Pressure Induced Disorder-Order Phase Transitions in the Al4Cr Phases

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Table S1. The Wyckoff positions of the centered atoms inside the Macky or pseudo-Macky cluster for the ε- and μ-Al_4Cr phase along with the η-$Al_{11}Cr_2$ phase.

Nanocluster Type	Phase	Center Atom Coordinates of Nanocluster
Macky (1@12@42)	ε-Al_4Cr 1@12@42	Cr10(0.50000,-0.06080,0.25000) (4*c*; m2m)
	η-$Al_{11}Cr_2$ pseudo-Mackay 1@12@38	Cr11(0.25000,0.75000,0.50000) (4*c*; -1)
	μ-Al_4Cr pseudo-Mackay 1@12@41	Cr2(0.00000,0.00000,0.25000) (2*b*;-6m2)
	θ-$Al_{45}Cr_7$ pseudo-Mackay 1@12@38	Cr3(0.50000,0.50000,0.50000) (2*c*; 2/m）
1@12@46	ε-Al_4Cr	Al13(0.50000, 0.18285, 0.25000) (4*c*; m2m) Al14(0.50000,0.07444, 0.25000) (4*c*; m2m) Al17(0.50000,0.25398,0.17920) (8*f*; m..) Al23(0.00000,0.19190,0.51390) (8*f*; m..) Al27(0.81860,0.14117,0.13300) (16*h* 1)
	η-$Al_{11}Cr_2$	Al36(0.44124, 0.64688, 0.49235) (8*f*; 1) Al28(0.75770, 0.85334, 0.80867) (8*f*; 1)
	μ-Al_4Cr	Al3(0.25590,0.36707,0.49559) (24*l*; 1) Al10(0.03077,-0.41351,0.15948) (24*l*; 1) Al22(0.50978,0.49022,0.25000) (6*h*; mm2) Al23(-0.23891,0.38054,0.25000 6h mm2)