

F-AlCoPdGe Alloy with Three Types of Pseudo-Mackay Clusters

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The structure of an *F*-AlCoPdGe alloy was determined by single-crystal X-ray diffraction analysis: space group $Pa\bar{3}$ (No. 205), Pearson symbol $cP1128-142.4$, $a = 24.4338(4)$ Å; $R1 = 0.0526$ for the observed 5106 reflections with $F_0 > 4.0\sigma(F_0)$. The *F*-AlCoPdGe alloy exhibited three types of pseudo-Mackay clusters (pMCs). The first shell of the Co(13)-pMC at $24d$ indicated a coordination polyhedron typically found in Al-Co binary approximants; the second shell was a combination of an M icosahedron and an Al icosidodecahedron, where M is a mixed site of Pd and/or Co. The first shell of the Co(14)-pMC at $4b$ consisted of 20 partially occupied Al positions arranged in a dodecahedral fashion; its second shell was also composed of an M icosahedron and an Al icosidodecahedron. The first shell of the Al(18)-pMC at $4a$ consisted of a combination of an M cube and an Al octahedron, resulting in the rhombic dodecahedral arrangement; its outer shell structure was similar to those of the other pMCs. The structure of the *F*-AlCoPdGe phase comprised an arrangement of these three types of pMCs together with interstitially placed Al icosahedra around the Pd/Al(1) and Pd/Al(2) sites.

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1. Introduction

Numerous complex intermetallic compounds have been reported as existing in the binary and ternary alloy systems of Al and transition metals. The Al-Co-Pd system is one of the most interesting alloy systems since a variety of crystalline phases associated with quasicrystals has been reported in conventionally solidified samples of this system [1]. Of the various crystalline phases noticed in the samples, the ε -phases have structures similar to that of the Al₃Pd (ε_6 -phase), which is an important crystalline approximant of decagonal quasicrystals with a period of 1.6 nm [2]. *W*-AlCoPd containing approximately 5 at.% Pd exhibits cell parameters similar to those of *W*-AlCoNi [3], and its structural characteristics are useful for understanding those of the columnar unit in the decagonal phase with a periodicity of 0.8 nm. On the other hand, a few crystalline phases probably associated with the icosahedral phase have also been found in this Al-Pd-Co system. The C_2 and *F* phases can be classified as belonging to this category, although their structures have not yet been determined. *R*-AlPdCo [4] is another alloy of the Al-Co-Pd system; its structure shows the presence two types of pseudo-Mackay clusters (pMCs) similar to those found in 1/1-AlCuRu [5] and trigonal χ -AlPdRe [6]. In this context, a series of structural investigations on the intermetallic compounds in Al-Co-Pd system would aid in determining the characteristics of the columnar unit in the decagonal phase as well as the atom clusters of the icosahedral phase. In a study on the Al-Co-Pd system, the addition of Ge into a ternary Al-Co-Pd alloy was found to encourage the formation of the *F* phase in a size large enough to allow for

structural analysis. This paper describes the structure of the *F*-AlCoPdGe alloy as determined by single-crystal X-ray diffraction analysis.

2. Experimental

An ingot of the alloy, which had a nominal composition of Al₆₅Co₂₀Pd₁₀Ge₅, was prepared from pure Al (99.999%), Co (99.9%), Pd (> 99.95%), and Ge (> 99.99%) in an atmosphere of purified Ar using a conventional arc melting furnace. A single-crystal specimen, which had the morphology of an elongated prism, was selected from the as-prepared ingot. The chemical composition of the specimen was determined by electron probe microanalysis (EPMA) (JEOL JXA-8621MX). The results indicated that the composition of the *F* phase was Al_{67.9}Co_{19.7}Pd_{9.8}Ge_{2.5} and quite similar to that of the starting alloy ingot. A block-shaped single crystal $44 \times 48 \times 65$ μm³ in size was cut from the alloy ingot and examined by single-crystal X-ray diffraction. Intensity data of 89172 reflections were collected using a Rigaku *R*-AXIS RAPID system and Mo K_α radiation ($2\theta < 54.9^\circ$) [7]. After Lorentz and polarization corrections, an absorption correction was carried out by taking into account the shape of the specimen along with the absorption coefficient, which was estimated from the chemical composition and structural model of the alloy specimen [8]. The lattice constants suggested to select a cubic cell with $a = 24.4338(4)$ Å. The observed reflections along with their intensity distribution led us to select the space group $Pa\bar{3}$. Analyzing the data on the basis of this space group yielded 5580 independent reflections. Among these, 5106 reflections met the condition $F_0 > 4.0\sigma(F_0)$.

The initial structural model was obtained by using the direct methods software package SIR97 [9]. The obtained structural model yielded 41 fully occupied sites; of these, 15 sites were suggested to be occupied by heavy met-

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Summary of experimental data.

TABLE I

chemical composition (EPMA)	Al _{67.9} Co _{19.7} Pd _{9.8} Ge _{2.5}
chemical composition (X-RAY)	Al _{68.9} Co _{18.7} Pd _{11.1} Ge _{1.3}
temperature [K]	298(2)
wavelength [Å]	0.71069
space group	$P\bar{a}3$
unit cell [Å]	$a = 24.4338(4)$
volume [Å ³]	14587.2(7)
D_x [Mg/m ³]	4.750
absorption coefficient [mm ⁻¹]	7.976
$F(000)$	19237
crystal size [mm ³]	$0.044 \times 0.048 \times 0.065$
$2\theta_{\max}$ [°]	54.94
R_{sigma}	0.0282
R_{sigma}	0.0131
h, k, l	$-29 < h < 31,$ $-31 < k < 30,$ $-31 < l < 31$
no. of measured reflections	89196
no. of independent reflections	5580
no. of observed reflections	5106
no. of parameters	393
goodness-of-fit on F^2	1.031
final R indices [$I > 2\sigma(I)$]	0.0526
final $wR2$ indices (all data)	0.1366
largest diff. peak and hole [eÅ ³]	4.78 and -1.93

als and the other 26 sites by Al. Each heavy metal site was surrounded by Al sites; this is a common feature in Al-based approximants of the binary Al–Pd and Al–Co systems [2, 10, 11].

Calculating the interatomic distances allowed us to classify the heavy metal sites into two groups. The Pd/Al(1) and Pd/Al(2) sites were placed in the first group, which corresponded to nearest-neighbor distances of greater than 0.260 nm. That the size of these two heavy metal sites was larger implied their preferred occupation by Pd and Al atoms. The nearest-neighbor distances of the other 13 heavy metal sites were less than 0.250 nm; this strongly suggested that they were fully or partially occupied by Co atoms. The results of several least-squares calculations, performed using the software SHELXL-97 [12], prompted us to employ a chemically disordered model for the 15 heavy metal sites. Therefore, we continued the least-squares calculations by introducing two Pd/Al, ten Co/Pd, and three Co sites so as to obtain reasonable displacement parameters for the heavy metal sites (hereafter, the ten Co/Pd and three Co sites are denoted as the M sites). A chemical disorder model was also introduced for the Al/Ge(16) and Al/Ge(17) sites because their displacement parameters became significantly smaller than the other Al sites when they were assumed to be fully occupied by Al atoms.

Difference Fourier maps obtained during the least-squares calculations indicated the presence of geometrically disordered areas in the present structural model. Next, four sets of partially occupied posi-

tions, Al(42)(a–b), Al(43)(a–b), Pd/Ge/Al(44)(a–c), and Al(45)(a–d), were introduced. The displacement parameters for Al(45)(a–d) sites were constrained to identical values. Further introduction of anisotropic displacement parameters for fully occupied sites converged at $R = 0.0525$ for the observed 5106 reflections.

Experimental data are summarized in Table I. The final atomic coordinates and equivalent displacement parameters are listed in Tables II and III. The converged structural model yielded the following chemical composition: Al_{68.9}Co_{18.7}Pd_{11.1}Ge_{1.3}. The chemical composition of the structural model agreed fairly well with that determined by EPMA. It should be added that the ordinary application of single crystal X-ray diffraction could not allow us to specify the detailed structural role of Ge in the structure.

3. Results and discussion

The alloy F-AlCoPdGe exhibits three types of pMCs; the Co(13)-, Co(14)-, and Al(18)-pMCs. The pMCs with a central atom could be further classified into three types: those having a first shell with (1) partial icosahedral symmetry; (2) 3-fold symmetry, with the local 5-fold symmetry being lost; and (3) others [13]. The Co(13)-, Co(14)-, and Al(18)-pMCs belong to types (3), (1), and (2), respectively. In particular, the Co(13)-pMC is a typical example, having an irregularly shaped first shell, which has a smaller transition metal as the central atom, such as Co and Re. On the other hand, the Al(18)-pMC is another fundamental structure with a larger central atom, such as Al and Pd.

Figure 1 shows a pMC around Co(13) at the 24d site (Co(13)-pMC). The first shell is an irregularly shaped polyhedron consisting of nine Al sites and some of the Co sites in binary Al–Co phases exhibit a similar geometry [10, 11]. The second shell has a radius of approximately 4.68 Å and could be divided into two subshells. One is an icosahedron of M sites (M icosahedron), with each vertex of the icosahedron being capped by five Al sites so as to form an Al icosidodecahedron. The Co(13)-pMC is surrounded by four Co(13)-pMCs by sharing the edges of the M icosahedron. At the same time, each pMC around the Co(14) and Al(18) sites also shares an icosahedral edge with the Co(13)-pMC.

The first shell of the pMC around the Co(14) site is a dodecahedron consisting of statistically occupied Al(45)(a–d) sites. Every site indicates the partial occupation and the concurrent occupation of the neighboring pairs are forbidden. Taking into account of the occupation parameters of these Al(45)(a–d) sites, it can be said that approximately seven Al atoms are located around the Co(14) site. The size of the second shell is approximately 4.65 Å, and it is composed of an inner M icosahedron and an outer Al icosidodecahedron. Since this pMC shows a point symmetry of $P\bar{a}3$, the Co(14)-pMC is surrounded by six Co(13)-pMCs. The arrangement of atoms in the shell structure of the Co(14)-pMC is shown in Fig. 2.

TABLE II

Atomic coordinates and equivalent or isotropic displacement parameters of $F\text{-AlCoPdGe}$.

Atom	site	occupation	x	y	z	$U_{\text{eq}} [\text{\AA}^2]$
Pd/Al(1)	8c	0.74(1)/0.26	0.15660(3)	x	x	0.0100(4)
Pd/Al(2)	24d	0.68(1)/0.32	0.00180(3)	0.40286(3)	0.24813(3)	0.0087(3)
Co/Pd(3)	8c	0.52(1)/0.48	0.25122(3)	x	x	0.0085(5)
Pd/Co(4)	24d	0.60(1)/0.40	0.00032(2)	0.53709(2)	0.59696(2)	0.0051(2)
Pd/Co(5)	8c	0.48(1)/0.52	0.05987(3)	x	x	0.0053(4)
Pd/Co(6)	24d	0.56(1)/0.44	0.09648(3)	0.50687(3)	0.33981(3)	0.0081(3)
Pd/Co(7)	24d	0.48(1)/0.52	0.00598(3)	0.65479(3)	0.39532(3)	0.0071(3)
Pd/Co(8)	24d	0.35(1)/0.65	0.34258(3)	0.09454(3)	0.80629(3)	0.0083(3)
Pd/Co(9)	24d	0.31(1)/0.69	0.49989(3)	0.15144(3)	0.09840(3)	0.0083(3)
Pd/Co(10)	24d	0.31(1)/0.69	0.00016(3)	0.35085(3)	0.09115(3)	0.0102(3)
Pd/Co(11)	24d	0.24(1)/0.76	0.05222(3)	0.24617(3)	0.25092(3)	0.0091(3)
Co(12)	24d	1	0.05927(4)	0.05749(3)	0.24953(3)	0.0041(2)
Co(13)	24d	1	0.40281(4)	0.15379(4)	0.24537(4)	0.0070(2)
Co(14)	4b	1	0	0	1/2	0.0057(4)
Co(15)	24d	1	0.31215(4)	0.15390(3)	0.39810(4)	0.0051(2)
Al/Ge(16)	24d	0.84(1)/0.16	0.55864(7)	0.09548(7)	0.15827(7)	0.0117(6)
Al/Ge(17)	8c	0.89(1)/0.11	0.30927(7)	x	x	0.012(1)
Al(18)	4a	1	0	0	0	0.0094(9)
Al(19)	24d	1	0.49873(9)	0.19276(9)	0.00239(9)	0.0125(5)
Al(20)	24d	1	0.06129(9)	0.21356(9)	0.15532(9)	0.0115(4)
Al(21)	24d	1	0.49727(9)	0.00404(9)	0.69403(9)	0.0109(4)
Al(22)	24d	1	0.15298(9)	0.24816(9)	0.0933(1)	0.0133(5)
Al(23)	24d	1	0.03622(9)	0.55916(9)	0.40228(9)	0.0111(4)
Al(24)	24d	1	0.40729(9)	0.46230(9)	0.25242(9)	0.0108(4)
Al(25)	24d	1	0.09835(9)	0.65780(9)	0.44342(9)	0.0109(4)
Al(26)	24d	1	0.06351(9)	0.09410(9)	0.15591(9)	0.0120(4)
Al(27)	24d	1	0.40244(9)	0.15155(9)	0.74812(9)	0.0112(5)
Al(28)	24d	1	0.16047(9)	0.55746(9)	0.40557(9)	0.0099(4)
Al(29)	24d	1	0.09520(9)	0.34120(9)	0.25214(9)	0.0128(5)
Al(30)	24d	1	0.44147(9)	0.09658(9)	0.84298(9)	0.0110(4)
Al(31)	24d	1	0.50198(9)	0.31290(9)	0.30968(9)	0.0101(4)
Al(32)	24d	1	0.19490(9)	0.00602(9)	0.80867(9)	0.0122(4)
Al(33)	24d	1	0.15217(9)	0.24718(9)	0.2163(1)	0.0129(5)
Al(34)	24d	1	0.5975(1)	0.4577(1)	0.25205(9)	0.0141(5)
Al(35)	24d	1	0.5617(1)	0.40275(9)	0.34359(9)	0.0142(5)
Al(36)	24d	1	0.4860(1)	0.1887(1)	0.1961(1)	0.0240(6)
Al(37)	24d	1	0.3191(1)	0.1877(1)	0.2981(1)	0.0264(6)
Al(38)	24d	1	0.3391(1)	0.1048(1)	0.6230(1)	0.0227(6)
Al(39)	24d	1	0.1609(1)	0.4317(1)	0.0994(1)	0.0315(7)
Al(40)	24d	1	0.3030(1)	0.0473(2)	0.7143(2)	0.056(1)
Al(41)	24d	1	0.3798(2)	0.2435(2)	0.2171(2)	0.073(2)
Al(42)a	24d	0.68(1)	0.3607(2)	0.0642(2)	0.2467(2)	0.038(1)*
Al(42)b	24d	0.32	0.3384(5)	0.0816(5)	0.2377(5)	0.039(3)*
Al(43)a	24d	0.68(1)	0.0239(2)	0.5966(2)	0.2705(2)	0.023(1)*
Al(43)b	24d	0.32	0.0644(3)	0.5578(3)	0.2513(4)	0.012(2)*
Pd(44)a	24d	0.47(1)	0.15390(5)	0.09680(5)	0.30816(5)	0.0136(4)*
Ge(44)b	24d	0.33(1)	0.3435(1)	0.15587(9)	0.1573(1)	0.0102(9)*
Al(44)c	24d	0.46(2)	0.3315(3)	0.1542(3)	0.1866(4)	0.040(3)*
Al(45)a	24d	0.39(2)	0.0901(4)	0.0034(4)	0.4634(4)	0.035(2)*
Al(45)b	24d	0.38(1)	-0.0919(4)	-0.0106(4)	0.4602(4)	0.035(2)*
Al(45)c	24d	0.31(2)	-0.0580(4)	-0.0562(4)	0.4435(4)	0.035(2)*
Al(45)d	8c	0.20(2)	0.5549(7)	x	x	0.035(2)*

* $U_{\text{iso}} [\text{\AA}^2]$

TABLE III

Anisotropic displacement parameters of *F*-AlCoPdGe.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	$U_{12} [\text{Å}^2]$
Pd/Al(1)	0.0100(4)	U_{11}	U_{11}	-0.0001(2)	U_{23}	U_{23}
Pd/Al(2)	0.0097(4)	0.0085(4)	0.0080(4)	0.0002(2)	-0.0012(2)	-0.0007(2)
Pd/Co(3)	0.0085(5)	U_{11}	U_{11}	-0.0014(2)	U_{23}	U_{23}
Pd/Co(4)	0.0058(3)	0.0055(3)	0.0041(3)	-0.0003(2)	0.0000(2)	-0.0001(2)
Pd/Co(5)	0.0053(4)	U_{11}	U_{11}	-0.0004(2)	U_{23}	U_{23}
Pd/Co(6)	0.0056(4)	0.0096(4)	0.0091(4)	-0.0038(2)	-0.0002(2)	-0.0005(2)
Pd/Co(7)	0.0069(4)	0.0054(4)	0.0091(4)	-0.0004(2)	-0.0024(2)	0.0003(2)
Pd/Co(8)	0.0083(4)	0.0062(4)	0.0104(4)	0.0001(3)	0.0041(3)	0.0001(2)
Pd/Co(9)	0.0077(4)	0.0104(4)	0.0067(4)	0.0020(3)	-0.0002(3)	0.0024(3)
Pd/Co(10)	0.0058(4)	0.0153(5)	0.0094(4)	-0.0065(3)	-0.0003(3)	-0.0003(3)
Pd/Co(11)	0.0110(5)	0.0065(4)	0.0097(5)	0.0002(3)	0.0043(3)	0.0013(3)
Co/Co(12)	0.0061(4)	0.0039(4)	0.0023(4)	-0.0004(3)	0.0003(3)	-0.0027(3)
Co/Co(13)	0.0080(4)	0.0061(4)	0.0070(4)	-0.0004(3)	0.0020(3)	-0.0018(3)
Co(14)	0.0057(4)	U_{11}	U_{11}	-0.0001(4)	U_{23}	U_{23}
Co(15)	0.0068(4)	0.0030(4)	0.0055(4)	0.0002(3)	-0.0007(3)	-0.0012(3)
Al/Ge(16)	0.012(1)	0.013(1)	0.0095(9)	0.0039(6)	0.0011(6)	0.0016(6)
Al/Ge(17)	0.012(1)	U_{11}	U_{11}	-0.0015(6)	U_{23}	U_{23}
Al(18)	0.009(1)	U_{11}	U_{11}	0.002(1)	U_{23}	U_{23}
Al(19)	0.014(1)	0.014(1)	0.009(1)	0.0013(8)	0.0019(8)	0.0002(8)
Al(20)	0.014(1)	0.012(1)	0.009(1)	-0.0012(8)	-0.0018(8)	0.0007(8)
Al(21)	0.010(1)	0.012(1)	0.011(1)	0.0017(8)	0.0030(8)	-0.0009(8)
Al(22)	0.008(1)	0.014(1)	0.018(1)	0.0007(9)	0.0018(8)	0.0039(8)
Al(23)	0.011(1)	0.010(1)	0.013(1)	-0.0005(8)	0.0009(8)	0.0005(8)
Al(24)	0.014(1)	0.009(1)	0.010(1)	0.0014(8)	0.0023(8)	-0.0015(8)
Al(25)	0.008(1)	0.013(1)	0.012(1)	-0.0002(8)	0.0013(8)	0.0004(8)
Al(26)	0.014(1)	0.013(1)	0.009(1)	0.0025(8)	-0.0001(8)	0.0012(8)
Al(27)	0.015(1)	0.013(1)	0.006(1)	0.0029(8)	0.0032(8)	0.0012(8)
Al(28)	0.010(1)	0.007(1)	0.012(1)	0.0004(8)	-0.0009(8)	-0.0009(7)
Al(29)	0.016(1)	0.011(1)	0.012(1)	-0.0037(8)	-0.0040(8)	-0.0002(8)
Al(30)	0.012(1)	0.009(1)	0.013(1)	-0.0018(8)	-0.0018(8)	-0.0009(8)
Al(31)	0.010(1)	0.009(1)	0.012(1)	-0.0008(8)	0.0023(8)	-0.0006(8)
Al(32)	0.011(1)	0.014(1)	0.012(1)	-0.0030(8)	0.0000(8)	0.0030(8)
Al(33)	0.013(1)	0.012(1)	0.014(1)	-0.0004(8)	-0.0010(8)	0.0025(8)
Al(34)	0.017(1)	0.016(1)	0.009(1)	-0.0011(8)	0.0022(8)	-0.0013(9)
Al(35)	0.020(1)	0.011(1)	0.012(1)	0.0021(8)	-0.0010(8)	-0.0046(9)
Al(36)	0.030(1)	0.024(1)	0.018(1)	-0.005(1)	0.008(1)	-0.014(1)
Al(37)	0.025(1)	0.032(1)	0.023(1)	0.009(1)	0.006(1)	0.012(1)
Al(38)	0.016(1)	0.022(1)	0.031(1)	-0.008(1)	0.011(1)	-0.006(1)
Al(39)	0.020(1)	0.045(2)	0.030(2)	-0.020(1)	-0.005(1)	0.005(1)
Al(40)	0.030(1)	0.087(3)	0.053(2)	0.042(2)	-0.014(1)	-0.004(2)
Al(41)	0.107(4)	0.030(2)	0.081(3)	0.031(2)	0.032(3)	0.013(2)

The structure for another type of Al(18)-pMC, which is located at 4a, is shown in Fig. 3. The first shell may be divided into two subshells of a cube of M(4) and M(5) and an octahedron of six Al(23) sites, by showing the local atomic arrangement of a rhombic dodecahedron. Al(23) is the vertex of the Al icosidodecahedron in the neighboring Co(13) pMC and the Al(18)-pMC is surrounded by six Co(13)-pMCs. The second shell can again be divided into two subshells: M icosahedron and an Al icosidodecahedron. The outer Al icosidodecahedron of the Al(18)-pMC is heavily distorted and different from the other

pMCs around Co. This is owing to the size of its central atom together with the unique bcc arrangement of the first shell. It should be noted that this type of pMC is also found in the 1/1-cubic approximant structure of *R*-AlPdCo [6] and α -AlCuRu [7].

Among the 17 heavy metal sites, the Pd/Al(1) and Pd/Al(2) sites are unique and are not the constituents of the three pMCs described above. Each of them is surrounded by 12 Al atoms, forming a regular Al icosahedron. These two Pd/Al icosahedra reside on the interstitial space of the pMCs since they share their peripheries.

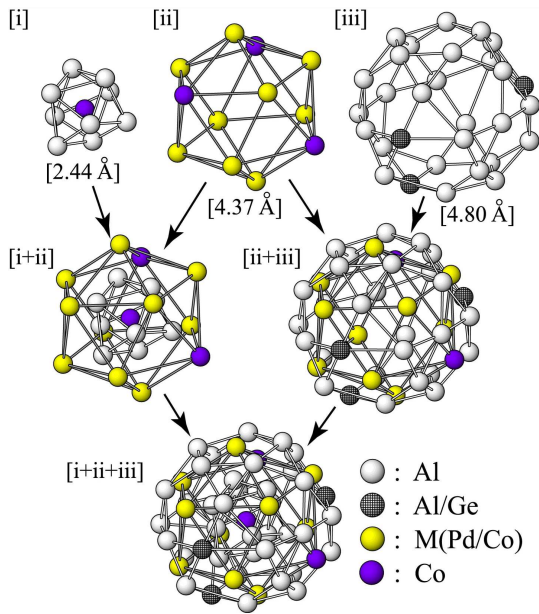


Fig. 1. The pseudo-Mackay cluster around the Co(13) site. The values in the parentheses are the averaged distances of the constituents from the central Co(13) atom. Some forbidden pairs with short distances arise from statistical disorder of several atomic sites. Therefore, this figure only shows the positions of Al(42)a, Al(43)a, Pd(44)a, Al(44)c and Al(45)b. The positions of Al(40) and Al(41) with relatively large anisotropic nature are the constituents of the disordered first shell.

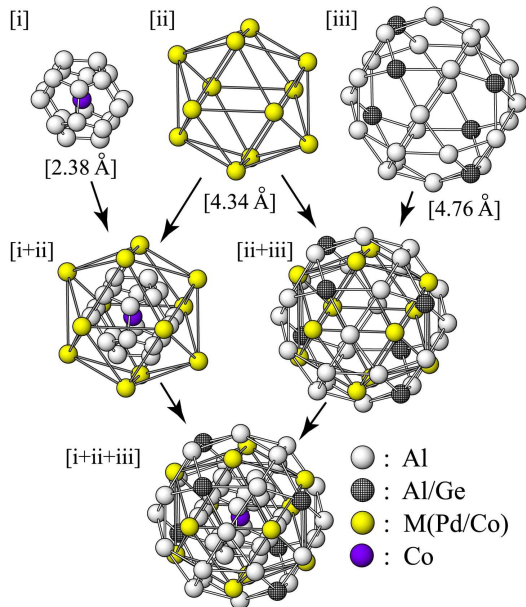


Fig. 2. The pseudo-Mackay cluster around the Co(14) site. The values in the parentheses are the averaged distances of the constituents from the central Co(14) atom. A dodecahedron consists of statistically occupied Al(45)(a–d) sites.

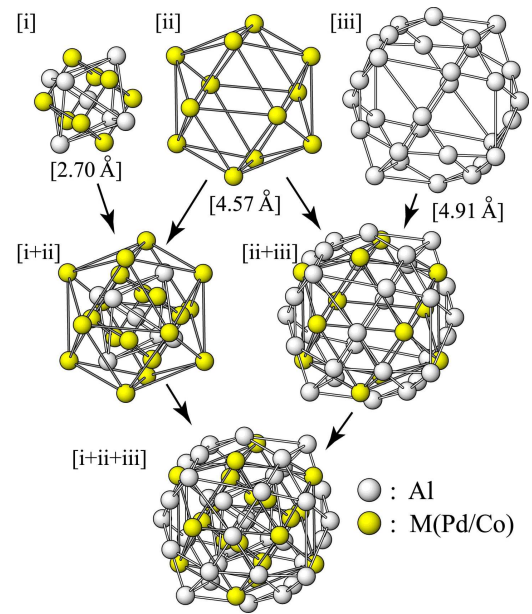


Fig. 3. The pseudo-Mackay cluster around the Al(18) site. The values in the parentheses are the averaged distances of the constituents from the central Al(18) atom.

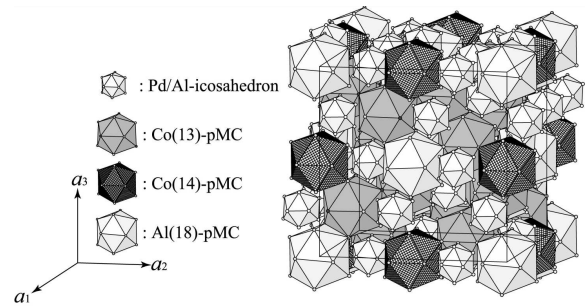


Fig. 4. The structure of the *F*-AlCoPdGe alloy, which consists of three types of pseudo-Mackay clusters and Pd/Al icosahedra.

With this fact in mind, the structure of the *F*-AlCoPdGe alloy could be pictured by the dense packing of the M icosahedra, which were representatives of the pMCs, and small Pd/Al icosahedra, as shown in Fig. 4. This figure also implies that the structure could also be represented by the penetration of three types of pMCs and the Pd/Al icosahedra, with no glue atoms being required.

4. Conclusion

The structure of the *F*-AlCoPdGe alloy was determined by single-crystal X-ray diffraction analysis. The structure contains three types of pMCs: those around the Co(13) sites, those around the Co(14) sites, and those around the Al(18) sites. These three types of pMCs could be ranked on the basis of the atomic arrangements of their first shells; nevertheless every outer shell was found to be a combination of an Al icosidodecahedron and an M icosahedron, being mainly composed of Co and Pd.

These pMCs interpenetrate each other owing to the sharing of the edges of the M icosahedra, and their interstitial space is subsequently filled by the smaller Al icosahedra around the Pd/Al(1) and Pd/Al(2) sites. These structural features suggest that the structure of F-AlCoPdGe can be represented suitably by linking the three types of pMCs and the smaller Pd/Al icosahedra without using any glue atom. It should be stressed here that the pMC with interstitial small icosahedra is one of the most important building units for the structure of icosahedral quasicrystal.

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