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Electronic Supplementary Information

Thermodynamic Predicting and Atomistic Modeling the Favored Compositions for Mg-Ni-Y Metallic Glasses

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Tables

TABLE S1 Lattice constants (a and c), cohesion energies (E_c), elastic constants (C_{ij}), and bulk moduli (B_0) of Mg, Ni, and Y that are fitted by potential and obtained from experiments. Lattice constants a and c are expressed in Å, cohesion energies E_c in eV/atom, elastic constants C_{ij} and bulk moduli B_0 in Mbar.

	hcp-Mg		*fcc*-Ni		*hcp*-Y	
	Fitted	Exp.	Fitted	Exp.	Fitted	Exp.
a	3.209	3.209[a]	3.524	3.517[a]	3.650	3.648[a]
c	5.235	5.211[a]			5.958	5.732[a]
E_c	1.508	1.510[b]	4.423	4.440[b]	4.361	4.370[b]
C_{11}	0.591	0.595[a]	2.385	2.418[a]	0.639	0.779[a]
C_{12}	0.270	0.261[a]	1.630	1.550[a]	0.348	0.285[a]
C_{13}	0.223	0.218[a]			0.294	0.210[a]
C_{33}	0.642	0.616[a]			0.703	0.769[a]
C_{44}	0.112	0.164[a]	1.217	1.242[a]	0.108	0.243[a]
B_0	0.362	0.354[a]	1.882	1.860[a]	0.428	0.415[a]

[a]Ref. 1; [b]Ref. 2

TABLE S2 Lattice constants (*a*, *b*, and *c*), cohesive energies (E_c), and bulk moduli (B_0) of the Mg-Ni,[3] Mg-Y[4] and Ni-Y compounds that are reproduced from the potential (first line) and derived from *ab initio* calculations (second line), together with some available experimental data for lattice constants of compounds (Ref. 5-8). Lattice constants *a*, *b* and *c* are expressed in Å, cohesive energies E_c in eV/atom, and bulk moduli B_0 in Mbar.

Compounds	Mg_3Ni	MgNi	$MgNi_3$	$MgNi_3$	$Mg_{24}Y_5$	Mg_3Y	Mg_2Y	MgY_3	Ni_3Y	Ni_2Y	NiY_3	NiY_3
Space group	$F4\bar{3}m$	$F4\bar{3}m$	$F4\bar{3}m$	$F4\bar{3}m$	$I4\bar{3}m$	$Pm\bar{3}m$	$P6\bar{3}/mmc$	$Pm\bar{3}m$	$Pm\bar{3}m$	$Fd\bar{3}m$	$Pm\bar{3}m$	*Pnma*
a or *a*,*c* or *a*,*b*,*c*	6.673	3.120	3.724	5.930	11.02	4.535	6.107, 6.107,9.885	5.011	3.903	7.250	3.456	7.308,9.427,6.375
	6.562	3.056	3.658	5.817	11.30	4.674	6.065, 6.065,9.878	4.973	3.967	7.310	3.517	7.053,9.704,6.461
					11.26[a]		6.038,9.800[b]			7.181[c]		6.920,9.490,6.360[d]
*E*c	2.277	3.161	3.816	3.781	2.060	2.329	2.533	3.637	4.507	4.695	4.288	4.439
	2.277	3.161	3.819	3.782	2.063	2.309	2.555	3.628	4.498	4.788	4.203	4.581
B_0	0.609	1.078	1.506	1.424	0.386	0.281	0.374	0.329	0.962	1.320	0.500	0.546
	0.594	0.889	1.367	1.366	0.425	0.316	0.436	0.376	3.903	7.250	3.456	0.788

[a]Ref. 5; [b]Ref. 6; [c]Ref. 7; [d]Ref. 8

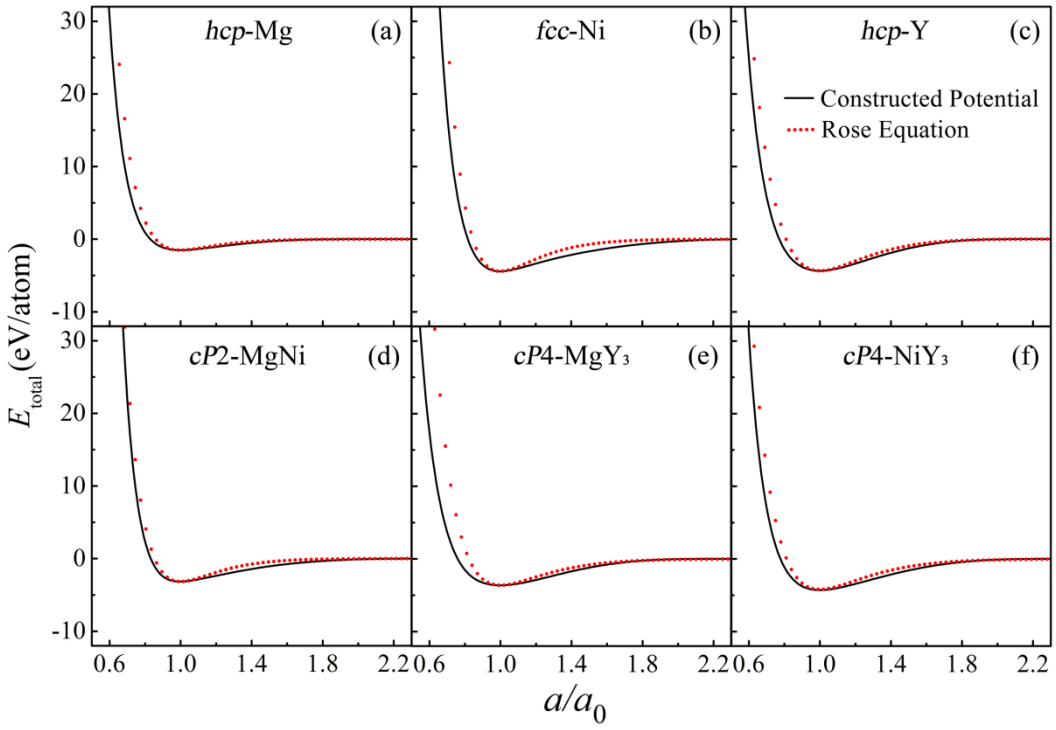

Figure S1 Equations of state calculated from the constructed potential (solid lines) and Rose equation (dotted lines) for (a) *hcp*-Mg, (b) *fcc*-Ni, (d) *hcp*-Y, (d) *cP*2-MgNi, (e) *cP*4-MgY_3, and (f) *cP*4-NiY_3.

References

1 D. R. Lide and T. J. Bruno, *CRC handbook of chemistry and physics*, CRC PressI Llc, New York, 2012.

2 C. Kittel and P. McEuen, *Introduction to solid state physics*, Wiley, New York, 1996.

3 Q. Wang, J. H. Li, J. B. Liu and B. X. Liu, *Phys. Chem. Chem. Phys.*, 2014, **16**, 19590-19601.

4 Q. Wang, J. H. Li and B. X. Liu, *Phys. Chem. Chem. Phys.*, 2015, **17**, 14879-14889.

5 E. Gibson and O. Carlson, *Trans. ASM*, 1960, **52**, 1084.

6 K. H. J. Buschow, R. C. Sherwood, F. S. L. Hsu and K. Knorr, *J. Appl. Phys.*, 1978, **49**, 1510-1512.

7 B. J. Beaudry, J. F. Haefling and A. H. Daane, *Acta Crystallogr.*, 1960, **13**, 743-744.

8 R. Lemaire and D. Paccard, *Bulletin de la société française de minéralogie et de cristallographie*, 1967, **90**, 311–315.