

Crystal structure of the Al₈Cr₅-type intermetallic Al_{7.85}Cr_{5.16}

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Supplementary materials include:

Table S1. Crystallographic information of all reported Al₈Cr₅ phases

Table S2. Lattice parameters for the standardization of crystal data for the γ_2' -Al₈Cr₅ phase based on the refined crystal data

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Table S1 Crystallographic information of all reported Al₈Cr₅ phases

Phase	Space Group		Lattice Parameters		Wyckoff positions					Ref.
	Symbol	number	<i>a</i> (Å)	α (°)	Atom site	<i>x</i>	<i>y</i>	<i>z</i>		
Al ₈ Cr ₅	<i>I</i> -43 <i>m</i>	217	9.0900	90.0000	Al1	24 <i>g</i>	0.3087	0.3087	0.0394	[1]
(1992)					Al2	8 <i>c</i>	0.1062	0.1062	0.1062	
					Cr1	8 <i>c</i>	0.1062	0.1062	0.1062	
					Al3	12 <i>e</i>	0.3522	0	0	
					Cr2	12 <i>e</i>	0.3522	0	0	
					Cr3	8 <i>c</i>	0.8300	0.8300	0.8300	
Al ₁₆ Cr _{9.5}	<i>R</i> 3 <i>m</i>	160	7.8110	109.1300	Al1	3 <i>b</i>	-0.3608	-0.3608	-0.0095	[2]
(1977)					Al2	3 <i>b</i>	0.0055	0.0055	-0.2096	
					Al3	3 <i>b</i>	-0.2709	-0.2709	-0.6270	
					Al4	3 <i>b</i>	0.3699	0.3699	0.0306	
					Al5	6 <i>c</i>	-0.3179	0.2982	0.0533	
					Al6	3 <i>b</i>	0.3608	0.3608	0.5720	
					Cr1	1 <i>a</i>	0.1795	0.1795	0.1795	
					Cr2	3 <i>b</i>	0.0055	0.0055	-0.2096	
					Cr3	1 <i>a</i>	-0.3071	-0.3071	-0.3071	
					Cr4	3 <i>b</i>	0.3699	0.3699	0.0306	
					Cr5	3 <i>b</i>	0	0	0.3451	

Al_8Cr_5	<i>R</i> 3 <i>m</i>	160	7.8050	109.1270	Cr1	1 <i>a</i>	0.1940	0.1940	0.1940	[3]
(1937)					Cr2	3 <i>b</i>	0.0030	0.0030	0.7940	
					Cr3	3 <i>b</i>	0.9980	0.9980	0.3400	
					Cr4	3 <i>b</i>	0.3550	0.3550	0.0060	
					Al1	1 <i>a</i>	0.6720	0.6720	0.6720	
					Al2	3 <i>b</i>	0.6540	0.6540	0.0120	
					Al3	3 <i>b</i>	0.3490	0.3490	0.5820	
					Al4	3 <i>b</i>	0.7220	0.7220	0.3560	
					Al5	6 <i>c</i>	0.0330	0.2880	0.6610	

Table S2. Lattice parameters for the standardization of crystal data for the γ_2' - Al_8Cr_5 phase based on the refined crystal data

Chemical Formula	Al_8Cr_5
Crystal system, space group	Hexagonal, <i>R</i> 3 <i>m</i>
<i>a</i> , <i>b</i> , <i>c</i> /Å	12.8717, 12.8717, 7.8408
α , β , γ /°	90, 90, 120
<i>V</i> /Å ³	1125.03

Table S3. The atomic positions for the standardization of crystal data for the γ_2' -Al₈Cr₅ phase based on the refined crystal data

Label	Site	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Al1	9b	0.5977 (12)	0.4023 (12)	0.0591 (9)	0.010871	0.7720
Cr1	9b	0.5977 (12)	0.4023 (12)	0.0591 (9)	0.010871	0.2280
Al2	9b	0.2150 (11)	0.7850 (10)	0.0770 (7)	0.011734	0.5000
Cr2	9b	0.2150 (11)	0.7850 (10)	0.0770 (7)	0.011734	0.5000
Al3	9b	0.0917 (14)	0.9083 (13)	0.2161 (9)	0.012218	0.9580
Cr3	9b	0.0917 (14)	0.9083 (13)	0.2161 (9)	0.012218	0.0420
Cr4	3a	0.0000 (10)	0.0000 (10)	0.0000 (7)	0.005509	
Cr5	9b	0.4444 (7)	0.5556 (7)	0.2062 (5)	0.003182	
Cr6	9b	0.7846 (8)	0.2154 (7)	0.2256 (6)	0.011041	
Cr7	3a	0.0000 (11)	0.0000 (11)	0.4368 (8)	0.009053	
Al4	18c	0.3732 (14)	0.0161 (14)	0.0334 (10)	0.018686	
Al5	9b	0.5501 (15)	0.4499 (16)	0.3699 (11)	0.014880	

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