crystals

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Article

Structure of Cubic $Al_{73.8}Pd_{13.6}Fe_{12.6}$ Phase with High Al Content

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Table 1. The crystallographic data of the C′-phase in space group *P23*.

Crystal data	
Chemical formula	$Al_{22.04}$ $Pd_{7.31}Fe_{0.69}$ ($Al_{73.4}$ $Pd_{24.3}Fe_{2.3}$)
Crystal system	Cubic
Space group	*P23*
a, b, c/Å	7.6401(3)
α, β, γ/°	90
V/Å^3	445.96(5)
Z	1
Intensity measurements	
Radiation	Mo-$K\alpha$, λ = 0.71073 (Å)
μ /mm^{-1}	8.819
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Radiation Absorption correction	Multi-scan
T_{min}, T_{max}	0.757, 0.870
No. measured reflections	14719
No. unique reflections	335
No. observed reflections(I > 2σ(I))	324
R_{int}	0.0355
(sin θ/λ)$_{max}$ (Å^{-1})	0.680
Refinement of the structure	
No. parameters used in refinement	30
No. reflections used in refinement	335
R_1 (F_{obs} > 4σ(F_{obs}))	0.0756
R_1 (all data)	0.0775
ωR_2 (F_{obs} > 4σ(F_{obs}))	0.2268
ωR_2 (all data)	0.2290
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	8.572, -2.046

Table 2. Geometric parameters: Bond lengths (Å) for C′-phase in space group $Pm\bar{3}$.

Pd1-Al1	2.7110(18)	Pd1-Al1	2.7110(18)
Pd1-Al1	2.7110(18)	Pd1-Al1	2.7110(18)

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Pd1-Al1	2.7110(18)	Pd1-Al1	2.7110(18)
Pd1-Al1	2.7110(18)	Pd1-Al1	2.7110(18)
Pd1-Al1	2.7110(18)	Pd1-Al1	2.7110(18)
Al1-Fe2	2.544(2)	Al1-Pd2	2.544(2)
Al1-Pd2	2.5789(19)	Al1-Pd2	2.5789(19)
Al1-Al2	2.618(4)	Al1-Al2	2.618(4)
Al1-Al4	2.633(12)	Al1-Al4	2.633(12)
Al1-Al1	2.777(4)	Al1-Al1	2.869(2)
Al1-Al1	2.869(2)	Fe1-Al5	2.36(3)
Fe1-Al5	2.36(3)	Fe1-Al5	2.36(3)
Fe1-Al5	2.36(3)	Fe1-Al5	2.36(3)
Fe1-Al5	2.36(3)	Fe1-Al5	2.36(3)
Fe1-Al5	2.36(3)	Fe1-Al5	2.36(3)
Fe1-Al5	2.36(3)	Fe1-Al5	2.36(3)
Fe1-Al5	2.36(3)	Al3-Al4	1.16(2)
Al3-Al4	1.16(2)	Al3-Al5	1.34(3)
Al3-Al5	1.34(3)	Al3-Al3	1.73(4)
Al3-Pd2	2.400(8)	Al3-Pd2	2.400(8)
Al3-Fe2	2.400(8)	Al3-Al2	2.524(13)
Al3-Al2	2.524(13)	Al3-Al2	2.524(13)
Al3-Al2	2.524(13)	Al2-Al5	1.620(15)
Al2-Al5	1.620(15)	Al2-Al5	1.620(15)
Al2-Al4	1.713(11)	Al2-Al4	1.713(11)
Al2-Al4	1.713(11)	Al4-Al5	1.40(2)
Al4-Al5	1.40(2)	Al4-Al5	1.70(3)
Al4-Al4	1.86(4)	Al4-Al4	2.78(2)
Al5-Al5	2.08(6)	Al5-Fe2	2.09(3)
Al5-Pd2	2.09(3)	Al5-Al5	2.59(4)
Al5-Al5	2.59(4)		

Table 3. Crystallographic information of C1, C2 and C phases.

Phase	Space Group		Lattice Parameters			Wyckoff positions				
	Symbol	number	*a*	*b*	*c*	Atom	site	*x*	*y*	*z*
C1	$Im\bar{3}$	204	15.398	15.398	15.398	Pd1	8*c*	1/4	1/4	1/4
						Pd2/Fe2	24*g*	0.14910	0.25955	0
						Pd3/Al3	16*f*	0.09624	0.09624	0.09624
						Fe1/Pd4	24*g*	0.34955	0.24479	0
						Fe2	6*b*	1/2	0	0
						Al1/Fe3	2*a*	0	0	0
						Al2	12*e*	1/2	0.1927	0

						Al3	48*h*	0.24965	0.16193	0.09800
						Al4	12*e*	0	0.1955	0
						Al5	48*h*	0.25629	0.34479	0.09604
						Al6	48*h*	0.4049	-0.0789	0.0954
						Al7	24*g*	0.3629	-0.0730	0
						Al8	24*g*	1/2	-0.0711	0.1366
C2	$Fm\bar{3}$	202	15.515	15.515	15.515	Pd1	8*c*	1/4	1/4	1/4
						Pd2	48*h*	0.7410	0.3518	1/2
						Pd3/Fe3	32*f*	0.0972	0.0972	0.0972
						Pd4/Fe4	4*b*	1/2	1/2	1/2
						Al5/Fe5	4*a*	0	0	0
						Al6	24*e*	0.8095	1/2	1/2
						Al7	96*i*	0.6590	1/4	0.5995
						Al8	32*f*	0.410	0.410	0.410
						Al9	48*h*	0.436	0.643	1/2
C	$Pm\bar{3}$	200	7.640	7.640	7.640	Pd1	1*b*	1/2	1/2	1/2
						Pd2/Fe2	6*f*	1/2	0.70685	0
						Fe1	1*a*	0	0	0
						Al1	12*k*	1/2	0.8048	0.6817
						Al2	8*i*	0.8154	0.8154	0.8154
						Al3	6*e*	0.387	0	0
						Al4	12*j*	0.705	0	0.878
						Al5	12*j*	0.723	0.864	0

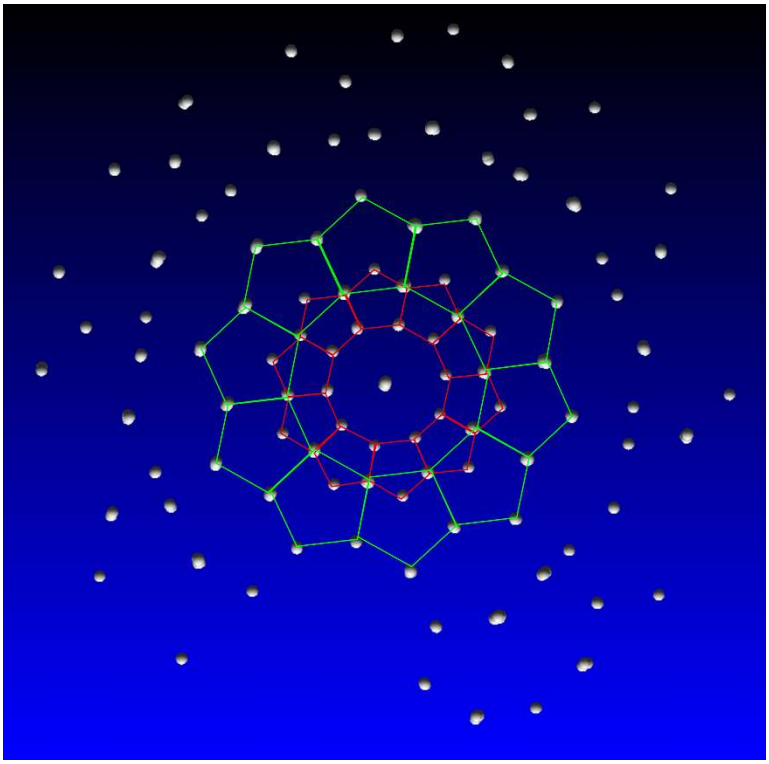

Figure 1. Projected diffraction patterns along the periodic direction of the quasicrystal phase.

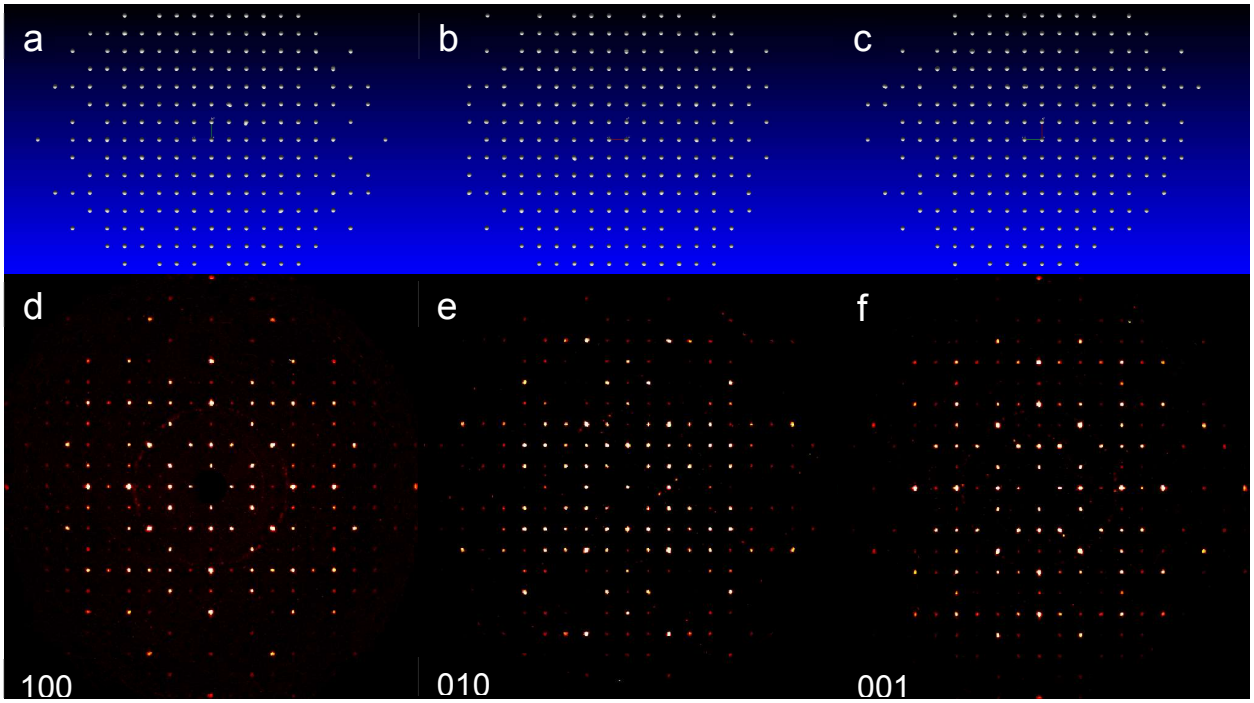

Figure 2. Projected diffraction patterns along a: <100>, b: <010> and c: <001> directions and the corresponding unwarp images along e: <100>, f: <010> and g: <001> directions for the C′-phase of Al-Pd-Fe.

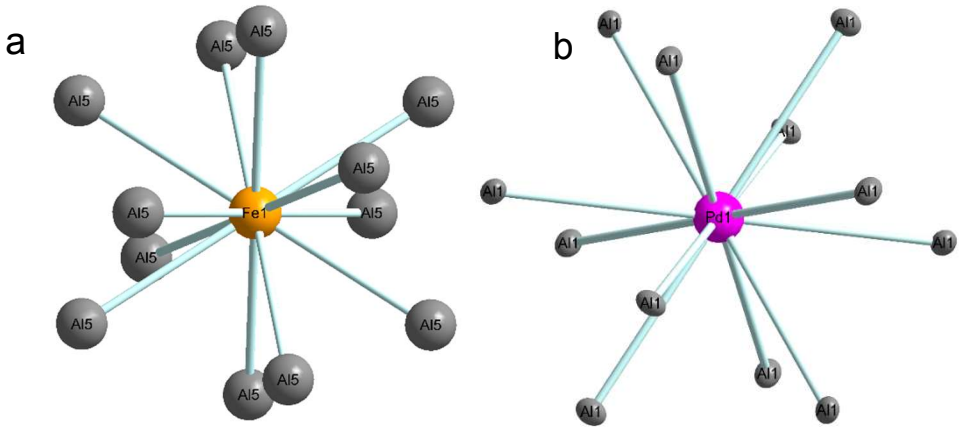

Figure 3. Environments of a: Pd1 and b: Fe1 atoms for the C′-phase.

(The distances to the vertices are 2.7110(18) Å and 2.36(3) Å for the Pd and Fe atoms, respectively.)