

Prediction of novel alloy phases of Al with Sc or Ta

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Supplementary Information

TABLE S1. Crystallographic information for the predicted stable alloy phases AlSc₃ and AlTa₇, their elastic constants (C_{ij}), bulk (B), shear (G) and Young (E) moduli and Poisson ratios (ν).

alloy	AlSc ₃	AlTa ₇
space group	194	210
a [Å]	6.307	10.501
c [Å]	5.030	
C ₁₁ [GPa]	119	302
C ₁₂ [GPa]	45	121
C ₁₃ [GPa]	33	
C ₃₃ [GPa]	128	
C ₄₄ [GPa]	49	46
C ₆₆ [GPa]	37	
B [GPa]	65	182
G [GPa]		46
G _{yz} [GPa]	49	
G _{xy} [GPa]	37	
E [GPa]		232
E _x [GPa]	98	
E _z [GPa]	115	
ν		0.29
ν_{zx}	0.20	
ν_{xy}	0.33	
ν_{yz}	0.17	