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Structure of quasicrystals – scaling in real and reciprocal space

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Quasicrystals are aperiodic structures and there are no unit cells for them in physical space. Recently it was shown that structure of quasicrystals can be successfully described in physical space by statistical approach. The normal unit cell is replaced by an Average Unit Cell (AUC) [1,2], where atoms occupy the positions with some probabilities. Knowing the probability distribution one can calculate the structure factor and use it for the structure refining procedure [2-4].

In the presentation the concept of AUC is discussed. It is also shown that:

1. Structure refinement of quasicrystals can be done in physical space only by using the AUC approach.
2. AUC can be easily supported by higher dimension analysis by an oblique projection method.
3. With the AUC approach one can go beyond quasicrystals, even to more complicated structures with singular continuous diffraction pattern.

For all crystalline structures (including quasicrystals) one can define an appropriate scaling factor. After scaling of all the distances by such factor the self-similar structure is obtained. The same holds in reciprocal space. When scattering vector of any diffraction peak is multiplied by the scaling factor, another diffraction peak is reached. For ordinary crystals the scaling factors are the integer numbers, which leads to the periodic lattice. For modulated structures the scaling factors can be either rational or irrational numbers leading to the commensurate or incommensurate structures. For the model quasicrystals, like the Fibonacci chain, Penrose tiling or 3D Amman-Kramer tiling, the scaling factor is equal to the golden mean value $\tau \approx 1.618$. The irrational value of the scaling factor results in an aperiodic structure. One can approximate this value by rational numbers which leads to some approximants.

In the AUC approach the scaling properties of quasicrystals give a particular probability distribution of atomic positions. The distribution is no-zero only along a line and such linear relation for perfect quasicrystals essentially simplify the complicated calculations of the corresponding structure factor. For some rational approximation of τ the non-zero distribution becomes broader which effects the intensity of the diffraction peak at the inflated position of scattering vector. The width of the distribution at AUC approach can be used as an order parameter for the description of the critical behaviour of diffraction pattern for different approximants when the scaling factor approaches the golden mean value.

For selected model structures of quasicrystals the critical behaviour is discussed and the critical exponents are determined. Analytical expression for the structure factor calculated in AUC is discussed in the vicinity of the critical point at golden mean value.

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To the Model of a Decagonal Al-Cu-Co

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It is attempted to produce a model of atomic positions of decagonal Al-Cu-Co using only the images of the phase in the direct space. Up till now, there is a large HREM (high-resolution electron microscopy) image of Al65-Cu15-Co20 [1] and a STEM (scanning transmission electron microscopy)image of Al64-Cu22-Co14 [2], both taken along the c-axis, perpendicular to the quasiperiodic structure.The atomic positions, seen on the images taken along the c-axis should be related to an ideal 2-dimensional pentagonal tiling T*(A4), obtained by the projection from the 4-dimensional A4 root-lattice [3]. In Ref [4] was shown that the Burkov model [5], based on the same tiling T*(A4) overestimates the density of certain pentagonal local atomic configurations. The tiling is now placed over different local pentagonal atomic configurations and improves the model with respect to both above mentioned images of quasicrystals [1,2]. The atomic positions are related to the prototiles of the tiling T*(A4) and sorted into five classes with respect to the pentagonal module.The use will be made of the single 2-dimensional pentagonal cluster of atomic positions suggested in Ref [2]. For the 2-dimensional cluster a possible splitting along the c-axis into 5fold planes is proposed.

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Physical properties of the Cd_6R 1/1 approximants

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Quasicrytalline 1/1 approximants Cd_6R (R=Ca, Y, rare earth elements) are known as cubic systems made up of Tsai-type clusters located at the bcc lattice points [1]. A Tsai-type cluster is composed of four succesive shells, i.e., from the cluster center, a Cd_4 tetrahedron, a Cd_{20} dodecahedron, a R_{12} icosahedron and a Cd_{30} icosidodecahedron. These compounds are reported to exhibit an order-disorder type phase transition, which is interpreted as ordering of the Cd_4 tetrahedron at the center of cluster below T_c [2]. Besides the structural phase transition phenomena, also interesting are their physical properties, especially the magnetic property of 4*f* magnetic moments sitting on the vertices of the R_{12} icosahedron. Recently, we have found an occurrence of three succesive anti-ferro magnetic phase transitions in Cd_6Tb approximant [3], which is in a contrast with the cases of the isostructual Ag-In-R where spin glass-like behaviors, not long-range orders, are observed at