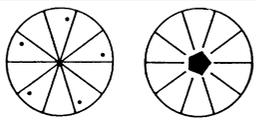
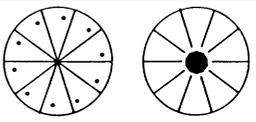
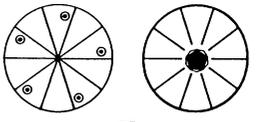
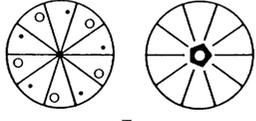
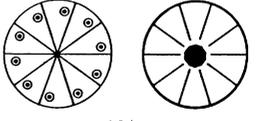
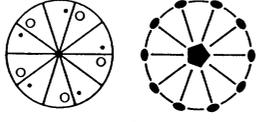
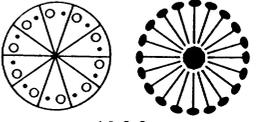
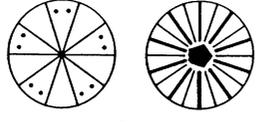
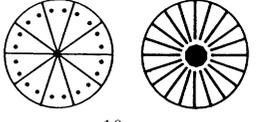
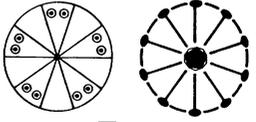
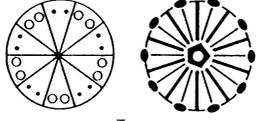
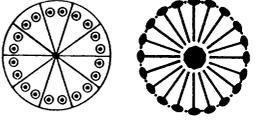


2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.15. Pentagonal and decagonal point groups constructed by analogy with trigonal and hexagonal point groups

This table is taken from Saito *et al.* (1992) with the permission of the Japan Society of Applied Physics.

| Pentagonal | Decagonal |
|---|---|
|  5 |  10 |
| — |  $\bar{1}0$ |
|  $\bar{3}$ |  $10/m$ |
|  5 2 |  10 2 2 |
|  $5m$ |  $10mm$ |
| — |  $\bar{1}0m2$ |
|  $\bar{5}m$ |  $10/mmm$ |

$10mm$. The whole pattern of Fig. 2.5.3.24(b), formed by HOLZ reflections, shows a fivefold rotation symmetry and a type of mirror plane, the resultant symmetry being $5m$. Figs. 2.5.3.24(c) and (d) show symmetries $6mm$ and $3m$, respectively. Figs. 2.5.3.24(e) and (f) show symmetry $2mm$. There are two icosahedral point groups, 235 and $m\bar{3}5$ (see Table 10.1.4.3 in *IT A*, 2005). The former is noncentrosymmetric with no mirror symmetry but the latter is centrosymmetric. Table 2.5.3.14 shows the diffraction groups expected from these point groups with the incident beam parallel to the fivefold or tenfold axis, and their symmetries appearing in the WP, BP, DP and \pm DP. Projection diffraction groups and their symmetries, in which only the interaction between ZOLZ reflections is taken into account, are given in the second row of each pair. Diffraction groups obtained for the other incident-beam directions are omitted because they can be seen in Table 2.5.3.3. The whole-pattern symmetries observed for better-quality images of $\text{Al}_{74}\text{Mn}_{20}\text{Si}_6$ have confirmed the result of Bendersky & Kaufman (1986), *i.e.* the point group $m\bar{3}5$. Fig. 2.5.3.25(a) shows a zone-axis CBED pattern taken at an electron incidence along the threefold axis. Figs. 2.5.3.25(b) and (c) show \pm DPs taken when tilting the incident beam to excite a low-order strong reflection. The pattern of

disc $+G$ agrees with that of disc $-G$ when the former is superposed on the latter with a translation of $-2G$. This symmetry 2_R directly proves that the quasicrystal is centrosymmetric, again confirming the point group as $m\bar{3}5$. The lattice type was found to be primitive and no dynamical extinction was observed. Thus, the space group of the alloy was determined to be $Pm\bar{3}5$.

Quasicrystals of Al–Mn alloys have been produced by the melt-quenching method and are thermodynamically metastable. Tsai *et al.* (1987) discovered a stable icosahedral phase in $\text{Al}_{65}\text{Cu}_{20}\text{Fe}_{15}$. This alloy has larger grains and is much better quality with less phason strain than $\text{Al}_{74}\text{Mn}_{20}\text{Si}_6$. The discovery of this alloy greatly accelerated the studies of icosahedral quasicrystals. It was found that the lattice type of this phase and of some other Al–Cu–TM (TM = transition metal) alloys is different from that of Al–Mn alloys. That is, Al–Cu–TM alloys display many additional spots in diffraction patterns of twofold rotation symmetry. The patterns were indexed either by all (six) even or all (six) odd, or by a face-centred (*F*) lattice. All the icosahedral quasicrystals known to date belong to the point group $m\bar{3}5$; none with the noncentrosymmetric point group 235 have been discovered.

2.5.3.5.2. Decagonal quasicrystals

The first decagonal quasicrystal was found by Bendersky (1985) in an alloy of Al–Mn using the electron-diffraction technique. This phase has periodic order parallel to the tenfold axis, like ordinary crystals, but has quasiperiodic long-range structural order perpendicular to the tenfold axis. The diffraction peaks were indexed by one vector parallel to the tenfold axis and four independent vectors pointing to the vertices of a decagon. Thus, the decagonal quasicrystal is described in terms of a regular crystal in five dimensions.

Two space groups, $P10_5/m$ and $P10_5/mmc$, have been proposed for the alloy by Bendersky (1986) and by Yamamoto & Ishihara (1988), respectively. However, owing to the low quality of the specimens, CBED examination of the alloy could not determine whether the point group is $10/m$ or $10/mmm$. Furthermore, identification of the space-group symmetry was not possible because observation of dynamical extinction caused by the screw axis and/or the glide plane was difficult. The Al–*M* (*M* = Mn, Fe, Ru, Pt, Pd, ...) quasicrystals found at an early stage were thermodynamically metastable. Subsequently, thermodynamically stable decagonal phases were discovered in the ternary alloys $\text{Al}_{65}\text{Cu}_{15}\text{Co}_{20}$ (Tsai *et al.*, 1989a), $\text{Al}_{65}\text{Cu}_{20}\text{Co}_{15}$ (He *et al.*, 1988) and $\text{Al}_{70}\text{Ni}_{15}\text{Co}_{15}$ (Tsai *et al.*, 1989b). However, space-group determination was still difficult due to their poor quasicrystallinity.

Tsai *et al.* (1989c) succeeded in producing a metastable but good-quality decagonal quasicrystal of $\text{Al}_{70}\text{Ni}_{15}\text{Fe}_{15}$. This alloy was found to be the first decagonal quasicrystal that could tolerate symmetry determination using CBED. The space group was determined to be $P\bar{1}0m2$ by Saito *et al.* (1992).

Fig. 2.5.3.26(a) shows a CBED pattern of $\text{Al}_{70}\text{Ni}_{15}\text{Fe}_{15}$ taken with an incidence parallel to the fivefold axis (*c* axis). The pattern clearly exhibits fivefold rotation symmetry and a type of mirror symmetry, the total symmetry being $5m$. The slowly varying intensity distribution in the discs indicates that the pattern is formed by the interaction between ZOLZ reflections. Thus, the projection approximation should be applied to the analysis of the pattern. Patterns that were related to Fig. 2.5.3.26(a) by an inversion were observed when the illuminated specimen area was changed, indicating the existence of inversion domains. Table 2.5.3.15 shows possible pentagonal and decagonal point groups, which are constructed by analogy with the trigonal and hexagonal point groups (Saito *et al.*, 1992).

It can be seen that the point groups that satisfy the observed symmetry $5m$ in the projection approximation are 52 , $5m$ and $\bar{1}0m2$. Point group 52 is a possibility because the horizontal