12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

12.01 – Quasicrystals and Incommensurate Crystal Structures

OCM-12.01.01 THE STRUCTURE OF DECAGONAL QUASICRYSTALS. By W.Steurer*, T.Haibach and B.Zhang, Institut für Mineralogie der Universität Hannover, Germany.

Basing on single-crystal X-ray structure analyses of decagonal phases in the systems Al-Ni-Co, Al-Cu-Co, Al-Mn, Al-Mn-Pd and Al-Cu-Fe-Cr, models for the two types of decagonal quasicrystal structures with 4 Å and 12 Å translation period, respectively, were derived. The structures were determined using the higher-dimensional embedding method. The qualitative 5-dimensional structure models obtained from the Patterson functions were refined by the least-squares technique to R-factors between 0.07 and 0.15 for up to 450 unique reflections. The phases of structure amplitudes obtained by this way were used as starting set for high-resolution electron density calculations employing the maximum-entropy method (MEM). From the resulting maps columnar clusters were identified as basic structural units in accordance with HRTEM results. Their quasiperiodic distribution can be interpreted in terms of a context dependent decorated rhombic tiling. A weak matching rule results from the formation of infinite networks of interconnected and interpenetrating closed and open icosagonal rings consisting of alternating pentagonal and rectangular structure elements (Fig. 1). This network may be realized in many ways stabilizing the quasiperiodic structure by entropy. Periodic structures can be generated using these unit tiles only by opening all icosagonal rings.

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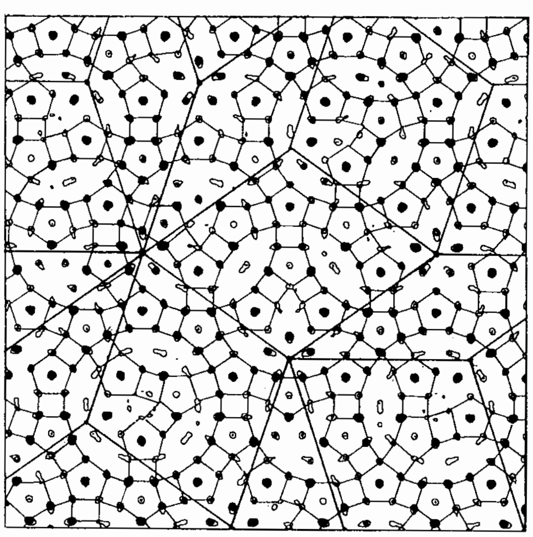

Fig. 1 60x60 Å^2 parallel space section at x_3=1/4 of the MEM electron density map of decagonal Al-Ni-Co showing the network of interconnected icosagonal rings of alternating pentagonal and rectangular structure elements. The rhombic tiling is also drawn in. The Y-like strips inside the icosagonal rings may flip to alternate positions.

OCM-12.01.02 ELECTRON DIFFRACTION AND ELECTRON MICROSCOPE STUDY ON DECAGONAL QUASICRYSTALS OF Al-Cu-Co ALLOYS. By K. Tsuda, K. Saito, M. Tanaka, *A.P. Tsai, *A. Inoue and *T. Masumoto, Research Institute for Scientific Measurements, Tohoku Univ., *Institute for Materials Research, Tohoku Univ., Japan.

Decagonal quasicrystals of $Al_{70}Cu_xCo_{30-x}$ ($x = 6, 8, 10, 12$) and $Al_{65}Cu_xCo_{35-x}$ ($x = 15, 20$) alloys have been investigated by convergent-beam electron diffraction (CBED), selected area diffraction (SAD) and the dark-field image method. These alloys were produced in ribbons using a single-roller melt-spinning apparatus. The CBED patterns taken at an incidence parallel to the decagonal axis (c-axis) clearly exhibited fivefold rotation and mirror symmetry. As a result, the alloys have been revealed to be noncentrosymmetric as well as the $Al_{70}Ni_{15}Fe_{15}$ alloy, which is the first noncentrosymmetric quasicrystal (M.Saito et al., Jpn. J. Appl. Phys., 1992, **31**, L109-L112.).
The alloys of Al-Cu-Co have been found to have a lattice period of 0.4nm in the c-axis from the SAD patterns. Using the dark-field image method, inversion domains with an antiphase shift of $c/2$ at the domain boundaries have been observed as was in the $Al_{70}Ni_{15}Fe_{15}$ alloy (K.Tsuda et al., Jpn. J. Appl. Phys., 1993, **32**,129-134; M.Tanaka et al., J. Noncrystalline Sol., 1993, to be published).
The alloys of $Al_{70}Cu_xCo_{30-x}$ ($x = 6, 8$) exhibited more high-order diffraction spots in the SAD patterns and better symmetry in the CBED patterns than the alloys with the composition of Cu $x \geq 10$. It is worth while to note that the electron-atom ratios (e/a) of $Al_{70}Cu_xCo_{30-x}$ ($x = 6, 8$) are respectively 1.77 and 1.82, and are nearer to a value of 1.75, which is proposed for the stable quasicrystals, than the other alloys of $x \geq 10$.

OCM-12.01.03 **STABLE DECAGONAL AlCuCoSi PHASE: A PHASON-PERTURBED QUASIPERIODIC CRYSTAL. By Z.Zhang*, H.L.Li, and K.H.Kuo, Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O. Box 2724, 100080 Beijing, P.R. China.**

X-ray diffraction (Steurer,W. and Kuo,K.H. (1990). *Acta Cryst.* B46, 703-712) and STM studies of the stable AlCuCo decagonal quasicrystal support the Penrose tiling model of quasicrystals. On the other hand, a previous electron-microscopic study supports the random tiling model (Chen,H., Burkov,S.E., He,Y., Poon,S.J. and Shiflet,G.J. (1990). *Phys.Rev.Lett.* 65, 72). However, our high-resolution electron microscopic images of the stable $Al_{62}Cu_{20}Co_{15}Si_3$ decagonal quasicrystal can be interpreted as a phason-perturbed Penrose tiling. If the centers of the small decagon subunits in an image are connected, a tiling of pentagons, 36° and 72° rhombi, and others is obtained. We index the vertices in this tiling by five integers and lift them to the 5D (five-dimensional) space and then project them onto the 2D perpendicular space. About 10% of them are lying outside of the decagon window, implying the presence of some phasons in this quasiperidic lattice. This is quite different from a previous study mentoned above, which is quite divergent and extends to a wide region. Another important property of this projection is the mean-square fluctuation of the perpendicular projection. For an ideal Penrose tiling this value is a constant. The random tiling theories claim a logarithmic increase of this quantity with N, the number of vertices. In the previous work, this has indeed been found, and was considered to be a strong evidence to support the random-tiling model. However, our experimental results show almost unchanged mean-square fluctuation with N. This favours the Penrose tiling model.

