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Decagonal Al-Cu-Co had been modelled by Burkov [1], based on the electron microscopy [2] and x-ray diffraction data [3]. A variant of the model was latter founded over the decagonal tiling of the two golden triangles, T*(A4) [4], projected from the 4-dimensional root lattice A_4. The recent STEM data of the same material [5] show that the previous models must be updated. We try to interpret the new data also as a decoration of the decagonal tiling T*(A4).

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Keywords: decagonal quasicrystal, modelling, tiling

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The pseudosymmetry of atomic structures in crystals of organic and organoelemental compounds

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A study of translational and inversion pseudosymmetry of crystal structures retrieved from the Cambridge Structural Database is presented. In this work, the results of translational and inversion pseudosymmetry investigation of 211162 crystal structures are given. The value of the pseudosymmetry determined as degree of invariance of crystal electron density function. The analysis method for pseudosymmetric structure was offered. The percentage of crystals with pseudo inversion (~18%) is higher than the percentage of crystals with translational pseudosymmetry (~5%). The increase in symmetry with respect to the inversion center has two mechanisms. The first one is special superposition of orbits which are invariant with respect to the inversion. The second one is the occupancy of special orbits by heavy atoms. Besides, there are some space groups where every orbit is invariant with respect to inversion. The crystal described by a locally centrosymmetric group will be pseudo-invariant with respect to the center of inversion if it has a heavy atom. In the case of translational pseudosymmetry, there are no groups where every orbit is invariant with respect to superlattice translation. In all the crystals, the increase in the symmetry depends on a special distribution of atoms in the unit cell. Heavy atoms occupy special positions whose location is pseudo-invariant with respect to pesudotranslations.

Keywords: pseudosymmetry, pesudotranslation, pseudoinversion

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Local structure study in decagonal quasicrystals

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Atomic short-range order (SRO) and size effect (SE) were investigated in Al-Ni-Co[1] and Al-Ni-Fe[2] decagonal quasicrystals. $Al_{72}Ni_{20}Co_8$ is described by an ideal Penrose tiling without a phason. $Al_{72}Ni_{20}Co_8$ possesses an order-disorder phase transition at high temperature. SRO diffuse scattering appeared around the ideal positions of superstructure reflections. Correlation length is estimated to be 2 nm. The SRO diffuse scattering disappeared completely above T_c. By anomalous X-ray scattering and quantitative analysis, total diffuse scattering is decomposed into three kinds of partial diffuse intensities, which are derived from SRO on a quasiperiodic lattice. Also, two significant points are found; i) SE is quite remarkable only between Al and transition metal (TM), not between TMs. ii) The partial diffuse intensity in TM pairs (Ni-Co or Ni-Fe) is largest. These suggest that decagonal quasicrystals suppress the additional strains, which are generated by SE. The effect is connected with the phase stability of an Al-based decagonal quasicrystal in addition to phason contributions. On the other hand, reverse Monte Carlo refinements can determine the Warren-Cowley SRO parameters. Here, SRO parameters are the conditional average of a pair-correlation function. SRO in decagonal quasicrystals develops over the medium-range, though SRO is very weak. It is considered that the peculiar feature is similar to medium-range order (MRO) in amorphous alloys. The idea of MRO parameters[3] will be applied to decagonal quasicrystals.

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Keywords: short-range order, diffuse scattering, size effect

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Structure refinement of a decagonal $Al_{72}Ni_{20}Co_8$ quasicrystal by convergent-beam electron diffraction

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In order to perform structure refinement of quasicrystals in a nanometer area, we have developed a structural refinement method of the quasicrystals by using convergent-beam electron diffraction (CBED). In the present study, we applied the method to an $Al_{72}Ni_{20}Co_8$ alloy, which is known as a highly ordered decagonal quasicrystal. Zero-loss CBED patterns of a water-quenched $Al_{72}Ni_{20}Co_8$ with an energy-selecting slit of 10 eV were taken at the [11110] incidence, which is one of the two-fold axes. The probe size of electron beam was 10 nm in diameter. A dynamical CBED simulation was carried out on the basis of the Bethe method with about 250 beams including strong reflections observed in experimental CBED patterns. The structural model used in the present study consists of pentagonal (P) and Star-shaped (S) clusters with about a 0.4 nm radius, which are located at vertex positions of two different hexagon-boat-star tilings whose scales are mutually different by τ times [1]. A high-dimensional description of

quasicrystal is used to parameterize the structure of $Al_{72}Ni_{20}Co_8$. 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 $Al_{72.5}Co_{18.5}Ni_9$ 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 $P10522$. 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 on 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℃ 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 potions 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 **v** in V can be written as **v** = **u** + **w**, where **u** is in V_E and **w** is in V_I. If the point group of the