

quasicrystal is used to parameterize the structure of $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$. Due to the constraint of the space group of $P10_5/mmc$, the atom positions in the clusters can be displaced only in the radial direction. These parameters were determined by minimizing a sum of residual square error χ^2 calculated from intensities of experimental and simulated CBED patterns. The final parameters show a good correspondence to the results of X-ray diffraction study [2].

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Keywords: quasicrystals, convergent-beam electron diffraction, structure refinement

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Superstructure solution of decagonal Al-Co-Ni using 5D and 3D approaches

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The structure study of Co-rich decagonal $\text{Al}_{72.5}\text{Co}_{18.5}\text{Ni}_9$ using 5D and 3D approaches is presented. Analysis of the reciprocal sections reveals that we have a well-ordered superstructure with double (four-layer) periodicity along the 10-fold axis with the 5D space group $P10_522$. Knowledge of the structure of the fundamental cluster(s) of this modification is the prerequisite for modeling the structure of all six known modifications of decagonal Al-Co-Ni as a function of the Co/Ni ratio. An average structure solution was obtained by 5D ‘charge flipping (CFM)’ and ‘low-density elimination (LDE)’ methods. To study the peculiarities of the real structure (superstructure) we used 3D pseudo-approximant technique together with the 5D ‘charge flipping (CFM)’ and ‘low-density elimination (LDE)’ for the structures with two-layer and with four-layer periodicity along the 10-fold axis. Based on the structure solution results we propose fundamental clusters for average and real structures for this modification.

Keywords: aperiodic structures, structure determination and analysis, X-ray diffraction

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New boron-based decagonal approximants

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Finding a nonmetallic quasicrystal is one of the biggest challenges in experimental quasicrystal research today as it will provide further insights into the mechanisms governing quasiperiodic order [1]. Boron-based ternary compounds are particularly promising. On the one hand, for B-Mg-Ru a decagonal quasicrystal has been predicted [2]. On the other hand, decagonal approximants have already been found in the systems B-Mg-Ru [3, 4] and B-Sc-Ru [5]. Another truly interesting, yet completely uninvestigated system is B-Ti-Ru, as the atomic radius of Ti is similar to those of Mg and Sc. Additionally, the higher melting point of Ti compared to Mg facilitates sample preparation considerably. The exact knowledge of new approximant structures will be a helpful tool on the way to a boron-based,

nonmetallic quasicrystal. Samples were prepared by mixing high purity powders of B and Ru with pieces of high purity Ti wire according to the composition of the predicted B-Mg-Ru quasicrystal. The samples were annealed at temperatures above 1000°C and water-quenched. Single crystal X-ray diffraction and subsequent refinement confirmed at least one new orthorhombic phase. It could be shown that replacing Mg or Sc by Ti leads to the formation of at least one stable decagonal approximant. It will be discussed how different structure types of boron-based approximants will be the basis of designing a nonmetallic quasicrystal.

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Keywords: approximants, boron-based quasicrystals, B-Ti-Ru

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X-ray analysis of phason strains for one-dimensional Al-Ni-Co quasicrystals

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Detailed examinations of peak profiles and positions of the Bragg peaks are carried out with the high-resolution single-crystal X-ray diffraction for one-dimensional quasicrystals of a Co-rich Al-Ni-Co decagonal phase. Due to a Q-perpendicular dependence of peak shifts from ideal Bragg peak positions, these quasicrystals were classified into some groups with different phason strains. These groups were identified as the ideal one-dimensional quasicrystal and some one-dimensional quasicrystals with small linear-phason strains. For the linear-phason strain along a D-direction, the same value of $\theta_1 = -\tau^{-8}$ was observed for all single crystals. On the other hand, for the linear-phason strain along a P-direction, $\theta_2 = 0$ (the ideal one-dimensional quasicrystal), $-\tau^{-13}$, and $-\tau^{-11}$ were observed. This suggests a structural relation between a one-dimensional quasicrystal and an approximant crystal for the Co-rich Al-Ni-Co decagonal phase.

Keywords: quasicrystals, single-crystal X-ray diffraction, phason strain

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Elastic properties of 2-dimensionally quasiperiodic and 1-dimensionally periodic quasicrystals

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Quasicrystals with two-dimensional quasiperiodic and one-dimensional periodic structure are considered whose symmetry can be described by embedding the three-dimensional (3D) physical space V_E in a 5D superspace V , which is the direct sum of V_E and a 2D internal space V_I . A displacement \mathbf{v} in V can be written as $\mathbf{v} = \mathbf{u} + \mathbf{w}$, where \mathbf{u} is in V_E and \mathbf{w} is in V_I . If the point group of the