

12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

PS-12.01.27 NEW CRYSTALLINE APPROXIMANTS OF DECAAGONAL QUASICRYSTALS IN Al-Co-Ni-Tb ALLOY, By R.C. Yu*, X. Z. Li, D. P. Xu*, Z. Zhang, W.H. Su* and K.H. Kuo, Beijing Laboratory of Microscopy, Chinese Academy of Sciences, P. O. Box 2724, Beijing 100080, P.R.China; * Department of Physics, Jilin University, Changchun 130023, P.R.China.

Four new orthorhombic approximants, C_1 , C_2 , C_3 , and C_4 , have been found in the $Al_{70}Co_{15}Ni_{10}Tb_5$ decagonal quasicrystals, which were prepared by the method of quenching from the fusion state under high static pressure 4.0 GPa. The lattice parameters of these orthorhombic phases are: C_1 , $a=2.28$ nm, $b=1.60$ nm, $c=5.46$ nm (B-type); C_2 , $a=6.1$ nm, $b=0.4$ nm, $c=8.4$ nm (P-type); C_3 , $a=6.1$ nm, $b=0.4$ nm, $c=8.4$ nm (B-type); C_4 , $a=3.68$ nm, $b=0.4$ nm, $c=3.2$ nm, respectively. The strong diffraction spots in the electron diffraction patterns of these phases show the same intensity modulation as those of the decagonal quasicrystals, implying a close structural relationship. The formation of these new crystalline approximants of the decagonal quasicrystals can be understood by substituting a rational ratio of two consecutive Fibonacci integers F_{n+1}/F_n ($F=1, 2, 3, 5, 8, 13, 21, \dots$) for the irrational $\tau=(1+\sqrt{5})/2$ in the two quasiperiodic directions in the decagonal quasicrystals. The larger the Fibonacci integer, the larger the lattice parameter and the closer the structure of the crystalline approximants to that of the decagonal quasicrystal. As $n \rightarrow \infty$, $F_{n+1}/F_n \rightarrow \tau$, the approximants \rightarrow the decagonal quasicrystal. In this context, the decagonal quasicrystal can be considered as the limiting case of this series of approximants with infinitely large lattice parameters.

PS-12.01.28 QUANTITATIVE EVALUATION OF PRIMARY AND SECONDARY AMMANN JAGS IN AN EIGHTFOLD QUASILATTICE. By J.C. Jiang*, H.L. Li and K.H. Kuo, Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, 100080 Beijing, China. Department of Materials Physics, University of Science and Technology Beijing, 100083 Beijing, China

The structure of $Mn_{80}Si_{15}Al_5$ octagonal quasicrystal on atomic scale was studied by high resolution electron microscopy (HREM) and image processing. A HREM image taken along the eight-fold axis shows numerous octagons consisting of eight bright image dots. As in electron diffraction patterns of this octagonal phase, the Fourier transform of the HREM image comprises both basic and satellite reflexions. The inverse Fourier transform of only basic reflexions gives a clearer image of octagons from which the basic quasilattice of the Mn-Si-Al octagonal quasicrystal can be obtained. By connecting all the bright dots in the Fourier filtered image, a tiling configuration of squares and 45° rhombi with an edge length of 2.5 \AA results. Both primary and secondary Ammann lines were drawn on this quasilattice and jags were clearly shown. They correspond to the tiling mistakes at the edge and vertex, respectively, of this eight-fold quasilattice. Consequently, phasons in this quasilattice can be quantitatively evaluated. Within an area of $58 \times 56 \text{ \AA}^2$, there are 254 squares and 349 rhombi. Of the 1206 edges and 672 vertices, altogether 66 primary and 34 secondary tiling mistakes have been found. Broadly speaking, this is a phason-perturbed Penrose or Ammann tiling with eightfold symmetry, but not a random tiling of squares and 45° rhombi.

PS-12.01.29 DYNAMICAL SIMULATIONS OF DIFFRACTION CONTRAST IMAGE OF DISLOCATIONS IN ICOSAHEDRAL QUASICRYSTALS. By Z.G.Wang**†, Z.Zhang, M.X.Dai‡ and R.Wang‡, Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, Beijing 100080, China, †Department of Material Physics, University of Science and Technology Beijing, Beijing 100083, China, ‡Department of Physics, Wuhan University, Wuhan 430072, China

In studies of defects in normal crystals, simulations of diffraction contrast images have been extensively used to characterize these defects quantitatively. Recently, the defects in quasicrystals (QCs) have also been observed by using electron diffraction contrast images. Due to the unusual contrast behaviors of these dislocations caused by the incommensurate nature of the quasicrystal, further simulations of these dislocations are necessary. In present paper, the contrast of dislocations in icosahedral QCs have been simulated by using a computer program based on the dynamical diffraction theory extended to QCs. For the simulation, we use a first order approximation of a strain field of a dislocation in icosahedral QCs. By variation of crystallographic parameters and imaging conditions, the diffraction contrast images of edge-, screw- and mixing-types of dislocations in icosahedral QCs were simulated systematically. The simulated results agree well with the experimental images.

PS-12.01.30 STRUCTURE OF ORTHORHOMBIC Al_3Co . By X.Z. Li*, X.L. Ma, and K.H. Kuo, Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P O Box 2724, Beijing 100080, China.

A new Al_3Co with an orthorhombic unit cell ($Pn\bar{m}n$, $a=1.444$, $b=0.812$, $c=1.225$ nm) occurs frequently together with the monoclinic $Al_{13}Co_4$ (Cm , $a=1.5183$, $b=0.8122$, $c=1.2340$ nm, $\beta=107.67^\circ$). $Al_{13}Co_4$ has a layer structure. Its (010) layer at $y=0$ being composed of a network of Co pentagons and 36° rhombi. By a shift of $0.39c$ along [001] or the length of a side of pentagon (marked by thick arrows), the pentagons and rhombi on the two sides of the boundary reunite and form a new tessellation conforming to the orthorhombic Al_3Co lattice (corners outlined). Other layers can be treated in the same way. In other words, these two phases have the same subunits of pentagonal prism and antiprisms (icosahedra) but differently arranged. Thus, the structure of Al_3Co was derived from that of $Al_{13}Co_4$, and this structure was confirmed by X-ray powder diffraction analysis and high-resolution electron microscopy.

