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Absolute structure-factor measurements of an Al–Pd–Mn quasicrystal

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A number of X-ray reflections from an icosahedral quasicrystal Al–Pd–Mn have been measured with great accuracy on an absolute basis by making use of Bragg-case diffraction. Since the specimen had high crystal quality, the dynamical theory was used for analyzing the results and to extract structure factors from measured integrated intensities. Good agreement was found between theory and experiment for strong reflections. Anomalous transmission was found to be strong in the 'good' regions of the quasicrystalline specimen and it was measured on an absolute basis, but the small residual strains present in the specimen prevented an accurate comparison between theory and experiment. A detailed discussion is presented on the parameters that mostly affect anomalous transmission in relationship to the adopted structural model.

1. Introduction

For several years, since the discovery of quasicrystals in 1984, the big question frequently asked in conferences and publications was: 'Where are the atoms?'.

One of the early attempts to answer this very basic question was a crystallographic study undertaken by Boudard *et al.* (1992). They measured 360 reflections and in this way they were able to fit a number of adjustable parameters in a 'cut and projection' model by comparing calculated and experimental intensities. They used a procedure to generate a large number of atomic sites (typically between 50000 and 100000), which were then used to calculate structure factors.

The quasicrystal used was a small sphere obtained by grinding and polishing, and the kinematic theory of diffraction was used to interpret the data.

The problem with this approach is that the quasicrystal is not an ideal mosaic, and the use of kinematic theory is questionable, especially for the strong reflections at low Q ($Q = 2\sin\theta/\lambda$). It is not clear then to what extent the atomic positions derived by Boudard *et al.* (1992) can reproduce the intensities of strong diffracted beams at low Q. A sensitive test of the accuracy of Boudard *et al.*'s (1992) model would be a diffraction experiment involving low-Q reflections, under conditions in which lattice imperfections could not play any role. The best quasicrystals available are Al–Pd–Mn alloys, which have been proved to exhibit anomalous transmission (Kycia *et al.*, 1993) and to yield rocking curves that are extremely sharp, 32″ wide (Lee *et al.*, 1996). Under the assumption that a good quasicrystalline specimen of Al–Pd–Mn diffracts as a perfect crystal, a Bragg-case diffraction experiment from a polished strain-free surface should yield a beam whose intensity can be calculated from first principles using dynamical theory. A more sensitive test can be performed using Laue-case diffraction, under conditions of anomalous transmission.

2. Experimental

The sample ($Al_{71.0}Pd_{20.5}Mn_{8.5}$) used for Bragg-case diffraction was a thick (∼3 mm) plate of triangular shape whose surface was perpendicular to a twofold axis. It was cut from a large Bridgman grown ingot. The side of the triangle was about 12 mm. Fig. 1 shows a Berg–Barrett topograph obtained with Cu $K\alpha$ radiation ($E = 8.04$ keV). The Bragg reflection was the $024\bar{0}24$, one of the strongest reflections. The quasicrystal appears to consist of three large grains. The uniform intensity across each grain is an indication of crystal perfection. The faint black lines present along the shorter grain boundary indicate stress. The reflectivity increases when stress is present. The measurements were all taken in the largest grain. The surface was diamond polished, and a circular region (about 8 mm in diameter) had been electropolished. The region, approximately circular, present in the middle grain, was smaller than the electropolished region, and had nothing to do with it. It was a black stained region, not well polished, and it was not used for measurements. The surprising result was that the reflectivity was the same over the diamond polished and the electropolished regions. In other words, there was no appearance of strain in the diamond polished region. The only plausible explanation for this result is that the Al–Pd–Mn quasicrystal is a very hard material, and so mechanical polishing with diamond does not introduce strain in the surface. Rocking curves were taken in the laboratory, using a double-crystal spectrometer, equipped with Ge(111) as

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monochromator, at several points on the surface. The cross section of the incident beam was about 1×1 mm. The integrated intensities obtained at several positions on the surface of the largest grain were quite uniform. Their average was used to get the values of structure factors given in Table 1 and their dispersion around the average was used to calculate the error bars. The rocking curves were always quite sharp, about $2'$ wide in the non-dispersive arrangement, corresponding more or less to the resolution of the spectrometer.

While we have no absolute proof that our quasicrystal specimen diffracts according to dynamical theory, all the indications we have point in that direction. True, uniform intensity in the diffracted beam is not a guarantee of crystal perfection. Usually, uniform intensity means that the crystal is perfect, except for some exceptional situations, of which we have no indications.

The FWHM of $2'$, measured on the first sample used for Bragg-case diffraction, corresponds to the resolution of the spectrometer, which was a laboratory installation (not synchrotron), with a sealed tube as X-ray source. In other words, a perfect silicon crystal would have produced diffraction peaks with the same FWHM. These crystals exhibit anomalous transmission, which is an indication of a high level of crystal perfection. We know that for moderate imperfections the effects on Bragg-case integrated intensities is negligible. What happens is that the diffraction peaks become broader, but the peak intensities decrease, so that the integrated intensity stays constant. The effect has been studied in detail by Patel *et al.* (1962). They show that a dislocation-free silicon crystal and a low dislocation density crystal (of the order of 100 dislocations cm^{-2}) exhibit the same integrated intensity for the 111 reflection, whereas their half-widths differ by 13.5%. In order to extract structure factors from measured intensities, we need to perform absolute measurements. It is a very well known classical method, called the 'rotating crystal method' (see, for example, Warren, 1969). Briefly, the quantity that can be directly compared with theory is a dimensionless number called P, the *integrated reflecting power*:

$$P = E\omega/I_O, \tag{1}$$

where E is the total number of counts collected by the counter as the crystal, during its rotation, goes through the Bragg reflection, ω is the angular velocity in rad s^{-1} and I_O is the power of the incident beam, namely, the number of counts s^{-1} in the incident beam.

The counter should be wide open, so that all diffracted photons contribute to E and the crystal should be large enough so that the incident beam is completely intercepted. The great virtue of equation (1) is that P does not depend on the structure of the incident beam, a quantity usually difficult to characterize. The only problem with this method is how to measure I_O. Usually the incident beam is strong enough to drive the counter, typically a scintillation counter, out of its linear range. The most common technique to measure I_O is to introduce a stack of attenuators, typically brass foils. Each foil should not attenuate more than 10%. The attenuation factor of each foil is accurately measured by using the linear region of the counter, and I_O is measured with all foils present on the beam. The problem with this technique is that usually there is some high-energy contamination in the beam, coming from harmonics transmitted by the monochromator. The high-energy component is strongly enhanced, compared to I_O, and in some extreme cases it may be impossible to discriminate electronically against the high-energy component. This extreme situation is rarely realized in laboratory installations, but is normally present in synchrotron beams. So, this is one of the rare cases in which a precise intensity measurement is

Table 1
Comparison of experimental and theoretical values for the structure factors of an Al–Pd–Mn quasicrystal.

The column to the right (Δ values) indicates the discrepancy factor, given by $\Delta = [(F_H^* - F_H)/F_H] \times 100$. The Debye–Waller factors have been taken out of the experimental values.

Reflection indices	$Q_\parallel$ (Å^{-1})	F_H (electrons Å^{-3}) experimental values	F_H^* (electrons Å^{-3}) calculated values	Δ
$04\bar{6}04\bar{6}$	0.78995	0.649 ± 0.03	0.596	−8
$02\bar{4}02\bar{4}$	0.48821	0.587 ± 0.008	0.494	−16
$04\bar{8}04\bar{8}$	0.97643	0.0115 ± 0.0005	0.0169	47
$\bar{2}20\bar{2}2$	0.30173	0.0833 ± 0.007	0.104	25
$\bar{2}24\bar{0}46$	0.67375	0.0271 ± 0.0009	0.176	549

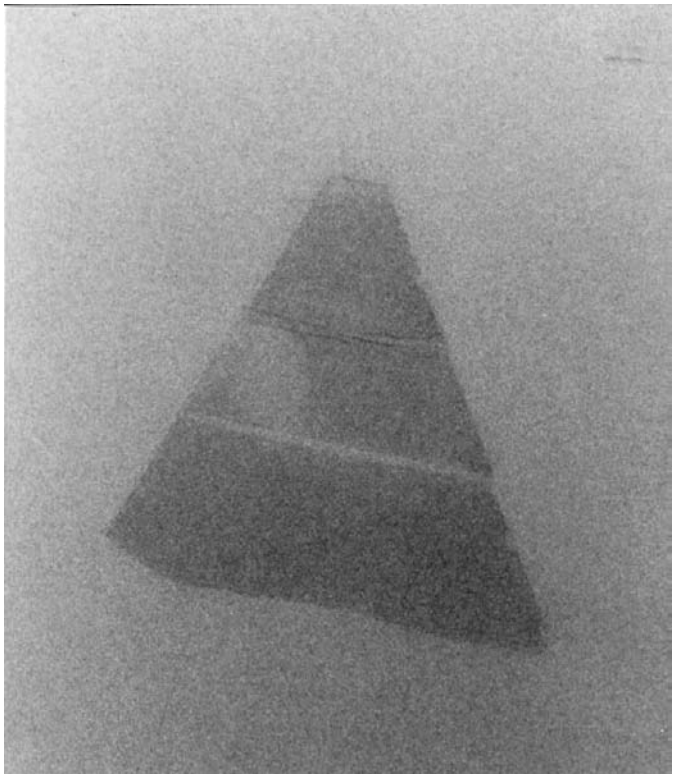

Figure 1
A Berg–Barrett topographic image of the Al–Pd–Mn quasicrystal sample which was used in the Bragg geometry measurements of structure factors. Three large grains extending several square millimetres in size could be identified. The uniform darkness indicates the perfect quality of the quasicrystalline sample.

Table 2
For the same reflections listed in Table 1, the Cartesian components of $\mathbf{Q}_\parallel$ are given, along with the relevant $q_\perp$ and M, N values (Cahn *et al.*, 1986).

The $q_\perp$ values have been calculated by means of equation 3.26*b* in Janot (1992).

Reflection indices	Components of $\mathbf{Q}_\parallel$: q_x, q_y, q_z	$q_\perp$ (Å^{-1})	M	N
$046\bar{0}46$	0.0, 0.0, 0.7899	0.027	336	208
$024\bar{0}24$	0.0, 0.0, 0.4882	0.044	128	80
048048	0.0, 0.0, 0.9764	0.088	512	320
$022\bar{0}22$	0.0, 0.0, 0.3017	0.071	48	32
$\bar{2}24\bar{0}46$	−0.1509, −0.1509, 0.6391	0.051	244	152

better done in the home laboratory, using a standard sealed tube set-up, rather than at a synchrotron installation.

There are ways to perform absolute measurements using synchrotron beams. A more elaborate technique suitable for synchrotron beams will be described later, in §4.

In order to extract the structure factor F_H from P, we make use of dynamical theory because we believe that the quasicrystal is perfect, as suggested by Fig. 1.

The formalism of dynamical theory is described in many books and papers. One convenient reference is the article by Hirsch & Ramachandran (1950).

In practice, we used a computer program written by one of us (Colella, 1974) for the solution of the problem of n-beam diffraction ($n = 2$, in this case), without approximations. The final results are presented in Table 1. The structure factors obtained from experiment do not contain the Debye–Waller factors. Those have been evaluated using the results of a separate experiment (Colella *et al.*, 2000), which are consistent with a Debye temperature equal to 312 K, and have been taken out from the F_H's obtained from the experimental integrated intensities. In other words, the structure factors obtained by fitting the experimental integrated intensities to the values calculated from dynamical theory have all been divided by the appropriate Debye–Waller factors $\exp(-M)$.

The indexing of Bragg reflections is consistent with the conventions established by Cahn *et al.* (1986). $Q_\parallel$ is defined to be $2\sin\theta/\lambda$. The $q_\perp$ values have been calculated by means of equation 3.26*b* in Janot (1992). The quantity Δ is a 'discrepancy index'. It is an indication of how far the experimental values are from theory.

It may be noticed that, while the first four reflections (from the top) are all located on a twofold axis, the last one, at the bottom, has its diffracting planes 18.5° away from the twofold axis. Asymmetry is properly taken into account in the dynamical theory program used to calculate the experimental values of F_H. The Cartesian components of $\mathbf{Q}_\parallel$, the value of $q_\perp$ and the M, N values (Cahn *et al.*, 1986) are given in Table 2.

3. Discussion

The data of Table 1 indicate that for most reflections the calculated and measured structure factors are off by no more than 50%. This is in itself a quite significant result, in view of the approximations and modeling that have been used in calculating the atomic sites and the structure factors.

The first reflection, the $046\bar{0}46$, is one of the strongest reflections, with a small value of $q_\perp$. It is expected to be dominated by multiple scattering and the mechanism of diffraction is dynamical. The fact that the measured value is only 8% above the calculated one is almost a miracle. The agreement between theory and experiment is indeed excellent.

The last reflection, with a larger $q_\perp$ value, is way off. We have no explanation for this huge discrepancy. The general trend emerging from Table 1 is that weak reflections (large $q_\perp$ values) tend to disagree with experiment more than strong reflections (say the first two in Table 1).

One of the key features of the theoretical model is the shape of the atomic surfaces in 6D space. It is known, in fact, that in the cut and projection method one has to specify a certain volume around each atom, in the form of a polyhedron (Bak, 1986). There are reasons to believe that the details of the atomic surfaces play a greater role in the weak rather than in the strong reflections (Gratias, 1991).

4. Anomalous transmission – experimental

A more sensitive test of the atomic sites calculated by Boudard *et al.* (1992) was attempted by making use of anomalous transmission (AT) of X-rays. The possibility of the existence of AT in a quasicrystal was predicted by Berenson & Birman in 1986. They considered a slab in which the spacing between atomic planes perpendicular to the slab is not uniform but rather given by a sequence of Fibonacci numbers. They showed that the conditions for AT can be realized even in such a situation. The experimental verification was obtained a few years later by Kycia *et al.* (1993). No attempt was made, however, to put the measurements on an absolute scale and to compare with theory.

We used one of our best slices, cut perpendicular to a twofold axis (within 0.25°) for a quantitative measurement of AT. The quasicrystal was a thin slab of $Al_{71.0}Pd_{20.5}Mn_{8.5}$, diamond polished on both sides. The thickness was 0.385 mm, as measured with a micrometer. Transmission and reflection topographs revealed a grain structure, with large grains (a few cubic millimetres each) and strained regions between the grains. A perfect region was selected, in which a high-energy ($E = 17.4$ keV) synchrotron beam from a perfect silicon-crystal monochromator, under conditions of normal transmission, would produce a sharp diffraction peak with no apparent broadening (about 30″ wide or less). The beam size was 0.8×0.8 mm. To make sure that the same region was used in all experiments, the quasicrystal was set against a thick copper plate with a 1.5 mm hole. Three bronze springs kept the slab gently pressed against the copper plate. The hole drilled in the copper plate had conical walls, with an angle of 41.5° between the lateral surface of the cone and its axis. The copper sample holder could be mounted on a standard eucentric goniometer head.

Table 3
The measured integrated reflections of the Al–Pd–Mn quasicrystal using anomalous transmission.

Theoretical calculations were done using a model of atomic locations developed by Boudard *et al.* (1992). The calculated integrated reflections were: 1.52×10^{-8} for the four upper equivalent reflections ($n = 1, 2, 3, 4$) and 1.42×10^{-9} for reflections 5, 6, 7, 8.

$Q_{\parallel}$ (Å^{-1})	Reflection indices	(q_x, q_y, q_z) (Å^{-1})	Integrated reflection R ($\times 10^{-11}$)	$q_{\perp}$ (Å^{-1})	M	N	No.
0.7899	$46\bar{0}60$	(0.7899, 0, 0)	3.01	0.027	336	208	1
0.7899	$\bar{4}\bar{6}04\bar{6}0$	(−0.7899, 0, 0)	2.11	0.027	336	208	2
0.7899	$046\bar{0}46$	(0, 0, 0.7899)	9.48	0.027	336	208	3
0.7899	$0\bar{4}6046$	(0, 0, −0.7899)	11.59	0.027	336	208	4
0.4643	$24\bar{2}\bar{2}22$	(0.3949, 0, 0.2441)	11.56	0.026	116	72	5
0.4643	$\bar{2}4\bar{2}22\bar{2}$	(−0.3949, 0, −0.2441)	5.23	0.026	116	72	6
0.4643	$22\bar{2}\bar{2}4\bar{2}$	(0.3949, 0, −0.2441)	10.00	0.026	116	72	7
0.4643	$\bar{2}22\bar{2}42$	(−0.3949, 0, 0.2441)	12.11	0.026	116	72	8
0.4882	$240\bar{2}40$	(0.4882, 0, 0)	Not observed	0.044	128	80	9
0.4882	$024\bar{0}24$	(0, 0, 0.4882)	Not observed	0.044	128	80	10

To make sure that the transmission was really anomalous, we decided to use a relatively low energy X-ray beam: 9 keV. At this X-ray energy, the linear absorption coefficient for the quasicrystal is 524.38 cm^{-1} as calculated using the program *FPRIME*, due to D. T. Cromer, based on a paper by Cromer & Liberman (1970). With a thickness of 0.385 mm, the product μt amounts to 20.19, and the normal absorption coefficient $\exp(-\mu t)$ is in the neighborhood of 1.7×10^{-9}. This is a much more stringent condition than the one used in the previous experiment by Kycia *et al.* (1993). They used higher X-ray energy ($E = 12$ keV). At this energy, the linear absorption coefficient μ is equal to 236.4 cm^{-1}, and with the thickness of 0.4 mm they used, the product μt amounts to 9.46 and the normal absorption coefficient $\exp(-\mu t)$ is close to 7.8×10^{-5}. In order to measure an integrated intensity on an absolute basis, we need to know I_O [see equation (1)], which is not easy for a synchrotron beam, in view of the extremely high power present in the beam.

Use of a large number of attenuators does not help because the high-energy contamination present in the incident beam, mostly due to $\lambda/3$, cannot be completely eliminated by electronic discrimination and makes the value of I_O unreliable.

One way to calibrate an incident beam is to measure the integrated intensity of a very weak reflection, for which the structure factor is known. Such is the case, for example, of the 222 reflection in Ge. This reflection is forbidden because the two f.c.c. lattices making up the Ge crystal structure are exactly out of phase. However, this result holds for spherical atoms. Since the bonding charges make the Ge atoms slightly aspherical, owing to a weak tetrahedral distortion, some weak intensity can be measured.

Several authors have measured the Ge 222 on an absolute basis using sealed X-ray tubes. We have adopted the value of $F_{222} = 1.08$ electrons (unit cell)$^{-1}$, measured several years ago by one of us (Colella & Merlini, 1966).

The 222 reflection in symmetric Bragg-case diffraction at the X18-A beamline of the National Synchrotron Light Source (NSLS) of Brookhaven National Laboratory was still quite intense and some calibrated Al attenuators were used to bring the counting rate of the scintillation counter into the linear range. Care was taken to avoid multiple Bragg scattering by judicious choice of azimuthal angles. Several measurements were taken in couples, with azimuths differing by 180°, in order to average out asymmetry effects owing to lack of parallelism between the (111) crystallographic planes and the physical surface of the crystal. In this way, the measurements done on the quasicrystal could be put on an absolute basis and compared to theoretical values, using structure factors calculated from atomic sites obtained by Boudard *et al.* (1992).

While, in principle, with $\mu t = 20.19$ the transmitted and diffracted beam are practically identical (Hirsch, 1952), we could not measure reliably the transmitted beam, owing to a strong high-energy contamination, even though a transmitted beam with X-ray energy = 9.0 keV, the unquestionable signature of AT, was clearly observed.

We could only observe AT for the first two reflections (in terms of intensity) observable in the Al–Pd–Mn quasicrystal. They are labeled 1 and 5 in Table 3, which shows all our results on AT. It also shows the structure factors calculated from Boudard *et al.*'s (1992) model, used for the calculations of theoretical integrated intensities.

We also attempted to observe the third reflection in Table 3, the $240\bar{2}40$, and its equivalent, the $024\bar{0}24$. We did not see any evidence for these two reflections, even though their $q_{\perp}$ value (0.044 Å^{-1}) is only slightly greater than the corresponding values for the first reflection ($q_{\perp} = 0.0259$ Å^{-1}), and for the second one ($q_{\perp} = 0.0272$ Å^{-1}). Reflections 1, 5 and 9 are the first three reflections, in terms of intensity, in the set of 360 reflections measured in 1992 by Boudard *et al.* for a crystallographic refinement.

After the initial observation of AT for reflection 1, we measured three more equivalent reflections (nos. 2, 3, 4). They are all crystallographically equivalent to 1. They all correspond to diffracting planes perpendicular to the quasicrystal slab we were using as specimen. We expected to find the same values, but unfortunately, as Table 2 shows, they vary quite a bit from a minimum of 2.11×10^{-11} to a maximum of 11.59×10^{-11}. Similar variations, to a smaller extent, were also found between reflections of the second set, nos. 5, 6, 7, 8, which are also equivalent among themselves. The only

possible explanation for these wild variations of intensity between equivalent reflections is the effect of imperfections and strain, which has indeed been proven to be true in a separate topography experiment done on the same specimen (Härtwig *et al.*, 2001). It is conceivable that strain will produce different effects on different sets of atomic planes, even though they are crystallographically equivalent. We will consider for our analysis the highest values of the integrated intensities given in Table 3, namely 1.16×10^{-10} for reflection 1 and 1.21×10^{-10} for reflection 2. The calculated values are considerably larger than the experimental values: 1.52×10^{-8} and 1.42×10^{-9}, respectively. In other words, the calculated values are greater than the experimental values by the following factors: 131 for reflection 1 and 11.7 for reflection 2.

In order to understand the possible origin of such large discrepancies, we must consider the parameters that mostly affect AT. It has been shown (Okkerse, 1962; Hirsch, 1952) that, in the case of $\mu t \geq 20$, the AT transmitted and diffracted beams are both proportional to a factor F:

$$F = \exp[-\mu t(1 - \varepsilon_H)], \tag{2}$$

where μ is the 'normal' absorption coefficient (= 20.19 in our case). t is the effective thickness ($= t_O/\cos\theta_B$) in the direction of the incident beam at the Bragg angle, and

$$\varepsilon_H = F''_H/F''_0, \tag{3}$$

where F''_H and F''_0 are the imaginary parts of the structure factor for the diffracted beam (F_H) and for the forward scattered beam (F_0). F_H contains the Debye–Waller factor, which is very close to 1 for reflections 1 and 2 in Table 2. Neglecting thermal motion, and assuming that all atoms scatter in phase, we have

$$\varepsilon_H = f^i_h/f^i_0, \tag{4}$$

where f^i_H and f^i_0 are the imaginary parts of the atomic scattering factors in the direction of the reflected and incident beams, respectively. If thermal motion is neglected and only inner-core electrons are involved in the absorptive processes, the electrons responsible for absorption surrounding every nucleus are confined within a point-like region.

If we remember the physical origin of AT, namely, the onset of a set of standing waves with antinodes centered *between* the atomic planes, it is clear that no absorption takes place in this situation because there are no electrons where the electric field is strong. This is the physical meaning of $\varepsilon_H = 1$, causing F (in equation 2) to be equal to 1 when all the atoms scatter in phase. This means zero absorption. If the atoms are out of phase, ε_H is less than 1 and AT is severely limited. This is the reason why, in a crystal like silicon, the 220 reflection, for which all the atoms are in phase, exhibits strong AT. The 333, on the other hand, for which the atoms are partially out of phase ($\varepsilon_H \simeq 0.7$), exhibits a very weak AT, not observable with traditional X-ray sources such as sealed tubes or rotating anodes. If we assume that most of the absorption involves inner-core electrons, there is no directional dependence and f^i_H, f^i_0 are practically identical.

If all the atoms scatter in phase, then ε_H is very close to 1 and equation (2) shows that the attenuation factor F is close to 1 (which means zero absorption). Equation (2) also shows how sensitive AT is to ε_H. Small departures of ε_H from 1 produce large effects on AT intensities when μt is large.

In our case, the key point to consider is the extent to which the atoms in the quasicrystal scatter in phase. Since there is no long-range ordering, it is not realistic to expect that all the atoms scatter in phase. It is worthwhile calculating ε_H for reflections 1 and 2 in Table 3, under the assumption of zero thermal motion, and assuming that $f^i_H = f^i_0$. The calculation is done using the atomic sites calculated by Boudard *et al.* (1992). The results are:

$\varepsilon_{H1} = 0.647$ for reflection 1;

$\varepsilon_{H2} = 0.812$ for reflection 2.

It is clear that small changes in structure (*i.e.* atomic sites) will produce some changes in ε_{H1} and ε_{H2}, which in turn will produce large effects on the AT intensities (diffracted and transmitted).

It appears then that AT can provide a sensitive test of structural information through the effect of ε_H, provided highly perfect quasicrystalline grains can be found.

5. Conclusions

A number of reflections have been measured quantitatively, on an absolute basis, by making use of Bragg-case diffraction, and compared with calculate values using a model of the icosahedral quasicrystal Al–Pd–Mn developed by Boudard *et al.* (1992). A quasicrystalline specimen of high perfection was used and good agreement between theory and experiment was found for strong reflections. Since these reflections were strongly affected by extinction, dynamical theory was used throughout the analysis of the results. On the other hand, disagreement between theory and experiment was found for weak reflections. This was probably because the details of the atomic surfaces in 6D space play a more important role for the weak reflections.

The anomalous transmission was also measured quantitatively on an absolute basis. Small residual imperfections in the quasicrystal caused large scattering of measured intensities for equivalent reflections, which made it difficult to assess the degree of agreement (or disagreement) between theory and experiment. Attention is called to a parameter ε_H which is a measure of the extent to which the atoms in the quasicrystal scatter in phase. This parameter is a sensitive function of the structural model adopted for the quasicrystal and can be calculated for a given model and also measured experimentally. If more perfect quasicrystals are available, the parameter ε_H may well turn out to be the most sensitive parameter for evaluating quasicrystal models.

References

Bak, P. (1986). *Phys. Rev. Lett.* **56**, 861–864.
Berenson, R. & Birman, J. L. (1986). *Phys. Rev. B*, **34**, 8926–8928.

Boudard, M., de Boissieu, M., Janot, C., Heger, G., Beeli, C., Nissen, H. U., Vincent, H., Ibberson, R., Audier, M. & Dubois, J. M. (1992). *J. Phys. Condens. Matter*, **4**, 10149–10168. Tables of observed intensities and calculated structure factors were kindly provided in the form of a private communication by M. de Boissieu and M. Boudard.
Cahn, J. W., Shechtman, D. & Gratias, D. (1986). *J. Mater. Res*. **1**, 13–26.
Colella, R. (1974). *Acta Cryst.* A**30**, 413–423.
Colella, R. & Merlini, A. (1966). *Phys. Status Solidi*, **18**, 157–166.
Colella, R., Zhang, Y., Sutter, J. P. & Ehrlich. S. N. (2000). *Phys. Rev. B*, **63**, 014202-1–5.
Cromer, D. T. & Liberman, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.
Gratias, D. (1991). Private communication.
Härtwig, J., Agliozzo, S., Baruchel, J., Colella, R., de Boissieu, M., Gastaldi, J., Klein, H., Mancini, L. & Wang, J. (2001). *J. Phys. D: Appl. Phys.* **34**, A103–A108.
Hirsch, P. B. (1952). *Acta Cryst.* **5**, 176–181.
Hirsch, P. B. & Ramachandran, G. N. (1950). *Acta Cryst.* **3**, 187–194.
Janot, C. (1992). *Quasicrystals. A Primer*. Oxford: Clarendon Press.
Kycia, S. W., Goldman, A. I., Lograsso, T. A., Delaney, D. W., Black, D., Sutton, M., Dufresne, E., Brüning, R. & Rodricks, B. (1993). *Phys. Rev. B*, **48**, 3544–3547.
Lee, H., Colella, R. & Shen, Q. (1996). *Phys. Rev.* **54**, 214–221.
Okkerse, B. (1962). *Philips Res. Rep.* **17**, 464–478.
Patel, J. R., Wagner, R. S. & Moss, S. (1962). *Acta Metal.* **10**, 759–764.
Warren, B. E. (1969). *X-ray Diffraction*, Section 4-2. New York: Addison-Wesley.