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PS-12.01.09 REPEATED ELBOW TWINNING OF $\text{Fe}_4\text{Al}_{13}$ SHOWING DIFFRACTION PATTERNS WITH DECAGONAL PSEUDOSYMMETRY.

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$\text{Fe}_4\text{Al}_{13}$ is formed by peritectic reaction at 1430 K from Fe_2Al_5 and the melt, C2/m, mC101, $a = 15.489$, $b = 8.0831$, $c = 12.476$ Å, $\beta = 107.72^\circ$ (Black, Acta Cryst., 1955, 8, 43-48 and 175-182). Multiple twinning was observed not only in $\text{Fe}_4\text{Al}_{13}$, but also in the isotypical compound $\text{Ru}_4\text{Al}_{13}$ (Edshammar, Acta Chem. Scand., 1965, 2124-2130) as well as in the ternary isotypical phase $\text{Ni}_3\text{Zn}_6\text{Ga}_4$ (Rajasekharan, Sarah & Schubert, Z. Metallkd., 1982, 73, 526-529). Twins and planar defects were recently observed in $\text{Fe}_4\text{Al}_{13}$ by means of HREM (Tsuchimori, Ishimasa & Fukano, Phil. Mag. B, 1992, 66, 89-108). In the present study $\text{Fe}_4\text{Al}_{13}$ was investigated in the concentration range from $x_{\text{Al}} = 0.75$ up to $x_{\text{Al}} = 0.77$ by means of X-ray diffraction, scanning electron and optical microscopy. In contrast to the neighbouring phase Fe_2Al_5 which does not show any polymorphic transformation, metallographic investigation of the structure of $\text{Fe}_4\text{Al}_{13}$ yielded an indication for a phase transformation. Hollow prismatic lamellae were observed in the $\text{Fe}_4\text{Al}_{13}$ alloys by the scanning-electron-microscopy investigations. They were interpreted as composite crystals formed by repeated elbow twins with the twin plane (100), (001) and (201). An atomistic model showing pentagonal pseudosymmetry is discussed in direct space for the repeated elbow twins of $\text{Fe}_4\text{Al}_{13}$. Guinier photographs of splat-cooled alloys $\text{Fe}_{100-x}\text{Al}_x$ ($x = 0.75 \dots 0.77$) showed diffraction lines of a new phase homoeotypic to $\text{Fe}_4\text{Al}_{13}$, oB50, $a = 7.733(3)$, $b = 4.021(2)$, $c = 23.688(9)$ Å, $c/a = \tan 72^\circ$. The relationship between this oB = q unit cell and the monoclinic unit cell of $\text{Fe}_4\text{Al}_{13}$ is $(a, b, c)_q = (a, b, c)_m(1/2, 0, 1/2; 0, 1/2, 0; 0, 0, 2)$, i.e. $a_q = a_m/2$ etc. The low-temperature monoclinic structure $\text{Fe}_4\text{Al}_{13}$ is a displacive variant of the high-temperature orthorhombic phase $\text{Fe}_4\text{Al}_{13}(h)$. A twinning model is discussed in reciprocal space for structures with orthorhombic face centred Bravais lattices oB (oA, oC) having an axial ratio $c/a = \tan 72^\circ$, ($b/c, b/a = \tan 72^\circ$), i.e. the ratio of the interplanar spacings $d_{002}/d_{101} = (1 + \sqrt{5})/2 = \tau$ ($d_{020}/d_{011}, d_{020}/d_{110} = \tau$) (golden mean). Composite crystals (repeated elbow twins) of these oB-structures which have the common direction $[010]_q = [010]_m$ and showing the twin plane $\{101\}_q$ i.e. twin planes $\{001\}_m$ and $\{201\}_m$ yield diffraction patterns $(h01)_q = (h01)_m$ of decagonal pseudosymmetry; cf. electron diffraction pattern of twinned $\text{Fe}_4\text{Al}_{13}$ (Fung, Zou & Yang, Phil. Mag. Lett., 1987, 55, 27-32, Fig. e).

PS-12.01.10 X-RAY DIFFRACTION PATTERNS OF ONE DIMENSIONAL QUASICRYSTALS. By H. Terauchi, M. Ishida, N. Sano, H. Kasatani and K. Sakaue, Department of Physics, Kansai-Gakuin University, Nishinomiya 662, Japan.

It is of great interest to study one-dimensional (1D) quasicrystals in which quasiperiodic orders may be established. The most typical 1D quasiperiodic order is found in the lattice with a second-order Fibonacci sequence, $S_r = S_{r-1} + S_{r-2}$. The lattice is fabricated by molecular beam epitaxy techniques with semiconductor materials. The diffraction pattern of the lattice shows many satellite peaks assigned by the golden mean τ related to a diagonal value of a regular pentagon (H. Terauchi *et al.*, J. Phys. Soc. Jpn., 1988, 57, 2416). Of course, quasiperiodic lattices with third-order Fibonacci sequences such as $S_r = 2S_{r-1} + S_{r-2} - S_{r-3}$ are fabricated and here the diffraction peaks are assigned by two diagonal values of a regular heptagon (H. Terauchi *et al.*, J. Phys. Soc. Jpn., 1990, 59, 405).

The other 1D quasiperiodic orders are seen in a Thue-Morse lattice (F. Axel and H. Terauchi, Phys. Rev. Lett., 1991, 66, 2223) and a dragon lattice (H. Terauchi *et al.*, J. Phys. Soc. Jpn., 1992, 61, 1141), where the sequences are given by $S_r = S_{r-1} + S_{r-1}$ and $S_r = S_{r-1} + X + S_{r-1}$, respectively. These 1D quasiperiodic lattices give the curious diffraction patterns.

The marked differences of the diffraction patterns in the above four quasiperiodic orders are discussed, in terms of the correlation lengths as well as the self-similarities.

PS-12.01.11 GEOMETRICAL MODE ANALYSIS OF INCOMMENSURATE RE-ENTRANT MODULATIONS: $(\text{C}_3\text{H}_7\text{NH}_3)_2\text{MCl}_4$ M=Cu, Mn, Cd. By N. Achiwa*, H. Ikeda and Y. Yamauchi, Department of Physics, Kyushu University, Fukuoka 812, Japan.

We have developed a geometrical method to analyse molecular modulation modes in incommensurate crystal structures. From the three dimensional locus of each modulated atom which are pulled back to the original unit cell, that of a special mode, for example translational molecular displacement is subtracted. Then, the remainder figure suggests the next main mode, for example, rotational molecular mode. So we can find successively minor modes orthogonal to the subtracted modes by the trial and error method. The family compounds $(\text{C}_3\text{H}_7\text{NH}_3)_2\text{MCl}_4$ (M=Cu, Mn, Cd) show the following phase sequence: $\alpha \rightarrow \beta \rightarrow \gamma \rightarrow \delta \rightarrow \epsilon \rightarrow \zeta$, with the two incommensurate ϵ and γ -phases. These incommensurate structures were extensively studied using superspace symmetry. We have applied the new geometrical method to find the displacive modulation modes in the γ and ϵ phases. Figure 1 and 2 show loci of modulated atoms of $(\text{C}_3\text{H}_7\text{NH}_3)_2\text{CuCl}_4$ in γ (superspace group, $Pbca:(\alpha 00)ss0$, Doudin and Chapuis, 1990 B46 180.) and ϵ (superspace group, $BP2_1/b11:(0, 0.5, \xi)1\bar{1}$, Ikeda and Achiwa) phases. The main modes in the γ and ϵ phases are a translational modulation along the c axis and a twisted intra-molecule mode of propyl ammonium base, respectively, though in both phases each orbit of atomic modulation consists of multi-molecular modes. Finally, the amplitude of each molecular mode can be refined by least squares fitting of satellite structure factors.

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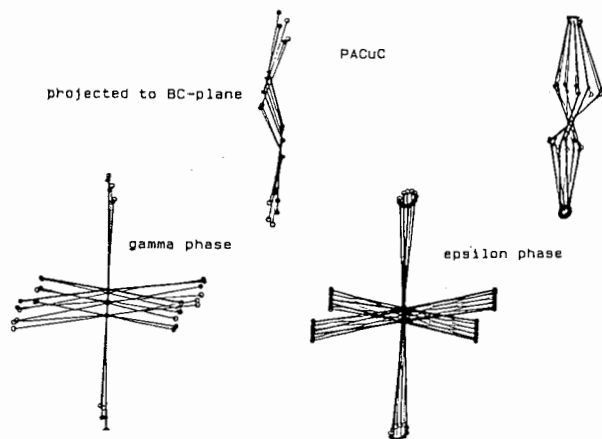


Figure 1 Loci of modulated atoms which are pulled back to the original unit cell of $(C_3H_7NH_3)_2CuCl_4$ in the γ (Fig.1) and ϵ (Fig.2) phases, looking from the a-axis.

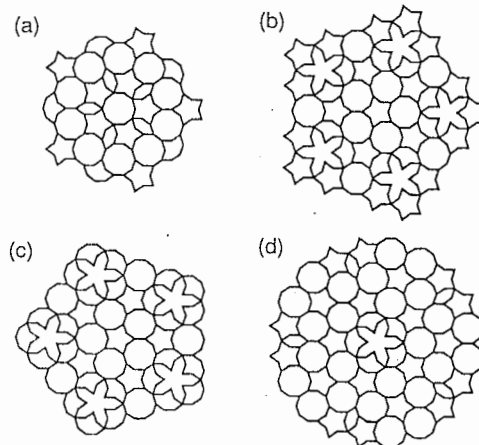


Fig. 1. The occupation domains of d-Al-Pd-Mn. (a) E at $z=0.25$, (b) D at $z=0.25$, (c) A at $z=0.38$ and (d) B at $z=0.44$.

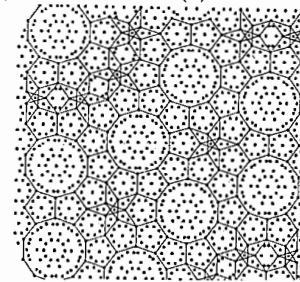


Fig. 2. The projection of d-Al-Pd-Mn along the 10-fold axis.

PS-12.01.12 A FIVE DIMENSIONAL MODEL OF DECAGONAL Al-Pd-Mn QUASICRYSTALS. By Akiji Yamamoto, Nat. Inst. Res. Inorg. Mat. Namiki 1, Tsukuba, 305, Japan

A structure model for decagonal Al-Pd-Mn quasicrystals (d-Al-Pd-Mn) is derived on the basis of theoretical considerations in 5-dimensional space. This can be considered to have a structure similar to d-Al-Mn. Both structures have a period of about 12 Å along the 10-fold axis. When the structure is described as a three-dimensional section of a five-dimensional decagonal crystal, the location of occupation domains is found from the Patterson map (Steurer, W., J. Phys. Condens. Matter, 1991, 3, 3397-3410). The occupation domains are derived based on the structure of Al_3Mn (Li, X. Z. et al, Phil. Mag. 1992, B 66, 331-340 and Hiraga, K. et al, Phil. Mag. 1993, to appear) and HREM images (Hiraga, K., Proc. Int'l. Conf. on Quasicrystals, St. Luis, 1992). The HREM images clarified that the arrangement of atom clusters is similar to that of pentagonal Penrose patterns with edge length of about 20 Å, while the crystal approximant Al_3Mn suggests the structure of the clusters and their linkage. The d-Al-Pd-Mn quasicrystal ($a=2.84$, $c=12.06$ Å, $P10_5/mmc$) consists of 10 flat (8 puckered) layers (Yamamoto et al. Acta Cryst, 1988, A44, 707-714), of which three layers at $z=0.25$, 0.38 and 0.44 are independent. The layers are composed of large occupation domains shown in Fig. 1 and additional small ones. If the layers composed of atoms derived from the domains E, A etc. in Fig. 1 are described as E, A etc., the layer stacking can be written as BA(E+D)ABCD'(E'+A')D'C, where C, D', E' and A' are layers coming from the occupation domains obtained from B, A, E and D by the screw axis 10_5 . The structure projected along the 10-fold axis is given in Fig. 2. The model has atom clusters proposed by Hiraga et al. (1993) and their arrangement seen in the HREM image (Hiraga, 1992).

PS-12.01.13 BURGERS VECTOR OF DISLOCATIONS IN $Al_{62}Cu_{25.5}Fe_{12.5}$ QUASICRYSTAL DETERMINED BY MEANS OF CONVERGENT-BEAM ELECTRON DIFFRACTION. By Renhui Wang, Mingxing Dai, Department of Physics, Wuhan University, 430072 Wuhan, China and Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O.Box 2724, 100080 Beijing, China

Since the discovery of quasicrystals(QCs) many authors studied defects, especially dislocations in QCs. However, there has been until now no work determining the indices of a six-dimensional Burgers vector \mathbf{b} of dislocations in icosahedral QCs without any presuppositions. Dislocations in $Al_{62}Cu_{25.5}Fe_{12.5}$ face-centered icosahedral QC were studied by means of the contrast experiment and defocus convergent-beam electron diffraction technique. The indices of the six-dimensional Burgers vector of the dislocations were determined at the first time to be $1/2 [1 -1 1 -1 0 0]$. The projection $b_{||}$ of this six-dimensional Burgers vector in the three-dimensional physical space is exactly parallel to a twofold axis of the icosahedron. The magnitude $|b_{||}| = 0.291$ nm was calculated when $a=0.896$ nm is taken for the lattice constant of the face-centered icosahedral QC. This is a complete experimental method which can be applied to any type of dislocations in QCs without any presupposition about the Burgers vector. This method may become a standard technique to determine Burgers vectors in QCs.