12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

PS-12.01.09 REPEATED ELBOW TWINSNING OF Fe₄Al₁₃ SHOWING DIFFRACTION PATTERNS WITH DECAgonAL PSEUDOSYMMETRY.  
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Fe₄Al₁₃ is formed by peritectic reaction at 1430 K from Fe₂Al₆ and the melt, C₂mA, n=101, a = 15.489, b = 8.0831, c = 12.476, α = 107.72° (Black, Acta Cryst., 1935, 8, 43-48 and 175-182). Multiple twinning was observed not only in Fe₄Al₁₃, but also in the isotypic compound Fe₄Al₁₃ (Eilhammer, Acta Chem. Scand., 1963, 2124-2130) as well as in the ternary isotypal phase Ni₄FeₓGa₃ (Tajasekhara, Sarah & Schuetz, Z. Metallkd., 1962, 73, 526-529). Twists and planar defects were recently observed in Fe₄Al₁₃ by means of HRTEM (Tsuchinori, Tsuchihara & Fukano, Phil. Mag. B, 1992, 66, 89-108). In the present study Fe₄Al₁₃ was investigated in the concentration range from 0.75 up to 0.77 by means of X-ray diffraction, scanning electron and optical microscopy. In contrast to the neighboring phase Fe₄Al₁₅ which does not show any polymorphic transformation, metallographic investigation of the structure of Fe₄Al₁₃ yielded an indication for a phase transformation. Holographic lamellae were observed in the Fe₄Al₁₅ 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 (010).

An atomic model showing pentagonal pseudosymmetry is discussed in direct space for the repeated elbow twins of Fe₄Al₁₃ (τ = 0.75...0.77) showed diffraction lines of a new phase homotypic to Fe₄Al₁₃, 0.490, a = 7.839(3), b = 4.011(2), c = 23.688(9) α, c/a = tan 72°. The relationship between this α-unit cell and the monoclinic unit cell of Fe₄Al₁₃ is (α,b,c) = (α,b,c)(1/2,0,1/2; 0,1/2,0,0,0,2), i.e. α = a/2 etc.

The low-temperature monoclinic structure Fe₄Al₁₃ is a disclike variant of the high-temperature orthorhombic phase Fe₄Al₁₃(α). A twinning model is discussed in reciprocal space for structures with orthorhombic face centred Bavaïs lattices (α, α, α) having an axial ratio c/a = tan 72°, (b/c, b/a = tan 72°), i.e. the ratio of the interplanar spacings d₂₀₁ = (1 + √5)/2 = τ (d₂₀₁ = 0.618), d₁₁₀ = (τ/2) (golden mean). Composite crystals (repeated elbow twins) of these α-structures which have the common direction [010] = [011] and showing the twin planes [011] i.e. twin planes [011], and [001] yield diffraction patterns (001) = (001) for decagonal pseudosymmetry; cf. electron diffraction pattern of twinned Fe₄Al₁₃ (Fung, Zou & Yang, Phil. Mag. Lett., 1987, 55, 27-32, Fig. e).

PS-12.01.11 GEOMETRICAL RE-ENTRY MODULATIONS: (C₅→N₅)₅Cr₄N₄. M = Cu, Mn, Cd. By M. Inoue, H. Ikeda and Y. Yamauchi, Department of Physics, Kyushu University, Fukuoka 812, Japan.

We have developed a geometrical method to analyze molecular modulation modes in incommensurate crystal structures. From the three-dimensional lattice of each adsorbed atom which are pulled back to the original unit cell, that if a special mode, for example translational molecular displacement is subtracted. Then, the remaining figure suggests the new 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 (C₅→N₅)₅Cr₄N₄ (M = Cu, Mn, Cd) show the following phase sequence: α → β → γ → δ → ε → ζ, with the two incommensurate ε and ζ-phases. These incommensurate structures were extensively studied using superspace symmetry. We have applied the new geometrical method to find the discrete modulation modes in the γ and ζ phases. Figure 1 and 2 show loci of modulated atoms of (C₅→N₅)₅Cr₄N₄ in (superspace group, Pcaλa(200)80, Doukid and Chaunu, 1990 B46 180) and c(8 superspace group, B2p₁b₄110.05.30.11) Ikeda and Achiba) phases. The main modes in the γ and ζ phases are a translational modulation along the a axis and a twisted intra-molecular mode of propyl ammonium base, respectively, though in both phases each orbit of atomic modulation consists of multiple molecular modes. Finally, the amplitude of each molecular mode can be refined by least-squares fitting of satellite structure factors.

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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 Al₅Mn (Li, X. Z. et al., Phil. Mag., 1992, 66, 331-340 and Hiraga, K. et al., Phil. Mag., 1993, to appear) and HREM images (Hiraga, K., Proc. Int. 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 approximation Al₅Mn suggests the structure of the clusters and their linkage. The d-Al-Pd-Mn quasicrystal (a=2.84 Å, c=12.06 Å, P10/mmm) consists of 10 flat (8 puckered) layers (Yamamoto et al., Acta Crystallogr., 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 B, C, E, etc. in Fig. 1 are described as B, A etc., the layer stacking can be written as BA(B+D)ADCD(E+E'A')D'C', where C, D', E' and A' are layers coming from the occupation domains obtained from B, A, B and D by the screw axis 10g. 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, K., 1992).

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 of dislocations in icosahedral QCs without any presuppositions. Dislocations in Al₅Cu₃Fe₅ face-centered icosahedral QC were studied by means of the contrast experiment and defect-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 | of 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.