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

quasicrystal is crystallographic, it is assumed that **w** transforms as a vector in the plane perpendicular to the direction in which the crystal is periodic, but differently if the point group is 5-, 8-, 10- or 12-gonal. From the Neumann principle follow restrictions on the form of the phonon, phason and phonon-phason coupling contributions to the elastic stiffness matrix that can be determined by combining the restrictions obtained for a set of elements generating the point group of interest. For the phonon part, the restrictions obtained for the generating elements do not depend on the system to which the point group belongs. This remains true for the phason and coupling parts in the case of crystallographic point groups but, in general, breaks down for the non-crystallographic ones. The form of the symmetric 12 x 12 matrix giving the phonon, phason and phonon-phason coupling contributions to the elastic stiffness is presented in graphic notation.

Keywords: quasicrystals, elastic properties, piezoelectricity

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Successive phase transition of a Cd-Yb 1/1 crystalline approximant under high pressure

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The phase study of a Cd-Yb 1/1 approximant crystal over a wide pressure and temperature range is crucial for the comparison study between periodic and quasi-periodic crystals. Our previous X-ray diffraction study revealed that the Cd4 tetrahedra, the most inner part of the atomic clusters, exhibit various structural ordering in the orientation sensitive to pressure and temperature [1]. Five ordered phases appear in a P-T span up to 5.2 GPa and down to 10K. In this study we surveyed higher pressure region up to 30 GPa at room temperature. Single crystal diffraction experiments at SPring-8 (BL22XU) using a helium pressure medium in a diamond anvil cell elucidated that the crystal undergoes successive structural phase transition with an alternation of the period. The bcc phase at ambient pressure transformed to a 3-fold ordered phase at about 12 GPa, and to 4-fold one at about 20 GPa. These phases are different from those found at the previous study. These transitions would be induced by charge order at the Yb ion site, while those at the lower pressure region at low temperatures are dominated by the orientational ordering of the Cd4 tetrahedra.
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Keywords: quasicrystals, phase transitions in solids, high-pressure diffraction

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Aperiodic tiling structure with ten-fold symmetry in B-Ti-Ru rapidly solidified alloy

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We have been searching for decagonal quasicrystal (DQC) in B-Mg-Ru system, where stable or metastable DQC is predicted to exist by Michalcovic and Widom [1]. Four new approximant crystals have been discovered to form stably at a high temperature [2]. All the structure models can be described with tessellation of two subunits Boat and Hexagon. No QC has yet been discovered in B-Mg-Ru system. Rather higher temperature or rapid quenching would be needed. B-Mg-Ru alloy cannot be melted at normal pressures, so that Mg was replaced with the other elements. More than two approximants formed in the annealed alloys. The alloys prepared by arc melting were melt-quenched by copper single roll. A structure very similar to DQC was observed in some of the samples. The EDP shows ten fold symmetry and the scaling rule of the golden ratio. Diffraction spots are broad and the density of spots is less than that of well-ordered DQCs. The HAADF-STEM images indicated the local structure to be described as tessellation of the subunits Hexagon, Boat and Star oriented in ten-fold direction. Clusters with decagonal framework about 1.4nm in diameter are predominant. The tiling is not domain of crystals like multiple twins but an aperiodic structure. Analysis in five demensional space indicates that the structure has no long-range translational order such as quasipiriodicity, but has long-range ten-fold bond orientational order to show ten-fold symmetry as a whole.
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[2] Y. Miyazaki, J. T. Okada and K. Kimura, Phil. Mag., 87, 2701 (2007)

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HRTEM observation of displacement fields around dislocations in quasicrystals

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Originating in the quasiperiodic translational order, quasicrystals have a special type of elastic degrees of freedom, termed as phason degrees of freedom. Dislocations in quasicrystals are generally accompanied by the phason displacement fields in addition to the conventional displacement fields[1]. According to a generalized elastic theory of quasicrystals, several groups have attempted to deduce analytical expressions of displacement fields around various types of dislocations in quasicrystals. In contrast, there have been no experimental studies of displacement fields around the quasicrystalline dislocations. In this study, we have observed the displacement fields by high-resolution transmission microscopy (HRTEM) and compared them with the theoretical displacement fields to examine the validity of the generalized elastic theory of quasicrystals. The effects of phason elastic constants on the displacement fields have been discussed and evaluation of their values has been attempted.
[1] For a review, see K. Edagawa and S. Takeuchi, ‘Dislocation in Solids’ ed.By F. R. N. Nabarro and J. P. Hirth (Elservier B. V. 2007), Chap.76, pp367

Keywords: quasicrystals, dislocations, TEM