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The $\text{Al}_3\text{Ni}_2$ Structure as Approximant of Quasicrystals

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Abstract. — The present paper discusses the approximant nature of the $\text{Al}_3\text{Ni}_2$ structure from the viewpoint of valence electron concentration (VEC) correspondence as well as from atomic structure correlation. Its VEC is close to that of corresponding quasicrystals and its atomic structure can be described by layers stacked along the direction corresponding to the 10-fold axis of the decagonal phase. A large orthorhombic pseudocell is proposed whose edges are integer multiplication of those of a basic CsCl unit along directions corresponding to the orthogonal 10-fold and two 2-fold axes of the decagonal phase. Thus its structure can be expressed in the form of $\text{Al}_3\text{Ni}_2-(1,3,3)$ or $\text{Al}_3\text{Ni}_2-(3,1,3)$, the integers being the multiplicity of the CsCl unit along the three directions. The generalization of this expression to several other approximants indicates that approximants can be related to each other by packing the basic CsCl pseudocells in different ways.

1. Introduction

The approximants of quasicrystals are defined in the light of hyper dimensional crystallography [1–3]. The approximants are periodic structures that arise from the projection of a hyper crystal along rational directions, whereas the corresponding quasicrystalline structures are projections along irrational directions. The term “approximant” was first introduced by Elser and Henley [1] to denote the crystalline structure generated from a hyper-cubic crystal using a rational ratio $p/q$ to substitute for the irrational golden mean $\tau = (1 + \sqrt{5})/2$. The projection scheme is, however, so versatile that even non-existent structures may be produced.

In practice, it is often difficult to distinguish approximants from common crystals, since a quasicrystalline alloy may well contain several crystalline phases of quite different structures. One example is the $\text{Al}_3\text{Ni}_2$ type of phase, a well-known vacancy-ordered CsCl superstructure, which exists in many quasicrystalline systems such as $\text{Al-Cu-Co}$ [4], $\text{Al-Cu-Fe}$ [5, 6], $\text{Al-Pd-Mn}$ [7], $\text{Al-Ni-Fe}$ [8], $\text{Al-Cu-Fe-Cr}$ [9, 10]. However, this kind of phase is relatively remote from quasicrystals in composition and apparently does not contain any structural characteristic of quasicrystals. Due to these reasons, the study on its relationship to quasicrystals has been largely ignored.

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In a recent paper [10], the discovery of an \( e/a \)-constant line was reported in ternary Al-Cu-Fe and pseudo-ternary Al-Cu-(Fe,Cr) phase diagrams, \( e/a \) representing valence electron concentration (VEC) per atom. Figure 1 illustrates schematically the composition chart for the Al-Cu-Fe system. The chemical composition of this line is \( C_{\text{Fe}} = 0.228 - 0.4C_{\text{Cu}} \) (\( e/a = 1.86 \)) when the outer electron number of Fe is taken as \(-2\) [11]. This means that there is only one degree of freedom in composition variation if \( e/a \) is constant. The composition zone of the Al-Cu-Fe icosahedral phase (I-AlCuFe) is also elongated along this line [11]. Similar \( e/a \)-constant lines can also be observed in the phase diagrams of other systems such as Al-Cu-Mn [12], Al-Cu-Co [4], Al-Pd-Mn [7] and Al-Cu-Ru [13]. Therefore, the existence of the \( e/a \)-constant line should be a general phenomenon for quasicrystalline phase diagrams.

It is noted that in Figure 1 the \( e/a \)-constant line passes by not only the composition zones of I-AlCuFe and its well-known approximants \( \lambda \)-Al\(_{13}\)Fe\(_4\) but also some CsCl-based structures such as \( \phi \)-Al\(_{10}\)Cu\(_{16}\)Fe with Al\(_3\)Ni\(_2\) structure and \( \zeta \)-Al\(_3\)Cu\(_4\) with a modified \( \gamma \)-brass structure. Therefore, we tend to consider all these crystalline phases as approximants. As suggested earlier, the approximants are those Hume-Rothery crystalline phases that possess approximately the same valence electron concentration as that of the corresponding quasicrystal [14]. This introduced a new criterion to the usual definition of Elser and Henley [1] which is entirely based upon crystallographic correlation. The Hume-Rothery characteristic of quasicrystals has been established since 1987 [15], and the new definition of approximants stresses both the crystallographic and electronic structure correspondence between quasicrystal and approximants.

The CsCl superstructures, having the same VEC as their corresponding quasicrystals, represent an important group of approximants, as contrasted to those having complex structures (e.g. Al\(_{13}\)Fe\(_4\) and Al\(_4\)Mn). However, their structural relationship to quasicrystals is usually unknown. As an example, this paper will deal with the Al\(_3\)Ni\(_2\) structure. As a matter of fact this phase is a decomposition product of metastable Al-Ni decagonal phase prepared by rapid quenching [16]. The \( \gamma \)-brass structure will be discussed in a separate paper [17].
Table I. — A comparison between phases of the Al₃Ni₂ type and two related quasicrystals in the Al-Cu-(Fe, Co) systems. Atomic density \( \rho \) is in \( \text{Å}^{-3} \). \( N \) represents VEC per unit volume. The last column shows \( d_0 \), the interatomic distance that corresponds to the edge of the basic CsCl pseudocell. For the Al₃Ni₂-type phases, \( d_0 = (V_{\text{cell}}/3)^{1/3} \) is the average size of the CsCl pseudocell. The icosahedral and decahedral phases have respectively \( d_0 = a_\tau / \cos(18^\circ)/\tau \) and \( d_0 = a_\tau \times 2 \times \cos(18^\circ)/\tau \) that are edge lengths of the basic pentagons. Since the lattice parameters and atomic densities about \( \phi \)-Al₃₁₀Cu₁₀Fe and \( H \)-Al₃(Cu,Co)₂ are not known, those of Al₃Cu₂ [24] are used instead.

<table>
<thead>
<tr>
<th>phase</th>
<th>composition (at. %)</th>
<th>parameters (Å)</th>
<th>( \rho(\text{Å}^{-3}) )</th>
<th>( e/a )</th>
<th>( N )</th>
<th>( d_0(\text{Å}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₃Cu₂</td>
<td>Al₆₀Cu₄₀</td>
<td>( a = 4.106 ) ( c = 5.094 )</td>
<td>0.0672</td>
<td>2.2</td>
<td>0.148</td>
<td>2.903</td>
</tr>
<tr>
<td>( \phi )-Al₁₀₅Cu₁₀Fe</td>
<td>Al₄₇.,₆₁₄₄₆Fe₄,₈</td>
<td>( a = 4.106 ) ( c = 5.094 )</td>
<td>0.0672</td>
<td>1.81</td>
<td>0.122</td>
<td>2.903</td>
</tr>
<tr>
<td>I-AlCuFe</td>
<td>Al₆₂.,₃₂₄₂₄,₈Fe₁₂,₂₈</td>
<td>( a_\tau = 4.465 )</td>
<td>0.0660</td>
<td>1.86</td>
<td>0.123</td>
<td>2.902</td>
</tr>
<tr>
<td>H-Al₃(Cu,Co)₂</td>
<td>Al₆₀Cu₃₀Co₁₀</td>
<td>( a = 4.106 ) ( c = 5.094 )</td>
<td>0.0672</td>
<td>2.0</td>
<td>0.134</td>
<td>2.903</td>
</tr>
<tr>
<td>D-AlCuCo</td>
<td>Al₆₈Cu₁₁Co₂₁</td>
<td>( a_\tau = 2.437 )</td>
<td>0.0724</td>
<td>1.94</td>
<td>0.140</td>
<td>2.865</td>
</tr>
</tbody>
</table>

2. Approximant Nature of the Al₃Ni₂ Phase

2.1. Crystallographic Structure. — The structure of this type of phase was known long time ago [18]. It has a rhombohedral structure with space group P-3m1. It is characterized by vacancy-ordering in a CsCl superlattice. One unit cell contains three CsCl pseudocells, with cell formula Al₃Ni₂\( \square \), \( \square \) representing one vacancy site. The vacancy sites are ordered into hexagonal network on a \{111\} plane of the CsCl pseudocell with three-layer period, determining the diagonal of the rhombohedral cell or in the hexagonal coordination, the length of the axis \( c \). See Pearson [19] for its detailed structural description.

This phase is the prototype of a series of vacancy-ordered \( \tau \) phases, uncovered by Lu and Tang [20] and studied in detail by Van Sande, De Ridder, Van Landuyt and Amelincx [21], whose structure can be described in terms of a basic CsCl type of cell with ordering along the [111] direction. Chattopadhyay, Lele, Thangaraj and Ranganathan [22] first pointed out the possible link between the vacancy-ordering and 1-dimensional quasiperiodicity. They noted that the vacancy layers in the \( \tau \) phases follow a Fibonacci sequence. The Al₃Ni₂ structure, designated as \( \tau_3 \), has a vacancy-layer period of three layers.

2.2. VEC Correspondence. — In order to illustrate the VEC correspondence, we have calculated the VEC per atom \( (e/a) \) and per unit volume \( (N) \) for this kind of phase and two related quasicrystals in the Al-Cu-(Fe, Co) systems. The results are shown in Table I. For the Al-Cu-Fe system, the agreement both in VEC and interatomic distances between the \( \phi \)-Al₁₀₅Cu₁₀Fe phase with Al₃Ni₂ structure and the I-AlCuFe phase is excellent indeed. By using the free electron model, we obtain the corresponding Fermi sphere diameters of the two phases to be \( 2k_F = 3.066 \text{ Å}^{-1} \) \( (d = 2.050 \text{ Å}) \) and \( 2k_F = 3.077 \text{ Å}^{-1} \) \( (d = 2.042 \text{ Å}) \), respectively. The intense reflections \{110\} \( (K = 3.060 \text{ Å}^{-1}, d = 2.053 \text{ Å}) \) and \{102\} \( (K = 3.034 \text{ Å}^{-1}, d = 2.071 \text{ Å}) \) of the \( \phi \) phase define a Brillouin zone (BZ) similar to the second-order \{110\} BZ of the CsCl phase but with lower symmetry. Note that these planes correspond to the \{110\} planes of the CsCl phase. For the Al-Cu-Co system, the \( N \) values of H-Al₃(Cu,Co)₂ and
D-AlCuCo are quite close to each other, too. However, these values are slightly larger than in the case of the Al-Cu-Fe system. This can be attributed to smaller negative $e/a$ contribution ($e/a = -1$) and smaller atomic radii (1.25 Å) of Co than those of Fe ($e/a = -2$, atomic radii = 1.27 Å). These two factors increase overall $e/a$ value as well as atomic density.

Therefore, the approximant identity the Al$_3$Ni$_2$ structure can be established from the VEC correspondence to quasicrystals.

2.3. Atomic Structure Correspondence. — According to the orientation relationship between an AlCuFeCr approximant with complex orthorhombic structure (O1$_{\text{AlCuCrFe}}$) and a CsCl surface layer induced by ion-beam milling, it has been suggested that a deformed pentagonal network, resembling the Penrose Tiling, can be defined on \{110\} planes of the CsCl phase [23]. This pointed out a possible mechanism that the two distinctively different structures can be mutually transformed. Structural relationship of the Al$_3$Ni$_2$ type of phases to that of quasicrystals can be resolved in a similar fashion, since this is a vacancy-ordered superstructure based on the CsCl pseudocell.

Figure 2 shows the atomic structure of the Al$_3$Cu$_2$ phase with Al$_3$Ni$_2$ structure [24]. Its hexagonal lattice parameters are $a = 4.106$ Å, $c = 5.094$ Å. The upper plot is a stereo view of its hexagonal unit cell together with one rhombohedrally distorted CsCl pseudocell. and the lower plot illustrates the [010] projection. Special attention is paid to the \{102\} and \{−120\} planes that correspond to the CsCl\{110\} planes and hence quasi-periodic planes of the decagonal phase (or the plane normal to a 5-fold axis in the case of the icosahedral phase). For this reason the (102) and (−120) planes are marked out in Figure 2. The atomic configurations on these two planes are very similar to each other.

There may be two possible orientation relationships which are based respectively on these two planes. Wang [16] has observed that after annealing the metastable decagonal AlNi phase is transformed into the Al$_3$Ni$_2$ phase. Though the orientational relationship between them are not yet known completely, the experimental results support at least the second \{−120\} scheme but do not exclude the first \{102\} scheme.

The two orientation relationships are best illustrated in the [010]-projected structure of Figure 2 (the lower plot). In the first (102)-based scheme, the [212] direction, being perpendicular to the (102) plane, is supposed to be parallel to the 10-fold axis of the decagonal phase or a 5-fold axis of the icosahedral phase. The 3-fold [001] direction of the Al$_3$Cu$_2$ phase is placed parallel to a 3-fold axis of quasicrystals. The angle between [212] and [001] is 35.61°, close to that between 5- and 3-fold axes. In the second (−120)-based scheme, the [−2 −11], [212], [010] directions are respectively parallel to 2P-fold, 2D-fold, and 10-fold of the decagonal phase.

The relationships among CsCl, Al$_3$Ni$_2$, icosahedral and decagonal phases can be summarized as follows:

<table>
<thead>
<tr>
<th>CsCl</th>
<th>$\tau_3/(102)$</th>
<th>$\tau_3/(-120)$</th>
<th>decagonal</th>
<th>icosahedral</th>
</tr>
</thead>
<tbody>
<tr>
<td>{110}</td>
<td>[212]</td>
<td>[010]</td>
<td>10-fold</td>
<td>5-fold</td>
</tr>
<tr>
<td>{−110}</td>
<td>[212]</td>
<td>[010]</td>
<td>2-fold D</td>
<td>2-fold</td>
</tr>
<tr>
<td>[001]</td>
<td>[−2 −11]</td>
<td>[−2 −11]</td>
<td>2-fold P</td>
<td>2-fold</td>
</tr>
</tbody>
</table>

Figure 3 presents the atomic arrangement in the (102) and (−120) planes of the Al$_3$Cu$_2$ phase together with one similar atomic configuration of the decagonal phase in Al-Mn system (abbreviated as D-AlMn). Exactly speaking, the (102) plane is not a flat layer: some atoms fluctuate above and below the plane, however the displacements are very small as compared to the interatomic distances (about 2-3%). The unit cell on (102) plane consists of three deformed
Fig. 2. — Structure of the Al$_3$Cu$_2$ phase of Al$_3$Ni$_2$ type. The hexagonal system is chosen to show this rhombohedral phase. Large circles represent Al atoms and the small ones Cu atoms. The upper plot is a stereo view of a hexagonal unit cell, inside is drawn a rhombohedrally deformed CsCl basic unit. The lower plot is the [010] projection, where its crystallographic relationship with quasicrystals is indicated. The (102) plane is marked out which corresponds to the quasi-periodic planes of the decagonal phase.

CsCl rectangles. One of the rectangles contains a vacancy site so that the composition on the layer is Al$_3$Cu$_2\Box$, or Al$_{50}$Cu$_{33}\Box_{17}$ in atomic percentage, the same as the cell formula. The unit cell on (−120) plane also consists of three deformed CsCl “rectangles”. The stacking of the (102) plane along [212] direction and (−120) plane along [010] direction has a six-layer periodicity, or 12.426 Å.

The D-AlMn structure (originally proposed by Steurer [25] and recently modified by Beeli and Horuchi [26]) presents similar local atomic configurations (Figs. 3, 4). It is formed with two kinds of layers, one flat B (and its 10-fold rotation image b) and the other puckered A
Fig. 3. — Atomic arrangement in the (102) and (−120) planes of the Al₃Cu₂ phase (left) and a similar atomic configuration from D-AlMn (right). Some interatomic distances and the displacements above and below the plane are marked. Large circles represent Al atoms and the small ones Cu (Mn) atoms.

Fig. 4. — Part of the flat quasi-periodic plane of D-AlMn where one can see traces of the Al₃Ni₂ structure feature (the shaded areas). The atoms are relinked to resemble the CsCl-(110) atomic grid. The original structure is taken from Beeli et al. [26].

(and its 10-fold rotation image a), which are stacked along the 10-fold direction in the stacking sequence of ABAaba. Part of the flat quasi-periodic plane is shown in Figure 4. The atoms are relinked to resemble the CsCl-(110) atomic grid. Such a reorganized linkage reveals the
following important points:

1. The shaded areas on the flat plane present Al₃Ni₂ characteristic: three deformed CsCl “rectangles” with the central site vacant. This implies that the Al₃Ni₂-type of structure retains indeed certain structural properties of quasicrystals.

2. The Al₃Ni₂ phase is formed by stacking six (102) or (−120) layers, while D-AlMn also has a six-layer stacking sequence along the 10-fold axis.

3. Quasicrystals are vacancy-ordered based on CsCl basic pseudocell. The vacancy sites are not distributed in random. Such an ordering should play an important role in the stabilization of quasicrystals.

4. The vacancy concentration VC of the Al₃Ni₂ structure is comparable to that of quasicrystals. On the flat and puckered layers of D-AlMn, VC values are respectively 21% and 11%(1). The average value is about 14%. The Al₃Ni₂ structure has a slightly higher VC of about 17%.

3. Unified Expression for CsCl-based Approximants

A periodicity of 12.426 Å along the [212] direction is achieved by stacking six (102) layers (refer to the [010] projection in Fig. 2). Adding the periodicity along the [010] direction of 4.106 Å and that along [−2 − 1] of 8.748 Å, a larger orthorhombic pseudocell can be constructed which shows a simple crystallographic correlation to the decagonal quasicrystal:

\[ A_{\text{Al₃Ni₂}} = 4.106 \text{ Å}, \quad [010]_{\text{hexagonal}} \quad // \quad 2\text{-fold } D, \]
\[ B_{\text{Al₃Ni₂}} = 12.426 \text{ Å}, \quad [212]_{\text{hexagonal}} \quad // \quad 10\text{-fold.} \]
\[ C_{\text{Al₃Ni₂}} = 8.748 \text{ Å}, \quad [-2 - 1]_{\text{hexagonal}} \quad // \quad 2\text{-fold } P \]

when using the orientation relationship based on the (102) plane, or:

\[ A_{\text{Al₃Ni₂}} = 12.426 \text{ Å}, \quad [212]_{\text{hexagonal}} \quad // \quad 2\text{-fold } D, \]
\[ B_{\text{Al₃Ni₂}} = 4.106 \text{ Å}, \quad [010]_{\text{hexagonal}} \quad // \quad 10\text{-fold,} \]
\[ C_{\text{Al₃Ni₂}} = 8.748 \text{ Å}, \quad [-2 - 1]_{\text{hexagonal}} \quad // \quad 2\text{-fold } P \]

when using the orientation relationship based on the (−120) plane.

This orthorhombic cell is half that of the Al₄Cu₉ phase with γ-brass structure. As discussed in another paper, the Al₄Cu₉ phase is an approximant of quasicrystals and it can also be described by stacking two kinds of layers, one flat and one puckered, along a < 110 > direction in a stacking sequence similar to that of D-AlMn [17]. The large “orthorhombic” pseudocell developed from it follows the same orientation relationship to quasicrystals as the above, i.e.,

\[ A_{\text{Al₄Cu₉}} = 12.31 \text{ Å}, \quad [-110]_{\text{cubic}} \quad // \quad 2\text{-fold } D, \]
\[ B_{\text{Al₄Cu₉}} = 12.31 \text{ Å}, \quad [110]_{\text{cubic}} \quad // \quad 10\text{-fold,} \]
\[ C_{\text{Al₄Cu₉}} = 8.7068 \text{ Å}, \quad [001]_{\text{cubic}} \quad // \quad 2\text{-fold } P. \]

(1) These values may vary in different part of the quasi-periodic planes as well as in different alloy systems. We have counted an area of 33 × 39 Å² of the D-AlMn model of Steurer-Beeli [25, 26].
In this way, the CsCl-based approximants $\text{Al}_3\text{Ni}_2$, $\text{Al}_4\text{Cu}_9$ and CsCl can all be expressed in larger "orthorhombic" cells with three edges parallel to the orthogonal 2-fold D, 10-fold and 2-fold P directions of the decagonal phase. A schematic illustration on the construction of the pseudocells is presented in Figure 5.

If the orthorhombic pseudocell of the basic CsCl structure is taken as the unit with edges $A_0 = a_{\text{CsCl}} \times \sqrt{2}$, $B_0 = a_{\text{CsCl}} \times \sqrt{2}$, $C_0 = a_{\text{CsCl}}$, the other two can be regarded as superstructures with integral multiplication of the basic edges. For the $\text{Al}_3\text{Ni}_2$ structure, $A_{\text{Al}_3\text{Ni}_2} = 1 \times A_0$, $B_{\text{Al}_3\text{Ni}_2} = 3 \times B_0$, $C_{\text{Al}_3\text{Ni}_2} = 3 \times C_0$. For the $\text{Al}_4\text{Cu}_9$ phase, $A_{\text{Al}_4\text{Cu}_9} = 3 \times A_0$, $B_{\text{Al}_4\text{Cu}_9} = 3 \times B_0$, $C_{\text{Al}_4\text{Cu}_9} = 3 \times C_0$. Then, these CsCl superstructures can be expressed into the following simple forms: CsCl-(1,1,1), $\text{Al}_3\text{Ni}_2$-(1,3,3)/(3,1,3), $\text{Al}_4\text{Cu}_9$-(3,3,3). The three figures represent
respectively the multiplication of the basic CsCl unit along the directions 2-fold D, 10-fold and 2-fold P of the decagonal phase.

Furthermore, this type of formula is not confined to these commonly accepted CsCl superstructures. The approximants are divided into two groups according to their positions in phase diagrams [10, 14], one consists of complex approximants (lying to the left of I-AlCuFe in Fig. 1) and the other the CsCl superstructures (lying to the right of I-AlCuFe in Fig. 1). The phases in the former group can also be expressed in a similar way with help of the basic CsCl pseudocell. In the Al-Cu-Fe system, only one phase is included in this group, i.e., the Al$_{13}$Fe$_4$ phase. It has C2/m as its space group and the following lattice parameters: $a = 15.489$ Å, $b = 8.0831$ Å, $c = 12.476$ Å, $\beta = 107.72^\circ$ [27]. Its approximant nature has been extensively discussed [28]. Its monoclinic cell can be transformed by a twinning operation into an orthorhombic pseudocell containing two original monoclinic unit cells. Such a twinning mode is often observed experimentally. Now the edges are $A_{Al_{13}Fe_4} = c = 3 \times A_0$, $B_{Al_{13}Fe_4} = b = 2 \times B_0$, $C_{Al_{13}Fe_4} \approx 2 \times \cos(18^\circ) \times a = 10 \times C_0$, or in the simplified form Al$_{13}$Fe$_4$-(3,2,10). In the Al-Cu-Fe-Cr system, there are a series of complex approximants [9, 29]. Two examples are O$_1$AlCuFeCr (B-face centered orthorhombic, $a = 32.54$, $b = 12.27$ and $c = 23.64$ Å [9, 23]) and O$_3$AlCuFeCr ($a = 14.582$, $b = 12.320$, $c = 12.363$ Å [30], isostructural with Al$_3$Mn [31]). The edges being parallel to the three directions mentioned above, they can be expressed as O$_1$AlCuFeCr-(8,3,8) and O$_3$Al$_3$Mn-(3,3,5), as shown in Figure 5.

4. Summary

We have analyzed the valence electron concentration and atomic structure correspondence between the Al$_3$Ni$_2$ type of phase and two relevant quasicrystals. The results support the conclusion that this type of CsCl superstructure is an approximant of quasicrystals, in spite of its relatively simple atomic structure. Its structure can be described by a six-layer stacking of (102) planes that corresponds to a CsCl-(110) plane or to the quasi-periodic planes of the decagonal phase. Such a description leads to a larger orthorhombic pseudocell with edges being parallel to the orthogonal 10-fold and two 2-fold directions of quasicrystals. The pseudocell edges are integer multiplication of those of the basic CsCl unit so that this phase can be simplified into the expression Al$_3$Ni$_2$-(1,3,3) or Al$_3$Ni$_2$-(3,1,3). The three integers being the multiplicity of the basic CsCl pseudocell along the three axes of the decagonal phase. This form of expression can also be applied to other approximants so that it can be treated as a unified way to relate approximants to the basic CsCl units.

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