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Orientation relationship of decagonal quasicrystal and tenfold twins in rapidly cooled Al-Fe alloy

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We have found that decagonal quasicrystal and tenfold twins of monoclinic $Al_{13}Fe_4$ coexist in rapidly cooled Al-Fe alloy. The tenfold axis of the decagonal phase is parallel to the pseudotenfold [010] axis of the twins. There is good coincidence between the strong spots of the decagonal twofold diffraction patterns and the corresponding diffraction patterns of $Al_{13}Fe_4$. This orientation relationship is also observed when the decagonal phase transforms into a $Al_{13}Fe_4$ twin on heating in an electron microscope. This shows that the decagonal quasicrystal is not a set of twins although they are closely related in structure.

Although the existence of quasicrystal has been widely accepted, the alternative multiple-twin explanation is still controversial.[1] Besides the icosahedral phase with $m\bar{3}\bar{5}$ symmetry,[2] decagonal phases with $10/mmm$ symmetry have also been found in Al-Mn, Al-Pd, Al-Fe, and V-Ni-Si alloys.[3-5] In the mean time, tenfold twins have been observed in NiZr and Al-Fe alloys.[6,7] Fivefold twins have also been found in Al-Pd.[8] In the study of rapidly cooled Al-14-at.% Fe alloy by transmission electron microscopy, we have found that not only the decagonal phase coexists with tenfold twins of $Al_{13}Fe_4$, but also they have a definite orientation relationship. Moreover, such an orientation relationship has also been observed *in situ* in the transformation of the decagonal phase into the $Al_{13}Fe_4$ phase.

Figures 1(a) and 1(b) show the tenfold diffraction patterns of the decagonal phase and tenfold twins in Al-Fe alloy in the same scale. The decagonal phase is a two-dimensional quasicrystal with translational periodicity along the tenfold axis. But normal to the tenfold axis, there is no translational periodicity. Figure 1(b) is taken from heavily faulted tenfold microtwins which are similar to the case of NiZr. The tenfold twin pattern can be obtained by superposing the [010] diffraction pattern [Fig. 1(c)] of differently oriented $Al_{13}Fe_4$ twins.[7] $Al_{13}Fe_4$ has the monoclinic $C2/m$ space group with lattice parameters $a = 1.5489$, $b = 0.8083$, $c = 1.2476$ nm, and $\beta = 107.71°$.[9] Figure 2 shows the intergrowth of the decagonal phase and the tenfold twins. Although the specimen is rather thick, the twins can be identified by their fringes which are related by 36° rotation. Five sets of fringes are clearly visible in the enlarged micrograph. The twins grow around a fringe-free region marked T which is the decagonal phase. This is confirmed by microdiffraction. The corresponding selected area diffraction pattern is shown in Fig. 1(d). It is clear that the [010] axis of the twins is parallel to the tenfold axis of the decagonal phase. Figure 1(d) is, in fact, a composite pattern of Figs. 1(a) and 1(b); the ten strong spots and the corresponding spots in Figs. 1(a) and 1(b) are marked by arrows. More often, it is found that the decagonal phase is in contact with one or two twins of

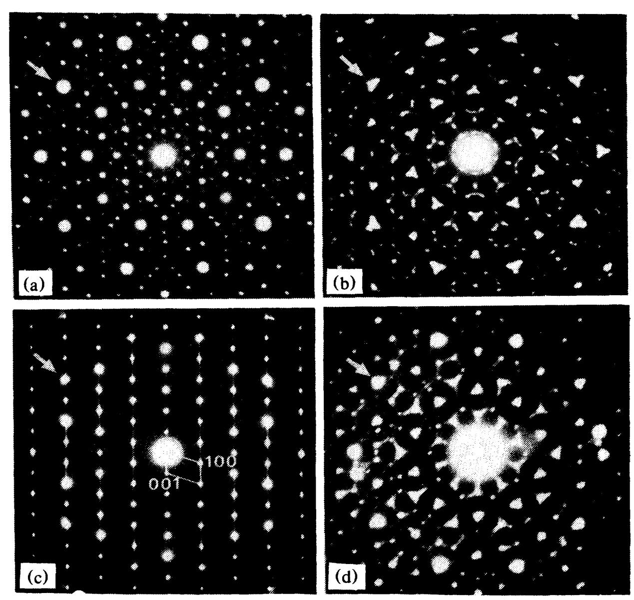

FIG. 1. Diffraction patterns from decagonal quasicrystal and $Al_{13}Fe_4$ twins: (a) decagonal tenfold axis, (b) tenfold twins [010], (c) single twin [010] (100 should read 200), and (d) decagonal tenfold and tenfold twins [010] axis.

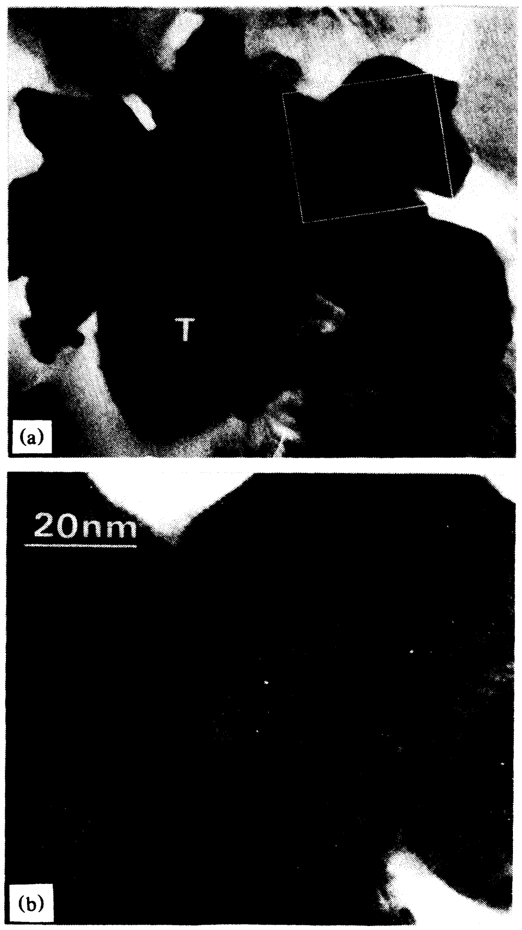

FIG. 2. (a) Intergrowth of decagonal quasicrystal (T) and tenfold twins of $Al_{13}Fe_4$. (b) The enlarged micrograph shows fringes of five twins rotated by about 36°.

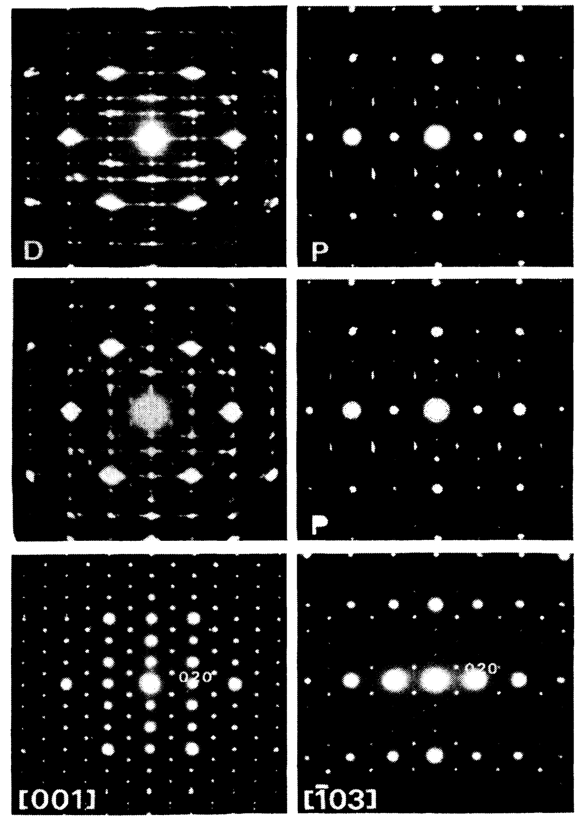

FIG. 3. Comparison of the twofold pseudohexagonal and pseudosquare patterns of the decagonal crystal (a), and the [001] and [$\bar{1}$03] patterns of the $Al_{13}Fe_4$ twin (c), and the composite patterns (b), showing good coincidence of spots.

$Al_{13}Fe_4$ with the above orientation relation. Diffraction patterns normal to the [010] axis in $Al_{13}Fe_4$ are alternatively D-like and P-like at approximately 18° intervals; the D and P axes are twofold axes normal to the tenfold axis in the decagonal phase.[4] The strong pseudohexagonal spots in the [001], [102], [504], and [100] patterns match those in the decagonal D pattern quite well. Similarly, the strong pseudosquare spots in the [$\bar{1}$03], [104], [506], and [301] patterns match those in the decagonal P pattern. It is found experimentally that the decagonal D and P axes are parallel to the [001] and [$\bar{1}$03] axes, respectively. Furthermore, the degenerate twofold, threefold, and fivefold and threefold patterns between the tenfold axis and the P axis are quite similar to the [1 104], [184], [134], and [114] patterns of the $Al_{13}Fe_4$ twin. Composite diffraction patterns from the decagonal phase and $Al_{13}Fe_4$ twin(s) show, indeed, that there is good coincidence between the strong pseudohexagonal and pseudosquare spots of the decagonal D and P patterns and the monoclinic [001] and [$\bar{1}$03] patterns. This is shown in Fig. 3. The coincidence of spots on the tenfold axis implies that the periodicity of the decagonal phase is related to the periodicity of the [010] axis of $Al_{13}Fe_4$. The orientation relationship between the decagonal phase and the $Al_{13}Fe_4$ twin is summarized in stereographic projection in Fig. 4. Note that the maximum deviation of the decagonal and monoclinic axes is 2.67°.

Heating the decagonal phase in a Philips EM420 electron microscope, the transformation of the decagonal phase into $Al_{13}Fe_4$ has been observed *in situ*. The trans-

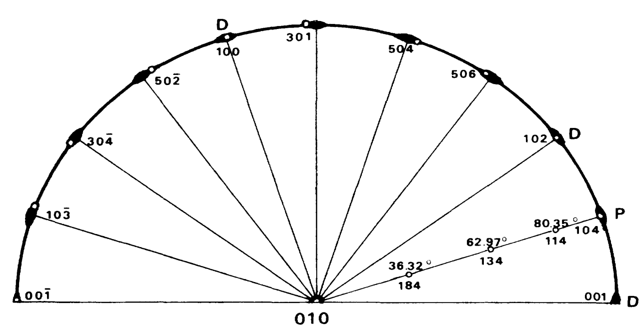

FIG. 4. Stereographic projection showing the orientation relationship between axes of the decagonal quasicrystal (solid symbols) and the $Al_{13}Fe_4$ twin (open circles).

formation takes place with the above orientation relationship. However, the decomposition of the decagonal phase into ten or five twins has not been observed yet. The specimens are heated steadily and aged at 400 and 450 °C for half an hour, respectively. As the temperature rises, especially above 400 °C, the diffraction patterns of the decagonal phase are gradually blurred by diffuse scattering. In real space, the outline of the grains is also gradually blurred. Heating to about 500 °C the tenfold pattern of the decagonal phase transforms to a blurred and faulted [010] pattern of $Al_{13}Fe_4$. Diffraction spots due to aluminum are also observed. Presumably, the decagonal phase decomposes into $Al_{13}Fe_4$ and excess aluminum. This transformation is therefore accompanied by the diffusion of atoms and reconstruction. It is similar to the transformation of the icosahedral $(Al_6Mn)_{1-x}Si_x$ into α-(Al-Mn-Si).[10] Such transformation shows that quasicrystals are not a set of twins, although they are closely related in structure. The structural characteristics relevant to quasicrystalline structure in $Al_{13}Fe_4$ have been noted by Henley.[11] Quasicrystal and crystal can readily be distinguished by transmission electron microscopy.

The decagonal phase, an intermediate phase between the icosahedral quasicrystalline and the crystalline phases, shows characteristic features of both phases. It has been shown that the decagonal phase grows epitaxially on the icosahedral phase in Al-Mn alloys.[12] It follows that the icosahedral phase is also not an aggregate of icosahedral twins. This is supported by the published high-resolution electron microscopic images and diffraction patterns. The different periodicity of the decagonal phases in Al-Mn, Al-Pd, and Al-Fe is probably related to their respective crystalline phases. The decagonal phase, being a two-dimensional quasicrystal, is a simpler system than the icosahedral phase and therefore easier to deal with. The study of the decagonal phases and the related crystalline structures will shed light on the structure of the icosahedral phase.

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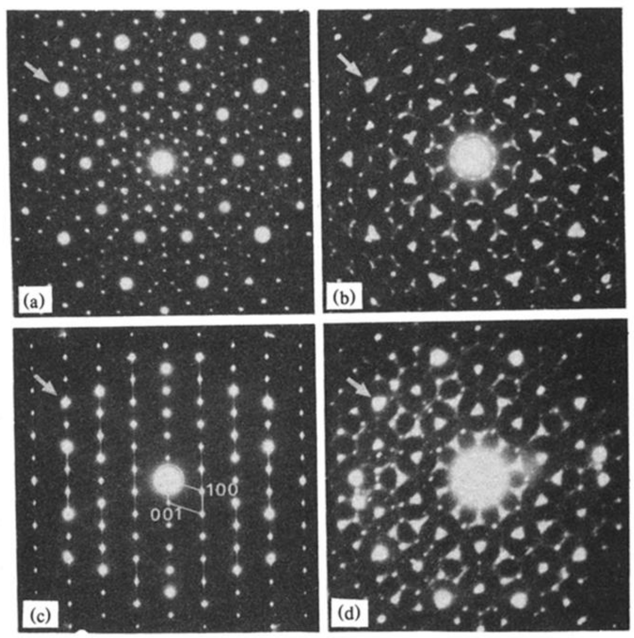

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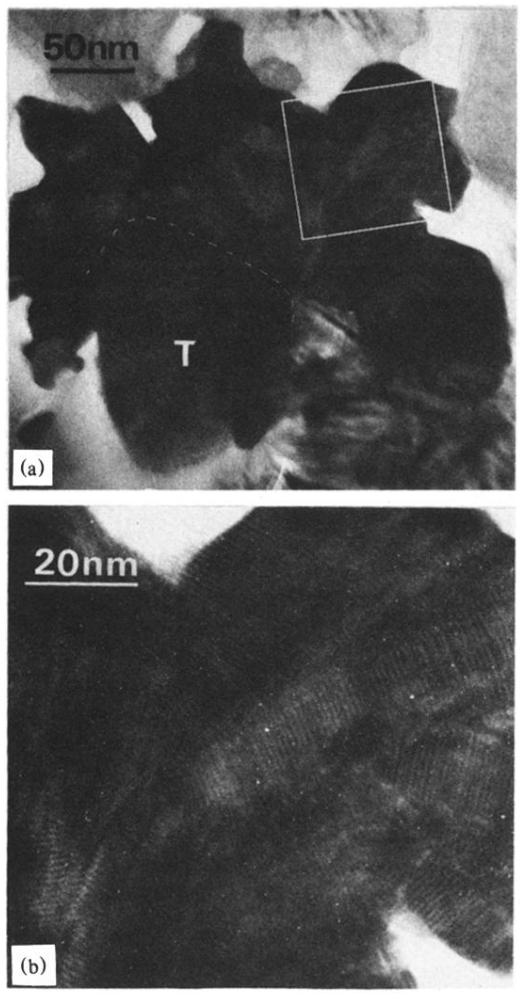

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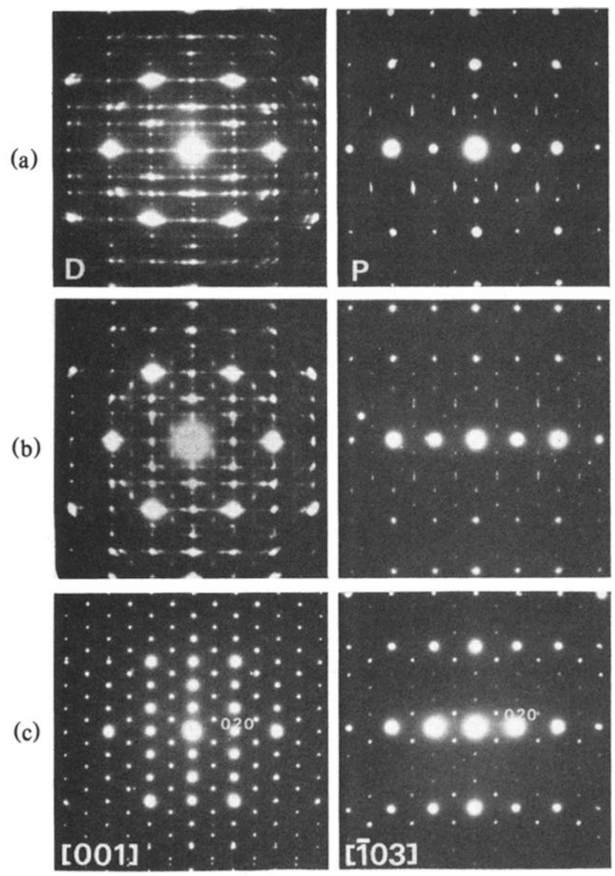

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