u)$ of atomic positions in respect to the reference lattice points. Fourier transform of such distribution gives the structure factor. The autocorrelation function of the average unit cell leads to the average Patterson function. This function can be also obtained directly from the diffraction pattern by its Fourier transform and contraction to the average unit cell.

In this paper it is shown that for higher-harmonic modulated structure given by

$$x_n = na + A\sum_{m=1}^{\infty} \frac{1}{m} \sin\left[m \frac{2\delta a}{b} n \right]$$

with $a=1+1/\tau^2$, $b=a\tau$ and $A=0.19673$, one gets the Fibonacci tiling of two bounds (S=1, L=t). In this case the average unit cell is described by the probability distribution of rectangular shape. The average Patterson function:

$$G_a(u) = \lim_{n_1 \to \infty} \left(\frac{1}{n_1} \sum_{n=0}^{n_1} G(x \mid x = u + n\lambda) \right)$$

(where $G(x)$ is a normal Patterson function obtained by Fourier transform of the diffraction pattern) is also an autocorrelation function of the average unit cell probability distribution:

For the analysed example the average Patterson function has a triangular shape, which leads to quasiperiodic diffraction pattern. Analysing of the structure for two reference lattices, one for a and the other one for b, brings to the probability distribution $P(u,v)$ which is non zero only along a line $v = -\tau^2 u$, which is characteristic for most of quasicrystals.

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