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HAL Id: jpa-00225747
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Submitted on 1 Jan 1986

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ICOSAHEDRAL ALLOYS: PHASE PURITY AND PHASON STRAINS

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Abstract - We present a survey of x-ray and electron diffraction studies of Aluminum-Transition Metal alloys. The icosahedral phase is found in Al alloyed with Mn, Cr, V, Mo, Ru, W, and Re. The effect of adding small amounts of Si and Ru to the binary alloys is discussed. We review the advantages and disadvantages of various indexing schemes. Distortions of electron diffraction pictures are described in terms of phason strains in a quasilattice.

I - Introduction

The discovery of an icosahedral phase (IP) in quenched alloys of Al with Mn, Cr, and Fe has presented an intriguing problem in crystallography. Icosahedral rotational symmetry is incompatible with periodic translational order, yet IP’s exhibit diffraction patterns with sharp spots, a property normally associated with periodic crystals. A possible resolution of these observations was suggested by Levine and Steinhardt, who introduced a class of structures which have long range bond orientational order and perfect quasi-periodic translational order. The calculated diffraction patterns of these icosahedral quasicrystals were found to be in close agreement with the electron diffraction patterns of the Al-Mn IP. Quasicrystals have since been investigated from several points of view and have been shown to include structures of arbitrary symmetry.

Another approach, first suggested by Sheshtman and Blech and more recently developed by Stephens and Goldman is to randomly pack icosahedra while maintaining orientational order. The structure factors of the random packing models are also in good agreement with the observed diffraction patterns. Random packing models are inherently disordered and their structure factors have peaks of finite width. This is distinct from quasicrystals, which have a perfectly quasiperiodic ground state. In the quasicrystal model, finite peak widths are considered to be generated by imperfections in the quasilattice.

The stability of icosahedral solids has been investigated from the point of view of Landau theory. These calculations have shown that quasi-periodic icosahedral structures may indeed be metastable, and possibly even globally stable, with respect to competing crystalline phases. It therefore seems plausible that the IP is not peculiar to Al-Mn, Al-Cr, and Al-Fe, but may be realized in many other systems, and indeed it has recently been reported in U$_{20}$Pd$_{80}$Si$_{14}$ and Al$_8$M$_6$Z$_{12}$Cu$_4$ alloys. We present here the results of a survey of quenched Aluminum-transition metal (Al-M) alloys. One intention of this study is to determine which Al-M systems form the IP and to investigate what factors favor its formation. We also address the question of disorder in these materials. Some of the present results have been presented elsewhere.

The remainder of this paper will proceed as follows: In Section II we discuss the advantages and disadvantages of different indexing schemes. In Section III-V we present the results of survey measurements on binary, ternary, and quaternary Al-M alloys. Finally, in Section VI...
we discuss mechanisms for peak broadening and shifting in x-ray and electron diffraction patterns.

II - Indexing of Diffraction Peaks

The electron diffraction patterns can be indexed by a set of six basis vectors taken as the vertex vectors of an icosahedron. The indexing procedure involves identifying a reflection of vertex symmetry in the electron diffraction pictures as a basis vector. The reciprocal lattice is then constructed from the basis vectors in the usual manner. An ambiguity arises since there is an infinite series of reciprocal lattice points scaled by \( r^2 \) (where \( r \) is the Golden Mean, 1.618...) in each vertex direction, any one of which could be taken as a basis vector. This is essentially a consequence of the self-similarity of the reciprocal lattice. We have arbitrarily chosen the most intense reflection in this series, which for Al-Mn occurs at 2.90 Å\(^{-1}\), as the fundamental vector, \((100000)\). One advantage of this choice of fundamental is that most of the intense diffracted peaks can be classified using a small number of nonzero indices. The structure factor of a simple quasi-lattice can be calculated by projection methods. It has been pointed out by several authors that, using the projection method, the ambiguity in the indexing can be resolved and that a comparison of experimental peak intensities along a \( r^2 \)-series should determine the choice of fundamental. Calculations based on a primitive, undecorated quasi-lattice with point scatterers show that intensities along a \( r^2 \)-series should monotonically increase towards a saturation value at large wave vector in such a way that there occurs an abrupt crossover from weak to strong peak intensity. The peak occurring just before the crossover should then be identified with the fundamental \((100000)\) vector. On the basis of these calculations, the strong peak at 2.90 Å\(^{-1}\) in the Al-Mn data should be indexed as the \((211111)\) and not as the \((100000)\), the fundamental being assigned to a weak peak scaled down by \( r^2 \), occurring at 0.88 Å\(^{-1}\).

While this analysis can in principle define a unique fundamental we have taken the view that such a determination makes assumptions about the structure that are not fully supported by the data. Specifically, the calculated structure factor assumes a primitive quasi-lattice and ignores the effects of decorations on scattering intensities. It is generally agreed that if the icosahedral phase is to be described by a quasicrystalline model, the precise structure corresponds to a non-trivial decoration. The effect of an arbitrary decoration would be almost certain to give a additional weight to intensities around 2.90 Å\(^{-1}\) since this wavelength corresponds roughly to interatomic distances. In fact, the structure factors of all crystalline, quasicrystalline, or amorphous Al-Mn alloys attain their largest amplitudes in this region. Whether the large peak intensity measured in the icosahedral phase is due to a geometrical structure factor or is the consequence of an intrinsic quasi-lattice might be resolved by examining intensities at larger wavevectors. However, the Al-Mn data have a limited range which does not extend to the next peak in the \( r^2 \)-series. It is noteworthy that the structure factor of icosahedral U\(_{20}\)Pd\(_{60}\)Si\(_{20}\), which closely resembles that of Al-Mn, has been measured out to this peak and the intensity is nearly two orders of magnitude less than predicted. This indicates that the effects of lattice decoration and disorder do play a strong role in modifying peak intensities.

The choice of fundamental has the further consequence of determining the size of rhombohedral cells which can be used to construct the quasi-lattice and, thus fixes a "quasilattice constant." It has been argued that the quasilattice constant of 1.1 Å implied by the choice of a fundamental of 2.90 Å\(^{-1}\) is unreasonably small and that the quasilattice constant of 4.6 Å which results if the indexing is scaled down by \( r^2 \) is more in accordance with atomic sizes. However, there is no a priori reason for assuming the rhombohedral cells to be the building blocks of a decorated quasi-lattice. As Levine, Socolar and Steinhardt have pointed out, the 3D Penrose quasi-lattice naturally decomposes into zonohedra of considerably larger size. Also, Jarić has discussed decorations with rhombohedra in which fractional occupancies are allowed.

Thus, while the suggestion that only one fundamental vector is "correct" remains intriguing, it rests on the assumption that the icosahedral phase can be described by the projection of a 6D periodic crystal. A rescaling of the indexing scheme may be indicated as study progresses. However, it must be considered for its implications not only in the context of quasicrystal theory but in the light of competing theories as well. For example, Landau theories would consider the most intense peak in the \( r^2 \)-series to be the fundamental. In the random packing model presented by Stephens and Goldman, the diffraction peaks are regarded not as true Bragg peaks but rather as interference maxima resulting from diffraction
from a partially random incorporating two length scales in the ration $1:~$; in this picture the strong diffraction peaks result when the wavevector is almost commensurate with both length scales, and no fundamental vector is preferred over any other.

III - Experimental Details

We now discuss techniques for the preparation and analysis of rapidly quenched Al-M alloys. Thin ribbon samples of these alloys were prepared by conventional melt-spinning techniques. In order to ascertain the relative tendency for IP formation in these systems, the spinning parameters were held fixed and chosen so that a stoichiometric Al-Mn alloy ($21.5-22\%$ Mn) would quench to nearly single phase icosahedral ribbons. X-ray scans from a number of such Al-Mn samples show identical diffraction profiles, indicating that the procedure is reproducible. Alloys were prepared by induction melting high purity (better than 99.95%, in most cases) elemental constituents in an Argon environment. The spinning apparatus consisted of a quartz nozzle suspended above a $23\,$cm Cu wheel rotating at 3600 revolutions per minute. Alloys were induction melted in the nozzle in gently flowing Argon, then propelled through a $0.4\,$mm aperture at the tip of the nozzle onto the wheel by a pressure burst of 40 pounds per square inch. This produced brittle ribbons several mm wide and 20-40 microns thick. The quench rate could be increased by increasing either the rotation speed of the wheel or the pressure above the molten alloy, with similar results. Our experience with Al-Mn has indicated that near stoichiometry other phases may compete with the IP. For this reason, samples for a number of systems were made at several Al-rich compositions.

Samples were characterized with electron diffraction and powder x-ray diffraction. The x-ray measurements employed MoK$_\alpha$ radiation from a Rigaku RU-200 rotating-anode generator, operating at $9\,$kW. The x-rays were monochromatized by Bragg reflection from a 2-inch bent graphite crystal and further collimated by slits before and after the sample, resulting in an instrumental resolution of $0.012\,$Å$^{-1}$ half-width at half-maximum (HWHM). Note that in most cases observation of weak peaks was limited, not by lack of x-ray intensity, but rather by intrinsic diffuse scattering from the sample. Samples for x-ray study were gently ground into a powder and suspended between pieces of Kapton tape. (It was found that grinding the sample too violently could result in substantial degradation of the x-ray spectra, presumably because of microscopic morphological changes). Diffraction scans for each sample were indexed to known equilibrium crystalline structures or the IP. In only two cases did there occur peaks that could not be indexed. Every occurrence of the IP was confirmed by single grain diffraction in an Phillips STEM 400T electron microscope. We emphasize that the survey determines the relative tendencies for formation of the IP in these systems. Since the x-ray scans cannot detect the presence of less than a few percent of the IP in a sample, a null result indicates only that its formation is unfavorable. A case in point is Al-Fe which shows no sign of icosahedral peaks in x-ray scans, yet is known to form the IP$^1$.

IV - Al-Transition Metal Binary Compounds

Initial studies$^{16}$ were done on rapidly quenched 6:1 Al-Mn samples. Quenching from the melt yields a mixture of fcc-Al and the IP. Electron microscopy studies show grains of the IP ranging up to several microns in size, embedded in an aluminum matrix. Electron diffraction from a single grain shows patterns of icosahedral symmetry. The presence of excess Al implies that the concentration of Mn in the IP is greater than 1:6, and measurements on other samples have put the Mn content of the IP at 21.5-22 atomic percent. Stoichiometric samples show no excess Al. However, as the Mn content is increased towards stoichiometry, competition from another metastable Al-Mn phase develops$^{23}$. This "decagonal phase" forms at slightly slower quenching rates than the IP and can be suppressed by appropriate adjustment of quenching parameters. Although the decagonal phase in itself merits further study, it poses problems for any measurements of bulk IP samples, since the decagonal phase and IP structures appear to be closely related. In particular, quantitative powder diffraction measurements of the IP may be unreliable if samples contain more than several percent of the decagonal phase, since many diffraction peaks of the two phases overlap.

The widths of peaks in high resolution x-ray scans range from $0.04\,$Å$^{-1}$ to $0.01\,$Å$^{-1}$, corresponding to translational correlation lengths on the order of 100Å . This should be compared with the extent of orientational order (grain sizes of several microns). The origins of x-ray line broadening will be discussed in more detail below. X-ray powder scans, which can reveal the presence of contaminant phases in bulk samples, also show considerable diffuse scattering around the most intense peaks.
**Figure 1** - X-ray powder diffraction profiles from rapidly quenched Al-M alloys. Note logarithmic scale. a) Al$_{78.4}$Mn$_{17.6}$Ru$_4$; b) Al$_{79.4}$Mn$_{19.6}$; c) Al$_{78}$Re$_{22}$; d) Al$_{78}$Ru$_{23}$; e) Al$_{85.7}$V$_{14.3}$; f) Al$_{92.3}$Mo$_{7.7}$.

**Figure 2** - X-ray diffraction profiles of ternary and quaternary compounds. a) Al$_{74.5}$Mn$_{21}$Si$_{4.5}$; b) Al$_{74.5}$Mn$_{21}$Si$_{4.5}$ (arrows indicate positions of $\beta$(AlMnSi) peaks); c) Al$_{80}$Mn$_{20}$ (slow quench); d) Al$_{79}$Mn$_{17}$Ru$_4$ (slow quench); e) Al$_{79}$Cr$_{17}$Ru$_4$; f) Al$_{75.8}$Mn$_{17.8}$Ru$_4$Si$_3$. 
We have identified the IP in seven of the Al-M systems surveyed (M=Mn, Re, Cr, Ru, V, W, Mo). We searched for, but did not find, evidence of the IP in binary alloys of Al with Ti, Fe, Co, Rh, Pd, Ta, and Pt. (Al-Pd and Al-Pt easily formed decagonal phase, however). In order to make comparisons between systems containing the IP, it is helpful to consider three different factors: 1) the degree of translational order as measured by the width of the sharpest diffraction peak, which is the I(10000) at 2.90Å⁻¹ in our indexing scheme. 2) the extent of orientational order as indicated by grain size, and 3) the relative phase stability as indicated by presence or absence of other phases. A representative set of diffraction scans is shown in Fig. 1. As a reference, Fig. 1a shows a diffraction profile from a stoichiometric (78.4% Al) Al-Mn sample which has been stabilized by the addition of a small amount of Ru, as discussed below. The IP can be recognized easily by the 3 pairs of strong peaks at approximately 1.7, 3.0, and 4.25Å⁻¹ and is indexed as shown. Note the use of a logarithmic intensity scale; plotting the data in this way emphasizes weak peaks and diffuse scattering at the expense of exaggerating noise and distorting peak shapes.

A typical scan from an Al-Mn binary alloy (Fig. 1b) has a similar diffraction profile but contains several low intensity peaks which cannot be icosahedrally indexed, and indicate the presence of contaminant phases. The sample composition is slightly Al-rich (80.4% Al) so that the excess fcc-Al has precipitated between IP grains, giving rise to the Al(111) reflection at 2.69Å⁻¹, as indicated. Two other peaks at 2.80 and 1.81Å⁻¹ signal the presence of decagonal phase, as does a slight broadening of the I(110000) which is nearly coincident with a third strong decagonal phase peak. As discussed above, it is this overlapping of numerous peaks between these two phases that hinders quantitative analysis of the scattering data. A scan from a stoichiometric Al-Re sample is shown in Fig. 1c. The sample is nearly single phase and peak widths are slightly broader than those seen in Al-Mn scans. A comparison with Fig. 1b shows that relative peak intensities are somewhat altered, a consequence of increased scattering from the heavy Re atoms. The Al-Mn and Al-Re systems are the best of the Al-M IPs that we have found.

The remaining five icosahedral Al-M binary alloys are of much poorer quality. An x-ray scan of an Al₂₇Ru₃₃ alloy is shown in Fig. 1d. The system is three-phase and indexes to the IP, fcc-Al and crystalline Al₁₃Ru₄. If the quenching rate is increased by increasing the wheel velocity, the amount of Al and of Al₁₃Ru₄ decrease, implying that single phase icosahedral Al-Ru might be formed at yet higher quenching rates. Both grain sizes and translational correlation lengths are noticeably smaller in these samples than in Al-Mn, and these do not improve at higher quenching rates. A stoichiometric Al-V alloy spun at our standard quenching rate produced a two-phase system of Al₃V and fcc-Al. The IP could only be formed at an Al-rich composition of > 85% Al. X-ray scans (Fig. 1e) show peaks from the two phases and a broad diffuse scattering intensity around 2.9Å⁻¹. As discussed earlier, this diffuse scattering occurs in all systems, but it is most pronounced in those of poorer quality. Finally, Fig. 1f shows a diffraction scan of Al₁₉₃Mo₇₇. Samples at 4:1 and 6:1 Al-Mo compositions both produced crystalline phases. The IP appears in this 12:1 sample, but clearly the icosahedral ordering is very poor. The peaks are broad and there is a large amount of diffuse scattering. Microscopy showed the grain sizes to be 1000Å or less. The Al-W system has similar characteristics.

The seven icosahedral binary alloys are formed with transition-metals which are grouped in the center of the periodic chart. Not surprisingly, they have similar phase diagrams with Al and share several isomorphic structures. These results suggest that Al-Tc and Al-Os would quench to the IP as well.

V - Ternary and Quaternary Compounds

It has been noted that the icosahedral ordering in Al-Mn is improved by the replacement of a few percent Al with Si in the sample composition. Diffraction intensities are altered slightly so that weak reflections, unseen in binary samples, become visible in electron diffraction pictures and micrographs of single grains show significantly reduced strains. Evidence for increased icosahedral order is also seen in the x-ray data. Peak widths sharpen noticeably, indicating a larger translational correlation length and the presence of decagonal phase is reduced. An x-ray scan of Al₇₄.₃Mn₇₃Si₄₅ (Fig. 2a) reveals almost no decagonal phase, with only the most intense reflection at 2.8Å⁻¹ appearing above the background scattering. However, the addition of Si has induced the growth of another phase, which becomes more prevalent with increasing Si content. An Al₇₁.₈Mn₇₅Si₇.₅ sample (Fig. 2b) shows more clearly a number of peaks from this phase which we identify as crystalline β(AlMnSi)₂⁵. At our standard quenching rate, the Si content which minimizes the decagonal and β(AlMnSi) phases is around 4%. At higher quenching rates the β-phase is suppressed so that single phase samples
are not restricted to such low Si concentrations. The effects of Si additions appear to be limited to the Al-Mn system. Inclusions of 4% Si in alloys of Al with V, Cr, Fe, Ru, Pd, and Re produced no significant changes in the diffraction profiles.

It is reasonable to consider a similar substitution for the transition-metal constituent, particular in light of recent Mössbauer (M. Eibshutz, private communication) and EXAFS measurements which suggest the presence of at least two Mn sites in icosahedral Al-Mn. We have investigated this question by replacing Mn with 2-11 atomic percent Ru and have found that the Ru addition greatly increases the IP stability relative to that of the decagonal phase. Fig. 2c and 2d compare the x-ray scans of Al-Mn and Al-Mn-Ru samples which have been spun at low quenching rates. The Al-Mn scan reveals large amounts of fcc-Al and decagonal phase whereas the Al-Mn-Ru is single phase. The decagonal phase suppression has been found to be strong in samples with 4 and 6% Ru. At a composition of 11 atomic % Ru, Al₁₋₃Ru₄ forms as a contaminant phase. The increased stability of the IP has been gained at the expense of translational order, as can be seen by the noticeably broader peak widths. This is not so for the Al-Cr system (Fig. 2e) for which the addition of Ru also suppressed a contaminant phase (not identified). The x-ray scans show that the width of the sharp (100000) peak actually decreases to 0.005A⁻¹, indicating an increased translational correlation length. Likewise, grain sizes measured from electron micrographs extend up to 25μ. Electron diffraction pictures from Al-Cr-Ru show an increased number of weak spots as in the case of Al-Mn-Si, and it has been possible to identify and index nearly 200 independent reflections. We have also observed up to 45 icosahedral x-ray powder pattern peaks in these samples. Finally, the addition of a few percent Si (Fig. 2f) to the AlMnRu samples sharpens the diffraction peaks without introducing any new additional phases.

We have also studied the effects of Ru additions to Al-V, Al-Fe, and Al-Pd and have found no noticeable difference in the tendency of these alloys to form the IP. Nevertheless, considering the significant effects observed in the Al-Mn-Ru and Al-Cr-Ru systems, it is plausible to suggest that the two transition-metals are occupying different sites, and that these sites are chemically as well as crystallographically distinguishable.

VI - Diffraction Peak Shifts and Broadening

In the remaining section of this paper we turn to the question of disorder in the icosahedral phase. The finite width of x-ray peaks signals the presence of considerable disorder in these materials and in particular the apparent symmetry dependence of the broadening indicates disorder or defects of an unusual nature. The peak broadening has been investigated from the point of view of both quasicrystalline and random packing models. It is found that both models can account for the broadening in a natural way. We have observed distortions in electron diffraction pictures that involve both the broadening and shifting of spots. We show here that, within the quasicrystalline model, the same mechanism that leads to peak broadening in the x-ray data can account for all the distortions seen in our electron diffraction.

We begin by considering scattering from a periodic crystal. In an ideal experiment a perfect crystal will have infinitely sharp Bragg peaks. If the crystal is described by a density

$$\rho(\vec{r}) = \sum_\Omega \rho_\Omega e^{i(\vec{G}_\Omega \cdot \vec{r} + \phi_\Omega)}$$

then the Bragg peaks will be located at the wavevectors \{\vec{G}\} which define the reciprocal lattice. The phases \(\phi_\Omega\) are given by \(\phi_\Omega = \vec{u} \cdot \vec{G}\) where \(\vec{u}\) is an arbitrary vector. The three degrees of freedom in the choice of \(\vec{u}\) result from the broken translational symmetry of the crystal; we can put the origin of the crystal wherever we choose. Suppose now we impose a smooth strain field on the crystal. This will shift the average positions of all the atoms. These displacements can be parametrized by the phases \(\phi_\Omega = \vec{u}(\vec{r}) \cdot \vec{G}\) so that the new atomic positions are given by

$$\rho(\vec{r}) = \sum_\Omega \rho_\Omega e^{i(\vec{G}_\Omega \cdot \vec{r} + \vec{u}(\vec{r}) \cdot \vec{G})}$$

As a concrete example, consider the special case of a linear field \(\vec{u}(\vec{r}) = \alpha \hat{x}\). This will impose a linear strain field which uniformly contracts or expands the lattice along the direction \(\hat{x}\). Clearly, this is equivalent to a small perturbation of the lattice and simply represents a transformation to another periodic structure. To see how this affects the scattering we write

$$\rho(\vec{r}) = \sum_\Omega \rho_\Omega e^{i(\vec{G}_\Omega \cdot \vec{r} + \alpha \vec{x} \cdot \vec{G})}$$

and let \(\alpha \vec{x} \cdot \vec{G} = \alpha \vec{G}_x \cdot \hat{x}\) where \(\vec{G}_x\) is the vector projection of \(\vec{G}\) along \(\hat{x}\). The crystal is now
described by a density

\[ \rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}} e^{i(\mathbf{G} + \alpha \mathbf{G}_s) \cdot \mathbf{r}} \]  

(4)

This just describes a new reciprocal lattice with vectors \( \{ \mathbf{G} + \alpha \mathbf{G}_s \} \). Bragg peaks will again be delta functions and will be found at these new positions, which in fact correspond to a uniform distortion of the original reciprocal lattice. The addition of non-linear terms will further affect the reciprocal lattice by broadening peaks. For instance, if a quadratic term is included in the strain field, along the same direction, we arrive at

\[ \rho(\mathbf{r}) = \sum_{\mathbf{G}} e^{i(\mathbf{G} + (\alpha + \beta x) \mathbf{G}_s) \cdot \mathbf{r}} \]  

(5)

Scattering from this crystal will give peaks shifted to the positions \( \{ \mathbf{G} + \alpha \mathbf{G}_s \} \) and broadened by the term \( \beta x \mathbf{G}_s \cdot \mathbf{r} \). In this case, the broadening will be in the same direction as the shifts. One can generalize this picture to the case of arbitrary strains; in general the peak shifts and broadening will still be proportional in magnitude to \( | \mathbf{G} | \).

We now carry out a similar analysis for the quasicrystal. The density is still given by Eq. (1), but now \( \{ \mathbf{G} \} \) span the icosahedral reciprocal lattice. Since there are six basis vectors instead of the usual three we have three additional phases, \( \phi_G \), to specify:

\[ \phi_G = \mathbf{u}(\mathbf{f}) \cdot \mathbf{G} + \mathbf{w}(\mathbf{f}) \cdot \mathbf{G}_1 \]  

(6)

The \( \mathbf{u}, \mathbf{G} \) term occurs as in the crystalline case. The second term is due to the fundamental incommensurability of the quasilattice, which contains an additional degree of freedom in the relative phases of density waves. Note that the vector field which describes this freedom (phason field) couples to the lattice through the conjugate variables \( \{ \mathbf{G}_1 \} \). These variables are distinct from and in one-to-one correspondence with the vectors \( \{ \mathbf{G} \} \), which are conjugate to \( \mathbf{u}(\mathbf{f}) \).

For further details see the article by J. Socolar in these proceedings and references therein. For our present purposes it suffices to note that the term \( \mathbf{w}(\mathbf{f}) \cdot \mathbf{G}_1 \) is formally equivalent to the usual \( \mathbf{u}(\mathbf{f}) \) term and that \( \mathbf{G} \) and \( \mathbf{G}_1 \) are related by a linear transformation. The phason variable, then, describes strains in much the same way as the \( \mathbf{u} \) variable. The effect on the reciprocal lattice will again be to shift and broaden spots. However, the amount a given spot is shifted is now proportional to \( \mathbf{G}_1 \), rather than to \( \mathbf{G} \). A linear phason strain will distort the reciprocal lattice (and hence electron diffraction patterns) so that:

1) Shifts in spots will be along the strain direction. 2) The magnitude of the shifts will be proportional to \( \mathbf{G}_1 \). The intensities of spots roughly decrease with increasing \( | \mathbf{G}_1 | \), so that the faintest spots will be shifted the most. 3) An additional non-linear component in the same direction will broaden spots and this broadening will be in the same direction as the shifts.

The electron beam generating the diffraction patterns illuminates a region 0.5μ in diameter. The phason strains are apparently unidirectional throughout the entire region. The only plausible origin of a preferred direction on this length scale is the growth direction of the icosahedral phase. Preliminary studies indicate that the phason strain does correlate with the growth direction. For example, a diffraction picture taken from a region centered on a grain nucleus is shown in Fig. 4a. This region contains dendrites which grow radially from the nucleus and should contain a distribution of strain directions. Note that there is now no preferred direction evident in the patterns and that the spots have an unusual triangular shape. In Fig. 4b we show a calculation of the diffraction pattern for the innermost ring in the presence of a radial distribution of phason strains. The calculation superposes shifts for twenty strain directions oriented in the plane at regular intervals of 18°. The close agreement between the calculation and the actual diffraction pattern strongly suggests a correlation between the phason strain and growth direction.
Figure 3 - a) A 5-fold pattern from an Al$_{78}$Cr$_{17}$Ru$_5$ sample showing large anisotropic phason distortion. b) Calculated spot shifting due to a linear phason strain.
Figure 4 - a) A 5-fold pattern from the AlCrRu sample. The diffraction aperture was centered on the grain nucleus. b) A calculation of spot shifts due to a radial distribution of phason strains (see text).
The phason broadening of x-ray powder peaks has been discussed elsewhere. We observe here that if the phason strains are largely linear in character the peak broadening can be asymmetric. In the most extreme case, peaks with large G could be split. We emphasize that, despite the good agreement with the quasicrystal model, the diffraction pattern distortions presented here may receive other interpretations. In fact, a purely linear phason strain describes a perfectly ordered structure (which may be quasiperiodic or periodic), much as a purely linear conventional strain describes a homogeneous perturbation of a crystal lattice. We are presently investigating the possibility that the phason strains arise when the IP locks into another nearby phase which may be commensurate or incommensurate.

Acknowledgements

We would like to thank T. Egami, A.I. Goldman, D. Kofalt, D. Levine, T.C. Lubensky, J.S. Socolar, P.J. Steinhardt, and P.W. Stephens for many useful discussions. This work was supported by the National Science Foundation Materials Research Laboratory Program under contract DMR-8216718.

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