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A cubic approximant of the icosahedral phase in the (Al–Si)–Cu–Fe system

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Abstract. We present a stable simple cubic structure in the quaternary system (Al–Si)–Cu–Fe with the composition $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ which corresponds to the $p/q = 1/1$ cubic approximant of the icosahedral Al–Cu–Fe phase. This cubic structure, with lattice parameter $a = 12.330 \text{ \AA}$ and density $\rho \approx 4.773 \text{ g cm}^{-3}$, contains roughly 135 atoms per unit cell. Preliminary studies of NMR and ME spectra as well as electric conductivity properties strongly suggest that this alloy shares most of the basic structural and physical properties of the parent icosahedral phase I-(Al–Cu–Fe).

1. Introduction

There are two major questions about quasicrystals which are still only partially answered: one concerns the accurate description of the atomic structure, and the other concerns the characteristics of the physical properties of quasicrystals as opposed to standard crystals.

In both cases, ‘approximant’ (periodic) structures have been shown to be very useful for understanding quasicrystals: immediately after the discovery of the icosahedral phase in the system Al–Mn [1], Elser and Henley [2] showed that a cubic crystalline phase, α -(Al–Mn–Si), studied long ago by Cooper and Robinson [3], could be seen as an ‘approximant’ to the icosahedral phase where the golden mean† $\tau = (1 + \sqrt{5})/2$ is simply replaced by its first rational approximant $\tau \approx p/q$ with $p = q = 1$. A very natural link between quasicrystals and ‘approximant’ crystals, and the number theory method of approximating real numbers by rational numbers had its root in the cut description where elementary geometry showed that any quasicrystal could be viewed as an ‘interpolation’ between crystals. This is because any irrational cut of a lattice can be viewed as an interpolation between rational cuts [4, 5]. The global result was that some specific crystalline structures should share, at least at medium-range distances, most of the atomic arrangements with the parent quasicrystal. For example, the cubic α -(Al–Mn–Si) phase can be described as a package of Mackay icosahedral clusters which do indeed seem to be the basic space-filling units in the icosahedral phase of the Al–Mn–Si system. In the same spirit, the R-(Al–Li–Cu) phase [6], discovered by Bergman in

† This is used to define the orientation of the 3D cut space in the standard 6D space representation of the quasicrystal.

the late fifties [7], is the result of a package of so-called Bergman icosahedral clusters on a cube-centred lattice, and has been shown by Elser and Henley to correspond to a cubic approximant of the icosahedral Al–Li–Cu quasicrystal. Both phases have about a hundred atoms per unit cell, and they have provided the basis for extensive structural studies of the icosahedral phases in these two systems [2, 8, 9, 10].

The discovery of the stable icosahedral phase by Tsai *et al* [11] in the ternary system Al–Cu–Fe posed a new problem in the sense that, unlike in the previous cases, no crystalline phase in the vicinity of the icosahedral phase in the phase diagram could be identified as a ‘simple’ approximant. The phase diagram has since been studied in great detail [12, 13, 14] and several approximant phases have been identified in a small region around the icosahedral phase [15–21], all with very large unit cells containing several hundreds of atoms. None of these phases have been totally determined by standard crystallography—not only because of their structural complexity, but also because of the metallurgical difficulty of extracting single-phased single crystals.

These studies showed how close quasicrystals and approximants can be with respect to their overall physical properties. Very careful examinations of the diffraction patterns are often required to distinguish a large-unit-cell approximant from its parent quasicrystal, and most of the electronic properties of quasicrystals and approximants are quite similar. For example, the transport properties of the icosahedral phase and its high-order approximants are almost indistinguishable [22–26] for the Al–Cu–Fe system. This is in agreement with the general idea that electronic transport properties in metallic alloys depend mostly on the short- and medium-distance atomic order.

The present paper reports a successful attempt to synthesize a high-structural-quality approximant of the Al–Cu–Fe icosahedral phase which is simple enough for a standard crystallography determination and could be a good candidate for extensive electronic band-structure calculations (see, for instance, [28]). This has been achieved by substituting a few per cent of silicon for aluminium in the quaternary system (Al–Si)–Cu–Fe. We present here experimental results for a sample of composition $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ which is icosahedral after a rapid quench (with some traces of the crystalline phase β) and becomes simple cubic ($Pm\bar{3}$, $P23?$) with a unit cell $a = 12.330 \text{ \AA}$ after being annealed for two hours at $650 \text{ }^\circ\text{C}$. The goal of the paper is to show that this cubic phase can indeed be qualified as the cubic approximant with $p/q = 1/1$ of the parent icosahedral phase.

2. Experimental conditions

The alloys were prepared from the pure elements (Al 99.99%, Si 99.999%, Cu 99.999%, Fe 99.99%) by induction melting in an alumina crucible under a controlled pure helium atmosphere flow. The entire ingots ($\approx 5 \text{ g}$) were remelted by induction heating in a silica nozzle and rapidly quenched by planar flow casting on a rotating copper wheel, under a pure helium atmosphere.

Several alloys with different percentages of silicon were prepared, by varying the ratio of substitution of Si for Al starting from the ‘canonical’ icosahedral phase $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$. Only the composition $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ will be discussed in this paper. The as-quenched state of this alloy is two phased: an ‘imperfect’[†] icosahedral phase, denoted as the I phase, is accompanied by a small amount of a simple cubic FeAl-type phase, denoted as the β -phase, rejected into the interdendritic regions. When this as-quenched alloy is annealed for

[†] This is in the sense that the full width at half-maximum (FWHM) of the x-ray reflections is larger than the instrumental resolution, and some peak locations are slightly shifted from their theoretical positions.

two hours at 650–680 °C, it transforms into a single-phased simple cubic state, denoted as the α -phase, with a density of $\rho \approx 4.773 \text{ g cm}^{-3}$.

3. X-ray results

Standard powder x-ray diffraction patterns were obtained on a Philips diffractometer equipped with a curved graphite monochromator in the diffracted beam, using Co $K\alpha$ radiation ($\lambda = 1.7902 \text{ \AA}$). The instrument resolution, measured by the FWHM of the (200) line from a standard CeO_2 powder sample, is about $0.08^\circ\theta$ ($\Delta q \sim 1.5 \times 10^{-3} \text{ \AA}^{-1}$, with $q = 2(\sin \theta)/\lambda$).

Table 1. The number ν of split orbits and multiplicities μ for the principal reflections of the icosahedral symmetry as a function of the point symmetry of the approximant.

Symmetry	Icosahedral $m35$		Cubic $m3$	
	μ	ν	μ	
A_5	12	1	12	
A_3	20	2	(8, 12)	
A_2	30	2	(6, 24)	

As described in [21], the first step in the identification of an approximant structure by x-ray diffraction is calculating from simple symmetry considerations how the icosahedral reflections with point group $m35$ split after a symmetry breaking to cubic $m3$. This is shown in table 1 for the main icosahedral reflections along five-, three- and twofold axes.

Figure 1(a) shows an x-ray powder diffraction pattern obtained for the cubic phase α ; there is an enlarged view in figure 1(b) of a small range of θ where the diffraction pattern of the as-quenched icosahedral phase (dashed lines) has been superimposed. Both the splitting and the locations of the cubic peaks match those of the expected x-ray diagram calculated for the cubic $p/q = 1/1$ approximant: the fivefold icosahedral reflection (7, 11) shows a simple peak shift with no split corresponding to the cubic reflection (320); the threefold icosahedral reflection (6, 9) splits into the two groups (310) and (222) of relative multiplicity 12 and 8; and the twofold icosahedral reflection (8, 12) splits into the two groups (321) and (400) with multiplicities 24 and 6 respectively. The observed intensities of the cubic reflections are in qualitative agreement with these multiplicities.

The computation of the expected peak positions of the cubic $p/q = 1/1$ approximant has been performed using the standard ‘shear’ formalism [30–34, 21], where each cubic peak, say Q_{\parallel} , is deduced from the corresponding icosahedral peak (q_{\parallel}, q_{\perp}) via the linear shear transformation:

$$Q_{\parallel} = q_{\parallel} + \varepsilon q_{\perp}. \quad (1)$$

The shear matrix ε in the cubic case is the following:

$$\varepsilon = \tan \varphi \text{ Id} \quad (2)$$

where the angle φ represents the amplitude of the shear and Id is the 3×3 identity matrix. The shear amplitude, $\tan \varphi$, is related to the integers p and q by

$$\tan \varphi = \frac{p - q\tau}{q + p\tau}. \quad (3)$$

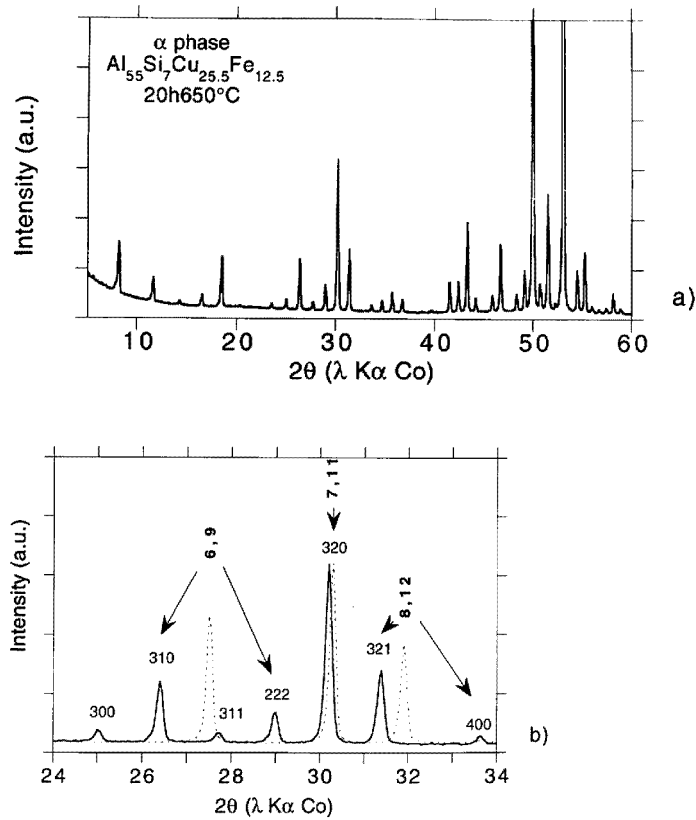


Figure 1. (a) The x-ray powder diffraction pattern of the cubic approximant α ($p/q = 1/1$) identified for the alloy $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ after annealing the as-quenched sample for 20 hours at 650°C . (b) For comparison between x-ray powder diffraction patterns of the previous α -phase and the I-phase—for the alloy $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$ obtained after annealing the as-quenched sample for 2 hours at 800°C —a portion of the previous pattern is enlarged (plain line) and the corresponding pattern of the I phase is superimposed (dashed line). The indexation of each phase is displayed, and a schematic representation shows how each icosahedral reflection [29] splits into cubic reflections.

The cubic unit cell is built on the three following 6D vectors:

$$\begin{cases} A = (q, p, 0, -q, p, 0) \\ B = (p, 0, q, p, 0, -q) \\ C = (0, q, p, 0, -q, p) \end{cases} \quad (4)$$

with the lattice parameter a as follows:

$$a = \frac{\sqrt{2}A(q + p\tau)}{\sqrt{2 + \tau}} \quad (5)$$

where A is the parameter of the (primitive) 6D lattice of the parent icosahedral phase.

Using the measured lattice parameter of the cubic α -phase, $a = 12.330 \pm 0.001 \text{ \AA}$, i.e. a 6D lattice parameter of $A = 6.3346 \text{ \AA}$, we calculated the expected x-ray peak positions for $\varphi = 13.05^\circ$ corresponding to $p/q = 1/1$. The deviations between experimental and

theoretical x-ray positions are never larger than $\Delta q \approx 10^{-4}$, which is within the experimental resolution, and all observed peaks are within this indexation scheme.

4. The icosahedral–cubic phase transformation

Differential scanning calorimetry (DSC) measurements on the as-quenched flakes were carried out using a Seiko 320 Differential Scanning Calorimeter. As-quenched flakes (20 mg) were put in alumina crucibles and heated at $10\text{ }^{\circ}\text{C min}^{-1}$ up to $1200\text{ }^{\circ}\text{C}$ under a 100 ml min^{-1} pure argon flow. The samples were then cooled at $10\text{ }^{\circ}\text{C min}^{-1}$ or quenched.

First of all, the substitution of Si for Al performed for the ‘canonical’ composition $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$ produces a decrease of the solidus temperature: it goes from $828\text{ }^{\circ}\text{C}$ in the case of the ‘canonical’ composition down to $769\text{ }^{\circ}\text{C}$ for the alloy $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$.

Figure 2(a) shows two DSC curves: the first one was obtained for flakes of as-quenched $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$ alloy and is presented for comparison with the second one which was obtained for flakes of as-quenched $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ alloy. A clear exothermic effect is observed for the second curve between $619\text{ }^{\circ}\text{C}$ and $705\text{ }^{\circ}\text{C}$ with an enthalpy change $\Delta H = 520\text{ J/g atom}$ which corresponds, as determined by x-ray diffraction, to the transformation from the icosahedral phase of the as-quenched state to the cubic approximant α -phase. This enthalpy change, which has never previously been detected in the transitions between the high-order approximants and the icosahedral phase in the Al–Cu–Fe ternary system, has a value of the order of magnitude of a standard order–disorder transition induced by chemical substitution [37] in metallic alloys.

To check the relative stability of the icosahedral versus cubic phases we performed the following DSC experiment (see figure 2(b)). The as-quenched icosahedral flakes were first slowly heated up to $710\text{ }^{\circ}\text{C}$ (the first heating curve in the figure) and then quenched. The exothermic peak is clearly observed, and x-ray diffraction shows that the icosahedral phase has entirely transformed into the cubic α -phase. A second heating in the same conditions showed a flat featureless DSC curve and no structural change on x-ray diffraction. Except for a fine crystallization of the β -phase above $700\text{ }^{\circ}\text{C}$, the cubic α -phase remains unchanged up to the solidus temperature. Hence, the icosahedral phase obtained by rapid quenching is a metastable phase which transforms into the stable cubic α -phase on heating: *the substitution of silicon for aluminium stabilizes the cubic approximant*. The kinetics of the transformation from icosahedral as-quenched structure to cubic is considerably faster than that observed with the approximants in the Al–Cu–Fe system. For example, the transition from the icosahedral to the rhombohedral phase in Al–Cu–Fe typically takes several days whereas, in the present case, two to three hours are sufficient, in the same range of temperature, for reaching the equilibrium state.

5. Transport properties of the cubic approximant α -phase

The low-temperature electrical conductivity was measured by the four-probe method for several samples of α -phase $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$. As presented in figure 3, the behaviour of the conductivity with respect to temperature is exactly opposite to what is expected for metallic alloys: the conductivity is low, with $\sigma_{4\text{K}} \approx 450\text{ }\Omega^{-1}\text{ cm}^{-1}$, and increases with temperature.

The value of $\sigma_{4\text{K}}$ is a particularly remarkable result for a crystalline phase with such a relatively small lattice parameter. As a comparison, the tetragonal ω - $\text{Al}_7\text{Cu}_2\text{Fe}$, with comparable unit-cell volume ($a = 6.34\text{ }\text{\AA}$, $c = 14.87\text{ }\text{\AA}$) and chemical composition, presents

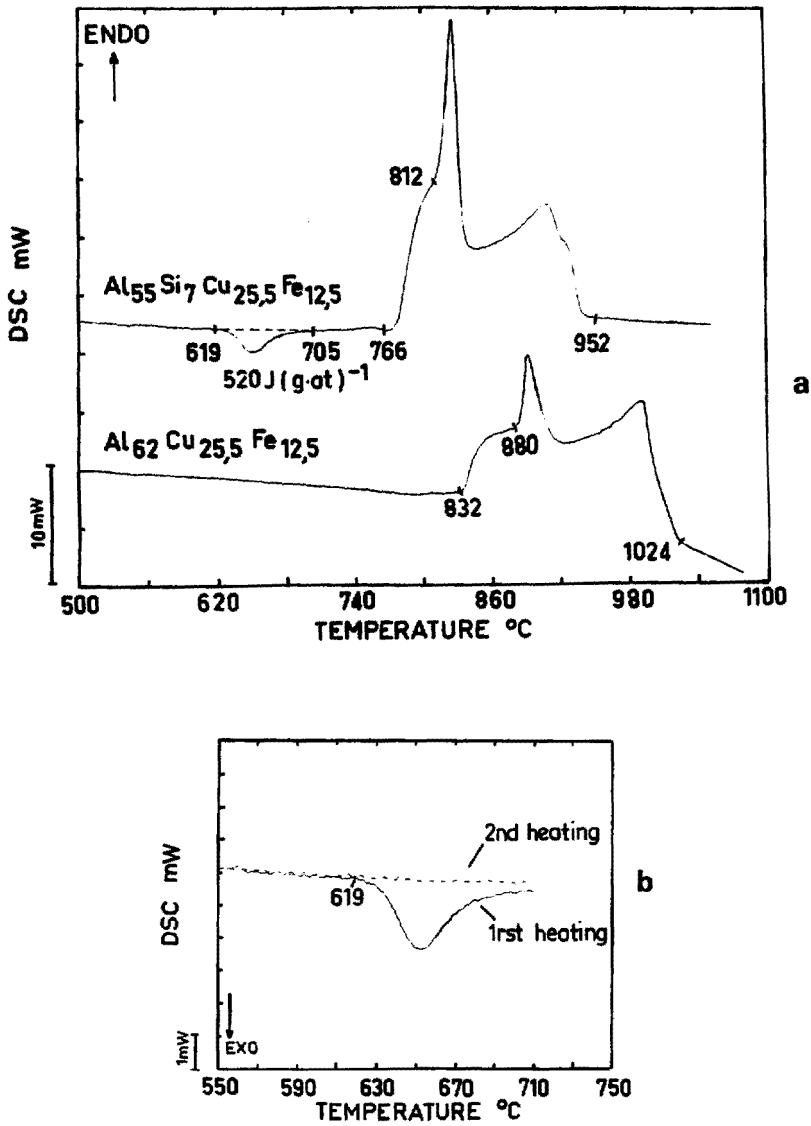


Figure 2. (a) DSC curves obtained for flakes of as-quenched $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$ and $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ alloys. (b) DSC curves obtained for as-quenched $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ alloys. The first heating was performed at $10\text{ }^\circ\text{C min}^{-1}$ up to $710\text{ }^\circ\text{C}$, then the sample was cooled at $100\text{ }^\circ\text{C min}^{-1}$, and then heated again at $10\text{ }^\circ\text{C min}^{-1}$ (second heating) up to $710\text{ }^\circ\text{C}$ and quenched.

a metallic behaviour with a conductivity $\sigma_{4\text{K}} \approx 46\,000\ \Omega^{-1}\text{ cm}^{-1}$, a hundred times higher than that for the cubic α -phase with a negative temperature dependence.

A second remarkable feature seen in figure 3 is that the temperature dependence of the conductivity $\delta\sigma(T) = \sigma(T) - \sigma_{4\text{K}}$ is the *same* (the inverse Matthiessen rule) as those of the other approximants and of the I-phase in the Al-Cu-Fe system.

These features show that the conductivity behaviour of the α -phase is typical of those

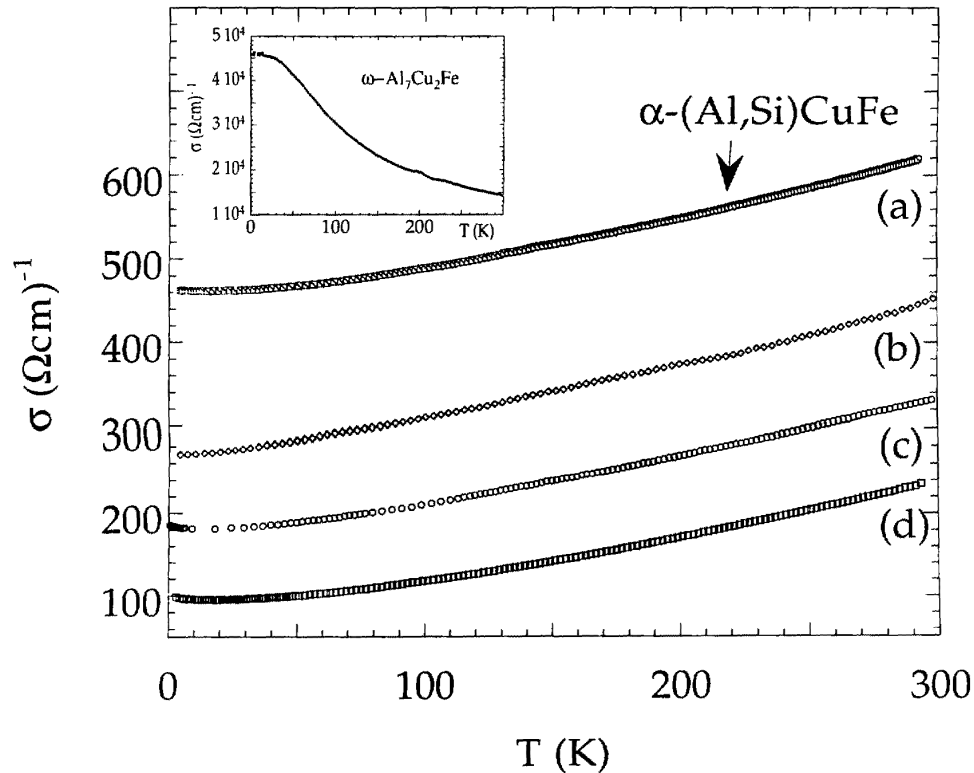


Figure 3. Electrical conductivity for icosahedral and approximant phases: (a) α -(Al, Si)CuFe; (b) the three approximant phases, namely orthorhombic O-Al_{60.4}Cu_{29.9}Fe_{9.7}, pentagonal P₁-Al_{63.6}Cu_{24.5}Fe_{11.9}, and rhombohedral R-Al_{63.6}Cu_{24.5}Fe_{11.2}; (c) icosahedral I-Al_{61.8}Cu₂₆Fe_{12.2}; (d) icosahedral I-Al_{62.5}Cu₂₅Fe_{12.5}. Inset: the conductivity of the (non-approximant) tetragonal ω -phase Al₇Cu₂Fe phase.

of the I-phase and of the standard large-unit-cell approximant in the Al–Cu–Fe system [23] (see figure 3). This speaks in favour of a similar conduction mechanism for all of these phases.

6. NMR and Mössbauer studies

In AlCuFe quasicrystals and high-order approximants, NMR and Mössbauer effect (ME) spectroscopies have proved to be valuable tools for investigating the local electronic properties as well as the local order, via the coupling of the quadrupolar moment with the local electric field gradient (EFG) (see, for instance, [25, 26, 27]). Other important properties include the Knight shift (NMR) and centre shift (isomer shift: ME).

The ⁵⁷Fe ME spectrum measured at room temperature in zero applied field and the ²⁷Al and ⁶⁵Cu NMR spectra observed at room temperature under 6.996 T in the α -phase Al₅₅Si₇Cu_{25.5}Fe_{12.5} are shown in figure 4.

The NMR spectra each consist of a single line corresponding to the $m = 1/2$, $m = -1/2$ nuclear spin transition superimposed on a much broader line due to the EFG splitting of the other nuclear transitions. Similar spectra have been observed for I-AlCuFe

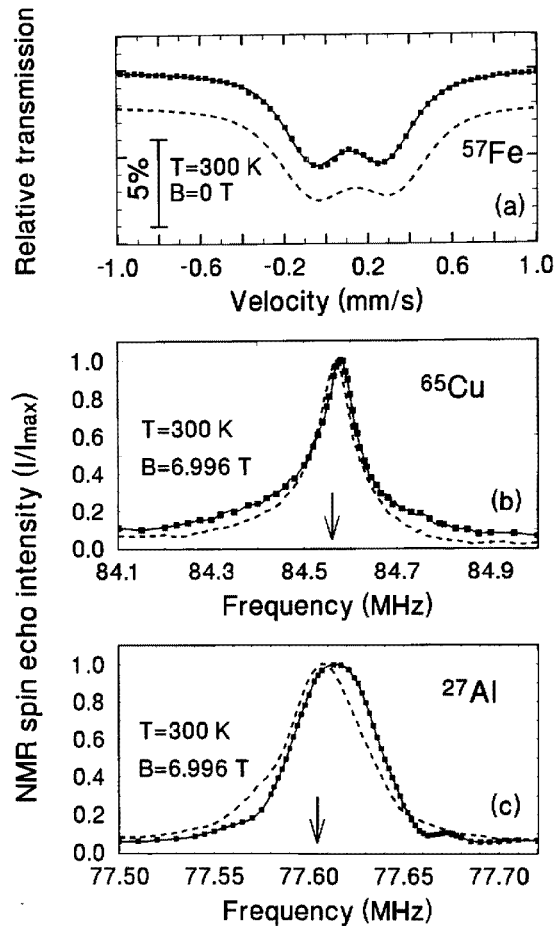


Figure 4. (a) The Mössbauer spectrum at room temperature in zero field, and (b) ^{65}Cu and (c) ^{27}Al NMR lines ($m = \pm 1/2$ transition only) at room temperature for $B = 6.996$ T, for the cubic $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ α -phase (solid boxes) and for the icosahedral $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$ phase (dashed line). In (a) the solid line is a fit of the Mössbauer line following the method described in [25]. In (b) and (c) the solid lines are only guides for the eye; the arrows indicate the reference frequencies in the applied field.

quasicrystal as well as for high-order approximants, and for all of the quasicrystalline alloys studied. To illustrate this point, spectra measured in identical conditions for the icosahedral $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$ phase [26] (with the same Cu and Fe content as the α -phase but without Si) have been given in figure 4. The absence of well-resolved quadrupolar satellites is characteristic of a broad distribution of local environments. In contrast, in the tetragonal ω - $\text{Al}_7\text{Cu}_2\text{Fe}_1$ phase the ^{27}Al NMR spectrum consists of many resolved peaks corresponding to the different crystallographic Al sites (F Hippert, unpublished results).

The shifts $K = (\langle \nu \rangle - \nu_{ref})/\nu_{ref}$ of the ^{27}Al and ^{65}Cu NMR lines are very small (less than 0.01%). Because of second-order quadrupolar effects (as explained in [25]), this small value does not reflect only electronic effects; however, it does indicate a small contribution of the s-electron density of states at the Fermi level in the α -phase on both

the Al and Cu sites, as confirmed by the long spin–lattice relaxation time T_1 measured. Both K - and T_1 -values are close to those measured for AlCuFe quasicrystals and high-order approximants [26, 27].

The fit of the ME spectrum of the α -phase, according to the method described in [25], shows that both the centre shift δ and the quadrupolar splitting ΔE_Q are quantities distributed around an averaged value: $\langle \delta \rangle = 0.2170 \pm 0.002 \text{ mm s}^{-1}$ and $\langle \Delta E_Q \rangle = 0.3367 \pm 0.002 \text{ mm s}^{-1}$ (δ is referred to α -Fe at room temperature). These values and the shape of the spectrum are quite close to those previously measured for AlCuFe quasicrystals and high-order approximants [26]. Thus, in the α -phase, the local environments of the Al, Cu and Fe sites are all broadly distributed.

At this preliminary stage of the study, it is difficult to comment on the tiny differences seen in the NMR and ME spectra between the α -phase and the icosahedral phase with the same Cu and Fe content but without Si. They could result from composition variation as well as from a possible influence of the long-range order, periodic or quasiperiodic. Only a comparison of the α -phase with a high-quality quasicrystalline phase for the very same composition would allow one to separate these two effects. In previous work [25, 26] we have shown that at the same composition the I-phase and its high-order approximants (rhombohedral, pentagonal or orthorhombic) could not be distinguished. However a significant composition dependence was also detected.

7. Discussion

The addition of a few per cent of Si substituting for Al in the Al–Cu–Fe canonical icosahedral phase stabilizes a cubic α -phase which corresponds to the cubic approximant $p/q = 1/1$ as suggested by the present structural analysis.

The α -phase can be easily obtained in single-phased form, and shows a remarkable crystallographic quality as deduced from the peak widths and profiles observed in the x-ray patterns.

Besides the composition we describe here, we made several other alloys by substituting Si for Al in various proportions starting from the canonical ternary icosahedral phase and for a composition corresponding to the rhombohedral phase of the ternary diagram. In all cases, we observed no structural changes for substitution of Si for Al lower than 2%. For substitutions larger than 2%, the cubic α -phase exists over a relatively large domain of composition and temperature, often in coexistence with the icosahedral or the rhombohedral phase.

With respect to structural features, it is interesting to observe that, from the experimental density, $\rho \approx 4.773 \text{ g cm}^{-3}$, and the composition, we obtain 135 atoms per unit cell with an average volume of 14.09 \AA^3 per atom (for comparison the idealized cubic phase $\text{Al}_9\text{Mn}_2\text{Si}_{1.8}$ proposed by Cooper and Robinson [3] has 138 atoms per unit cell and an average atomic volume of 14.77 \AA^3).

A striking point is that the 6D lattice parameter calculated from the actual cubic parameter in the framework of the shear method is significantly larger than the 6D parameter of the metastable as-quenched icosahedral phase of the quaternary alloy. On the one hand, the 6D parameter of this as-quenched phase in the quaternary alloy is $A = 6.3068 \text{ \AA}$ as compared to $A = 6.3173 \text{ \AA}$ for the canonical ternary icosahedral phase, which shows that Si substituted for Al contributes to a tiny contraction of the 6D unit cell. On the other hand, the 6D parameter calculated from the stable cubic phase is $A = 6.3346 \text{ \AA}$ which is, in contrast, 0.5% larger. This shows that the geometric description in terms of pure perpendicular shear—which has proved to be very accurate in the case of the pentagonal

and rhombohedral phases in Al–Cu–Fe—is here insufficient and should be corrected with a non-zero parallel component in the shear. This is not very surprising if one considers the group theory analysis proposed several years ago by Ishii [38] who showed that the symmetry breaking to cubic $m\bar{3}$ (or 23) contains the Γ_4 representation, thereby allowing a possible non-zero coupling between phason and phonon fields. In that scheme, we would expect the basic space-filling clusters of the α -phase to be slightly distorted versions of those of the canonical icosahedral phase. An analysis of the cubic phase in terms of shears developing along rational planes in 6D as proposed by Duneau [39] several years ago should certainly be interesting.

An important structural point that has not yet been addressed concerns the point symmetry of the cubic approximant. Qualitative examination of the intensities in the diffraction peaks observed by electron microscopy in the exact Laue orientation support the hypothesis of the high-symmetry point group $m\bar{3}$ (or 23). CBED electron microscopy experiments are in progress to eventually determine the point group.

For the atomic local environments as detected by NMR and ME spectroscopies, it is difficult to give an unambiguous physical interpretation of the results. It is very clear that the spectra are comparable to those observed for the I-phase and that many different local environments are present for all three chemical species in the α -phase. This may result either from a deviation of the composition from the still unknown ideal stoichiometry (inducing a chemical disorder by substitution), from a phason-like disorder, or, most probably, from a combination of the two effects.

From all of these structural results, we may reasonably expect the α -phase to have several atoms at critical atomic flip positions (which would make the structure cubic *on average*) exactly as in ‘phasons’ in quasicrystals (see [34]). This would make this alloy a very attractive candidate for quasielastic neutron scattering studies, such as those performed by Lyonard *et al* [40], and thus transposing the formidable problem of atomic hopping in quasicrystals to the relatively simpler hopping problem in crystalline material.

With respect to transport properties, the α -phase behaves—as does the cubic AlMnSi phase [35, 36]—as a relatively ‘poor quality’ quasicrystal, but still shows all the main features of the stable icosahedral phases. As the structural study suggests, the α -phase is most probably built with the same kind of space fillers or structural units as the I-phase. This would be consistent with the general idea that local atomic environments are of primary importance for the transport properties. Even at relatively small scale (≈ 15 Å), the long-range periodic order does not seem to modify much the particular conduction mechanism of these kinds of phase. This favours a similar conduction mechanism for all of these kinds of phase that would confirm the interpretation of [22] and [23] where it was proposed that the eigenstates near the Fermi energy are centred on the common structural units in the icosahedral and approximant phases. In that scheme, electron propagation is due to hopping between these units (roughly 15–20 Å apart from each other), induced either by elastic or by inelastic scattering.

It is thus tempting to say that the electronic hopping mechanism and the thermally induced process driving the conductivity behaviour are similar in both the I- and α -phases. It is thus reasonable to think that the hopping occurs between structural units that are similar in these two phases.

In conclusion, the preliminary experimental studies presented here strongly support the idea that the cubic α -phase $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ can be considered as a periodic phase approximant to I-phase AlCuFe as regards both structural and physical properties. Further studies of this phase, currently in progress, should help in understanding the atomic structure and the electronic properties of quasicrystals.

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