MS63.P06

Acta Cryst. (2011) A**67,** C624

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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Keywords: quasicrystal, structure, modeling

MS63.P07

Acta Cryst. (2011) A**67,** C624

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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Keywords: quasicrystal, decagonal, structure

MS63.P08

Acta Cryst. (2011) A**67,** C624-C625

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

low temperatures [4].

In the present work, we have prepared Cd_6R single grains by a self-flux method and have measured their physical properties such as electrical, thermal and magnetic properties. We have also performed high-magnetic field measurements up to ~50 Tesla at low temperatures down to 1.3 K.

For most of Cd_6R compounds, the magnetic susceptibility is found to obey the Curie-Weiss law, say, above 50 K, indicating that R atoms at the vertices of the R_{12} icosahedron are well localized in a trivalent state. At low temperatures, heat capacity exhibits peaks attributed to occurrences of long-range magnetic orders. In Cd_6Tb, measurements under high-magnetic field show two clearly meta-magnetic transitions below 10 Tesla. This result suggests that several magnetic states are nearly degenerate at low temperatures. Detail of the physical properties of Cd_6R will be discussed in the presentation.

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Keywords: quasicrystal, magnetism

MS63.P09

Acta Cryst. (2011) A**67,** C625

Synthesis of single-grained $Zn_{88}Sc_{12}$ quasicrystal and its electrical resistivity

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$Zn_{88}Sc_{12}$ icosahedral qusicrystal (iQC) has recently been discovered by Canfield et al.[1] It is a stable binary iQC and is expected to contain no chemical disorder. An interesting feature about the iQC is that two different shapes, i.e., morphologies, of single grains are obtained depending on the initial composition, the reason of which has not been understood[1]. In this study, we have prepared $Zn_{88}Sc_{12}$ single grains and investigated the electrical properties of the $Zn_{88}Sc_{12}$ single grains having two different morphologies.

Single-grained $Zn_{88}Sc_{12}$ quaicrystals were prepared using a self-flux method. Pure elements of Zn(6N) and Sc(3N) with initial compositions of $Zn_{100-X}Sc_X$ with X in the range between 1.5 and 4 were placed in an alumina crucible, sealed inside a quartz tube under argon atmosphere. The elements were melted at 860° C for 3h, and slowly cooled to 490～500 ° C . Then, single grains were separated from the melt using a centrifuge. The obtained grains are found to exhibit two types of growth morphologies as reported[1] depending on the initial composition; PD(Pentagonal Dodecahedron)-shaped grains were obtained for the initial compositions of $Zn_{96}Sc_4$, $Zn_{97}Sc_3$, $Zn_{97.5}Sc_{1.5}$, while RT(Rhombic Triacontahedron)-shaped grains were obtained for the initial compositions of $Zn_{98}Sc_2$ and $Zn_{98.5}Sc_{1.5}$.

Temperature dependences of the electrical resistivity ρ(T) are found to be almost the same for all the grains, exhibiting a negative temperature coefficient, which is a typical behavior of ternary iQCs. We note that the PD-shaped grains exhibit slightly higher values of the resistivity ratio ρ_{16K}/ρ_{290K} than the RT-shaped grains. In the presentation, the results on annealed grains will be also discussed.

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Keywords: quasicrystal

MS63.P10

Acta Cryst. (2011) A**67,** C625

Dislocation mobility in icosahedral quasicrystals

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A theoretical description of the dislocation motion in quasicrystals is developed. The hydrodynamic approximation is used in deriving the expression for dissipation losses of a moving dislocation. The continuum theory of dislocation mobility [1] and the dynamic equations of elastic and phason fields [2] are combined. Hence the dependence of dislocation mobility on vacancy concentration is found explicitly [3,4]. The numerical analysis of dislocation mobility shows that phason deformations make the major contribution to the drag of free dislocations in icosahedral quasicrysal Al-Pd-Mn. The influence of vacancies on dislocation mobility becomes noticeable only at very large vacancy concentration, $C_v > 10^{-3}$, and at very low dislocation velocity, $v_D < 10^{-8}$ cm/s.

The study of existing experimental data reveals the considerable contribution of mutual pinning of dislocations to their mobility in icosahedral quasicrystal. The expressions obtained for dislocation mobility are valid for temperatures close to the melting temperature since the role of mutual pinning decreases with the increase of temperature. Dislocation drag on pinning centers has a dominant role at lower temperatures.

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Keywords: quasicrystal, dislocation, mobility

MS63.P11

Acta Cryst. (2011) A**67,** C625-C626

Structural characterization of thin AlPdRe quisicristalline film formation during annealing process

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One of the possible ways to form ultrathin $Al_{70}Pd_{20}Re_{10}$ quasicristalline film is the annealing of 3-layer (Al/Pd/Re) structure. Layer-by-layer ion-plasma deposition allows forming thin quasicrystalline film with precisely controlled thickness and homogeneity. Deposition was performed in a vacuum system with a sputtering chamber in the form of a Penning cell by Kr assisted magnetron sputtering from separate pure materials targets. After deposition of a layered structure, the films were coated with a layer of aluminum oxide, which was formed by sputtering of aluminum in a krypton atmosphere with addition of oxygen. The aluminum oxide layer was deposited to prevent selective escape of elements from the film upon vacuum annealing. The concentration range for the films prepared coincided with the known range of quasicrystalline phase formation in bulk samples [1].

We have studied phase evaluation of Al/Pd/Re layered structures in-situ during heat treatment and layer intermixing on intermediate annealing steps ex-situ. In-situ phase evolution study was done with X-ray diffraction and ex-situ layers intermixing analysis was done with