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Supplementary Information

First principles study on the mechanical and thermodynamic properties of aluminium doped magnesium alloys

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The mechanical stability criteria of *hcp* Mg, *fcc* Al and Mg_xAl_y alloys are listed below.

Hexagonal phase ($C_{11}, C_{33}, C_{44}, C_{12}$ and C_{13})

$C_{44} > 0$, $C_{11} > |C_{12}|$, $(C_{11} + 2C_{12})C_{33} > 2C_{13}^2$

Cubic phase(C_{11}, C_{44} and C_{12})

$C_{11} > 0$, $C_{44} > 0$, $C_{11} > |C_{12}|$, $(C_{11} + 2C_{12}) > 0$

The formulas of elastic moduli of *hcp* Mg, *fcc* Al and Mg_xAl_y alloys are listed below.

Hexagonal phase ($C_{11}, C_{33}, C_{44}, C_{12}$ and C_{13})

$B_V = (1/9)[2(C_{11} + C_{12}) + 4C_{13} + C_{33}]$

$G_V = (1/30)(M + 12C_{44} + 12C_{66})$

$B_R = C^2/M$

$G_R = (5/2)[C^2C_{44}C_{66}]/[3B_VC_{44}C_{66} + C^2(C_{44}+C_{66})]$

$M = C_{11} + C_{12} + 2C_{33} - 4C_{13}$

$C^2 = (C_{11} + C_{12})C_{33} - 2C_{13}^2$

Cubic phase(C_{11}, C_{44} and C_{12})

$B_V = B_R = (C_{11} + 2C_{12})/3$

$G_V = (C_{11} - C_{12} + 3C_{44})/5$

$G_R = 5(C_{11} - C_{12})C_{44}/[4C_{44} + 3(C_{11} - C_{12})]$

It is worth noting that the structures listed in Tables S1, S2 and S3 are the metastable Mg_xAl_y except for $Mg_{11}Al_5$, Mg_5Al_3 and Mg_9Al_7. Listing the data of these structures in Supplementary Information was just for reference purposes if necessary. $Mg_{11}Al_5$, Mg_5Al_3 and Mg_9Al_7 are the most stable structures determined based on the formation energies and convex hull diagram, and their elastic properties, electronic properties and thermodynamic properties were discussed in the main text.

Table S1. The elastic constants (Gpa) of Mg_xAl_y structures.

Structure	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
$Mg_{15}Al_1$	64.6	24.3	22.8	71.8	18.7
Mg_7Al	66.9	29.1	24.6	73.4	21.1
$Mg_{13}Al_3$	62.6	32.2	25.0	66.2	15.1
Mg_3Al	69.6	31.7	30.5	84.7	14.5
MgAl	74.3	43.9	35.7	89.9	20.6
Mg_7Al_9	71.8	54.4	40.1	91.2	23.1
Mg_3Al_5	71.9	42.7	39.1	100.8	19.3
Mg_5Al_{11}	75.0	44.7	38.0	108.2	21.1
$MgAl_3$	81.4	45.4	43.5	114.1	19.9
Mg_3Al_{13}	67.3	47.5	54.2	104.0	23.4
$MgAl_7$	75.2	49.9	50.7	112.9	17.8
$MgAl_{15}$	82.2	48.3	58.3	106.1	17.2

Table S2. The elastic moduli with the unit of GPa (B_R and B_V represent the bulk moduli with the Reuss and Voigt averaging scheme, respectively; G_R and G_V represent the shear moduli with the Reuss and Voigt averaging scheme, respectively; *E*, *B* and *G* represent Young's modulus, bulk modulus and shear modulus with the Voigt-Reuss-Hill averaging scheme, respectively), Poisson's ratio (*v*), anisotropy (A^U) and hardness (H_v) of Mg_xAl_y.

Structure	B_R	B_V	G_R	G_V	*E*	*B*	*G*	*v*	*B/G*	A^U	H_v
$Mg_{15}Al_1$	37.82	37.87	20.10	20.25	51.4	37.8	20.2	0.27	1.88	0.04	3.8
Mg_7Al	40.42	40.42	20.65	20.81	53.1	40.4	20.7	0.28	1.95	0.04	3.7
$Mg_{13}Al_3$	39.51	39.53	16.07	16.36	42.8	39.5	16.2	0.32	2.44	0.09	2.4
Mg_3Al	45.19	45.48	17.60	18.34	47.6	45.3	18.0	0.32	2.52	0.22	2.5
MgAl	52.04	52.12	18.70	19.49	51.1	52.1	19.1	0.34	2.73	0.21	2.4
Mg_7Al_9	55.96	56.00	14.01	17.66	43.4	56.0	15.8	0.37	3.54	1.30	1.5
Mg_3Al_5	53.15	54.04	17.93	18.89	49.6	53.6	18.4	0.35	2.91	0.28	2.1
Mg_5Al_{11}	54.66	55.51	19.24	20.64	53.4	55.1	19.9	0.34	2.76	0.38	2.4
$MgAl_3$	59.02	60.19	20.37	21.19	55.9	59.6	20.8	0.34	2.87	0.22	2.4
Mg_3Al_{13}	57.21	61.16	14.37	16.85	43.1	59.2	15.6	0.38	3.79	0.93	1.4
$MgAl_7$	60.65	62.88	16.00	17.12	45.6	61.8	16.6	0.38	3.73	0.39	1.5
$MgAl_{15}$	64.37	66.70	17.18	17.31	47.6	65.5	17.2	0.38	3.80	0.07	1.5

Table S3. Theoretically calculated thermal properties of Mg_xAl_y alloys including longitudinal sound velocity (v_l), shear sound velocity (v_t) and average sound velocity (v_m) and Debye temperature (Θ_D).

Structure	v_l(m·s^{-1})	v_t(m·s^{-1})	v_m(m·s^{-1})	Θ_D (K)
$Mg_{15}Al$	6011.21	3355.94	3736.24	394.39
Mg_7Al	6077.94	3354.36	3737.87	397.21
$Mg_{13}Al_3$	5692.69	2931.37	3282.52	350.69
Mg_3Al	5928.49	3019.14	3383.16	365.86
MgAl	5945.14	2950.51	3311.36	367.42
Mg_7Al_9	5844.30	2648.40	2986.05	333.64
Mg_3Al_5	5839.48	2834.30	3184.89	356.82
Mg_5Al_{11}	5907.32	2918.80	3276.60	368.79
$MgAl_3$	6031.89	2942.58	3305.65	374.28
Mg_3Al_{13}	5705.09	2520.21	2844.63	323.88
$MgAl_7$	5773.07	2565.58	2895.11	331.43
$MgAl_{15}$	5852.68	2582.92	2915.52	335.97