12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

**PS-12.01.09 REPEATED ELBOW TWINSING OF Fe₄Al₁₃ SHOWING DIFFRACTION PATTERNS WITH DECAGONAL PSEUDOSYMMETRY.**

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Fe₄Al₁₃ is formed by peritectic reaction at 1430 K from Fe₂Al₃ and the melt, C₂₅₆, m = 15,649, b = 8,093, c = 12,476, α = 107,72° (Black, Acta Cryst., 1935, S, 42-48 and 175-182). Multiple twinning was observed not only in Fe₄Al₁₃, but also in the isotypic compound Fe₄Al₁₃ (Edhammer, Acta Chem. Scand., 1965, 2124-2130) as well as in the ternary isotypic phase Ni₂Fe₄Ga₄ (Zajkasehara, Sarah & Schubert, Z. Metallkd., 1962, 73, 526-529). Twinned and planar defects were recently observed in Fe₄Al₁₃ by means of HREM (Tsuchimori, Tsukimasa & Fukano, Phil. Mag. B, 1992, 66, 89-108). In the present study Fe₄Al₁₃ was investigated in the concentration range from Al₁₃ = 0.75 up to Al₁₃ = 0.77 by means of X-ray diffraction, scanning electron and optical microscopy. In contrast to the neighboring phase Fe₄Al₁₃ which does not show any polymorphic transformation, metallographic investigation of the structure of Fe₄Al₁₃ yielded an indication for a phase transformation. Hottow prismatic lamellas were observed in the Fe₄Al₁₃ 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 (011).

An atomic model showing pentagonal pseudosymmetry is discussed in direct space for the repeated elbow twins of Fe₄Al₁₃. Gaviner photographs of splat-cooled alloys Fe₀-₄₀Al₁₃ (r = 0.75...0.77) showed diffraction lines of a new phase homotopic to Fe₄Al₁₃, d₅₀, a = 7,739(3), b = 4,021(2), c = 23,688(9) Å, a/c = tan 72°. The relationship between this o8 = q unit cell and the monoclinic unit cell of Fe₄Al₁₃ is (a,b,c) = (1/2,0,1/2; 0,1/2,0; 0,0,2), i.e. a8 = a/2 etc. The low-temperature monoclinic structure Fe₄Al₁₃ is a discommensurate variant of the high-temperature orthorhombic phase Fe₄Al₁₃(h). A twinning model is discussed in reciprocal space for structures with orthorhombic lattice centred Bawnt cells (o8, o8, o8) having an axial ratio c8/a = tan 72°, (b/c, b/c = tan 72°), i.e. the ratio of the interplanar spacings d₂₀²₀/110 = (1 + √5)/2 = τ (d₂₀₂₀/001; d₂ₒ₂/110 = τ (golden mean). Composite crystals (repeated elbow twins) of these o8-structures which have the common direction [010]ₙ = [018]ₙ and showing the twin planes [011]ₙ i.e. twin planes [001]ₙ, and [011]ₙ yield diffraction patterns (011)ₙ = (011)ₙ of decagonal pseudosymmetry; cf. electron diffraction pattern of twinned Fe₄Al₁₃ (Fung, Zou & Yang, Phil. Mag. Lett., 1987, 55, 27-32, Fig. 4).

**PS-12.01.11 GEOMETRICAL MODE ANALYSIS OF INCOMMENSURATE RE-ENTRANT MODULATIONS: (Cr₃N,B₇)₃MC₄, M = Cu, Mg, Cd.**

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We have developed a geometrical method to analyze molecular modulation modes in incommensurate crystal structures. From the three-dimensional lattice of each modulated 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 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 (Cr₃N,B₇)₃MC₄, M = Cu, Mg, Cd show the following phase sequence: α → β → γ → δ → ε → ζ with the two incommensurate c and γ-phases. These incommensurate structures were extensively studied using superspace symmetry. We have applied the new geometrical method to find the displaceable modulation modes in the γ and c phases. Figure 1 and 2 show loci of modulated atoms of (Cr₃N,B₇)₃Cu₄ in γ (superspace group, P63/mcm, Doudin and Chapuis, 1990 B46 180) and c (superspace group, BP6₃/C11m(0.99,0.52,1) Ikekda and Achiba) phases. The main modes in the c and γ phases are a translational modulation along the c axis and a twisted intra-molecular 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.