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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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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