Thermodynamic modelling of the Al–Co–Mn system

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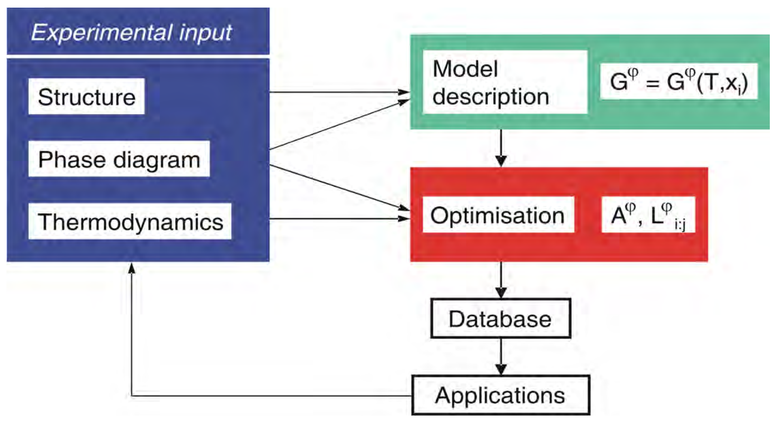
Objectives

- Model thermodynamically the Al–Co–Mn ternary system by using experimental data in the literature.
- Optimize the ternary interaction parameters in the Al–Co–Mn.
- Include the Al–Co–Mn ternary parameters in the high entropy alloy thermodynamic database to give a reliable calculation.

Methodology



Crystal structure

Table 1: Crystallographic information of Al–Co–Mn system.

Phase label	also known as	Prototype	Pearson symbol	Space group	Strukturbericht
fcc	γ	Cu	$cF4$	$Fm\bar{3}m$ (225)	$A1$
bcc	α	W	$cI2$	$Im\bar{3}m$ (229)	$A2$
hcp	ϵ	Mg	$hP2$	$P6_3/mmc$ (194)	$A3$
B2_BCC	β	CsCl	$cP2$	$Pm\bar{3}m$ (221)	$B2$
α-Mn		α-Mn	$cI58$	$I\bar{4}3m$ (217)	$A12$
β-Mn		β-Mn	$cP20$	$P4_132$ (213)	$A13$
Al_5Co_2		Al_5Co_2	$hP28$	$P6_3/mmc$ (194)	$D8_{11}$
O-$Al_{13}Co_4$		$Al_{13}Co_4$	$oP102$	$Pmn21$ (031)	
Y-$Al_{13}Co_4$		$Al_{13}Co_4$		$C2/m$ (012)	
M-$Al_{13}Co_4$		$Al_{13}Fe_4$	$mC102$	$C2/m$	
Al_9Co_2		Al_9Co_2	$mP22$	$P2_1/c$ (014)	
Al_3Co		Al_3Co			
γ_2-Al_8Mn_5		Al_8Cr_5	$hR26$	$R3m$ (160)	$D8_{10}$
γ_1-Al_8Mn_5		Cu_5Zn_8	$cI52$	$I\bar{4}3m$ (217)	$D8_2$
LT-$Al_{11}Mn_4$		$Al_{11}Mn_4$	$aP15$	$P\bar{1}$ (002)	
HT-$Al_{11}Mn_4$		Al_3Mn	$oP156$	$Pnma$ (062)	
λ-Al4Mn		Al4Mn-λ	$hP586$	$P6_3/m$ (176)	
μ-Al4Mn		Al4Mn-μ	$hP574$	$P6_3/mmc$ (194)	
Al_6Mn		Al_6Mn	$oC28$	$Cmcm$ (063)	$D2_h$
$Al_{12}Mn$		$Al_{12}W$	$cI26$	$Im\bar{3}$ (204)	
T-AlCoMn	ζ	$Al_{62}Mn_{12}Ni_4$	$oC156$	$Cmcm$	

Conclusion

- Al–Co–Mn ternary system was thermodynamically modelled.
- Liquidus and solidus datapoints were used to optimize ternary liquid parameters and calculate liquidus surface.

Acknowledgment

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References

[1] M Ostrowska and G Cacciamani. Critical evaluation and thermodynamic modeling of the Al–Co–Fe system. *J. Alloys Compd.*, pages 553–568, 2019.

[2] Y Du, J Wang, J Zhao, J C Schuster, F Weitzer, R Schmid-Fetzer, M Ohno, H Xu, Z K Liu, Sh Shang, et al. Reassessment of the Al–Mn system and a thermodynamic description of the Al–Mg–Mn system. *Int. J. Mater. Res.*, 98(9):855–871, 2007.

[3] W Huang. An assessment of the Co–Mn system. *Calphad*, 13(3):231–242, 1989.

[4] R Kainuma, M Ise, K Ishikawa, I Ohnuma, and K Ishida. Phase equilibria and stability of the B2 phase in the Ni–Mn–Al and Co–Mn–Al systems. *J. Alloys Compd.*, 269(1):173–180, 1998.

[5] T Gödecke and W Köster. The ternary system cobalt-mangenese-aluminum. *Z. Metallkd.*, 63:422–430, 1972.

Binaries: Al–Co, Al–Mn, and Co–Mn

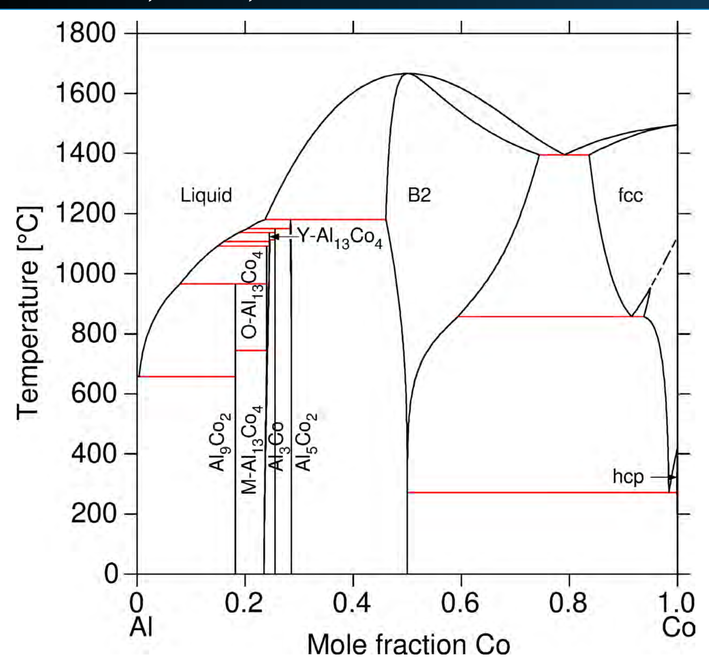

Figure 1: Calculated Al–Co phase diagram from Ostrowska and Cacciamani [1].

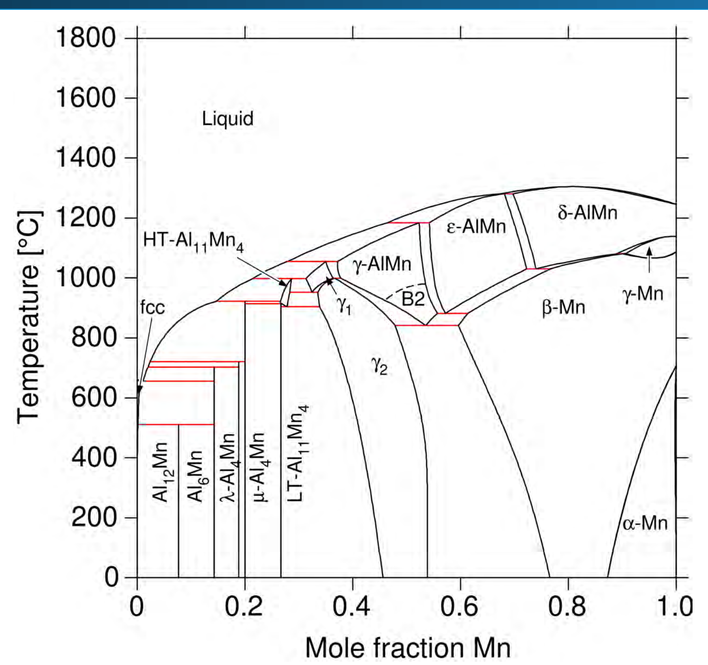

Figure 2: Calculated Al–Mn phase diagram from Du et al. [2].

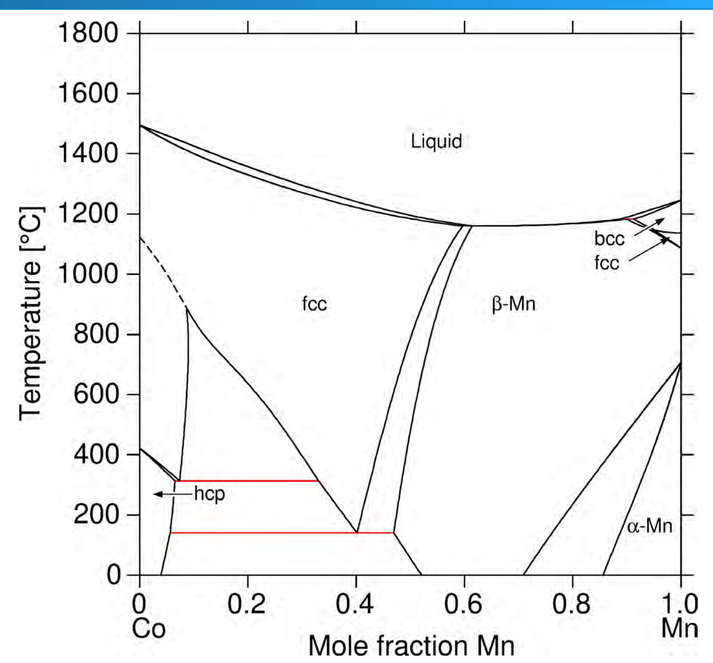

Figure 3: Calculated Co–Mn phase diagram from Huang [3].

Results: Isothermal sections

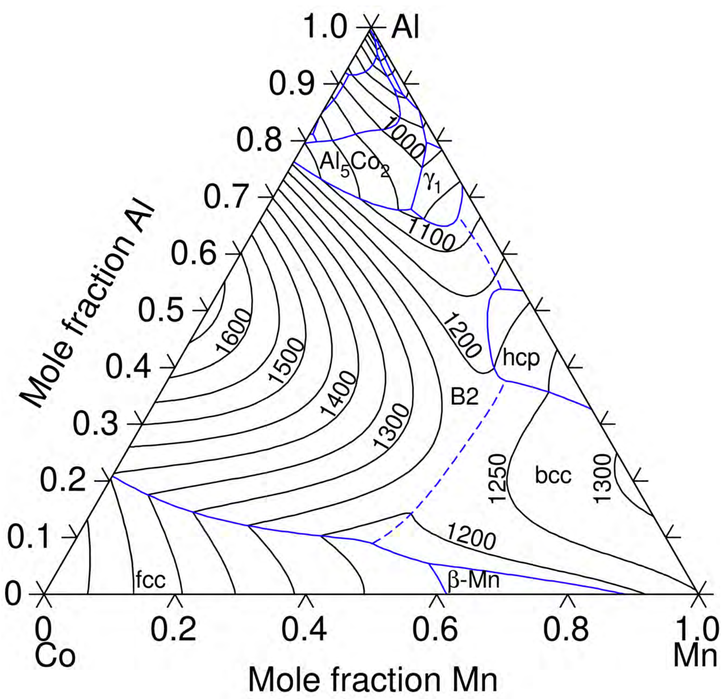

Figure 4: Calculated liquidus projection for Al–Co–Mn system. All the temperatures are in °C.

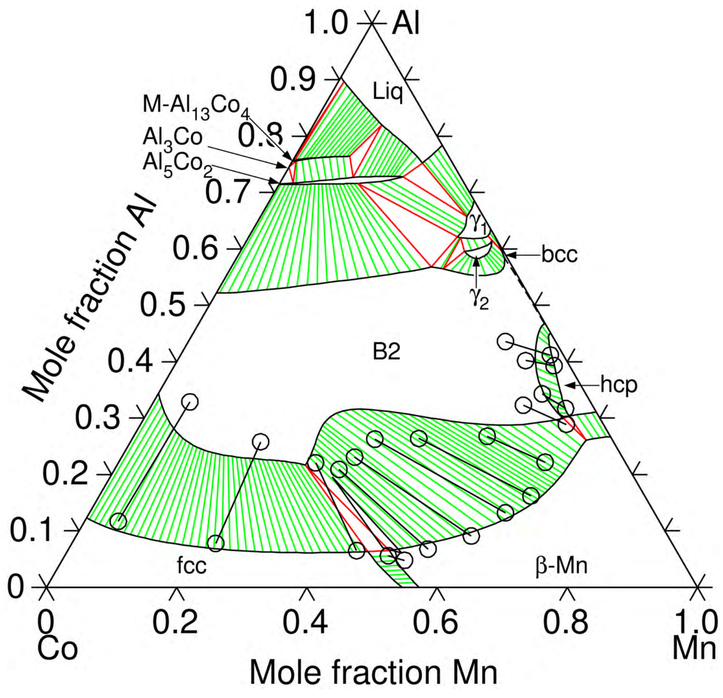

Figure 5: Calculated isothermal section of Al–Co–Mn at 1000 °C using experimental data from Kainuma et al. [4].

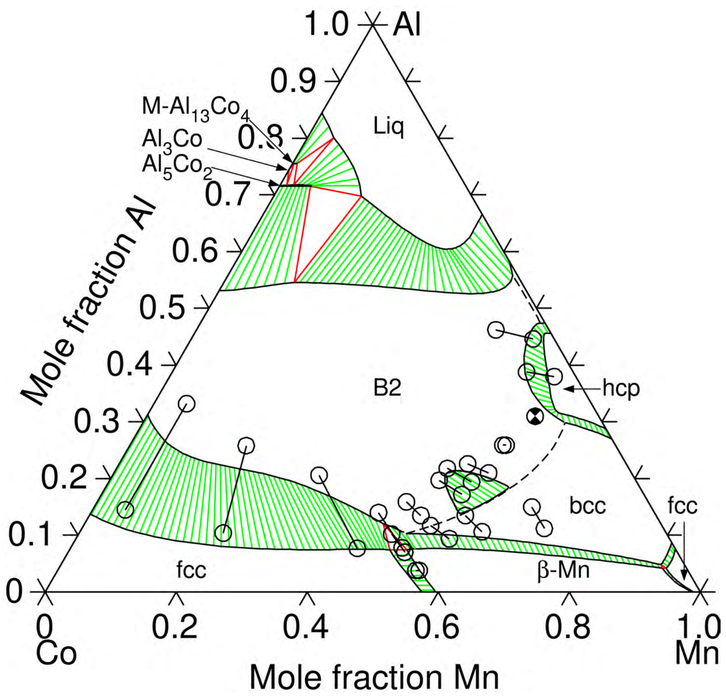

Figure 6: Calculated isothermal section of Al–Co–Mn at 1100 °C using experimental data from Kainuma et al. [4].

Results: Isoplethal sections

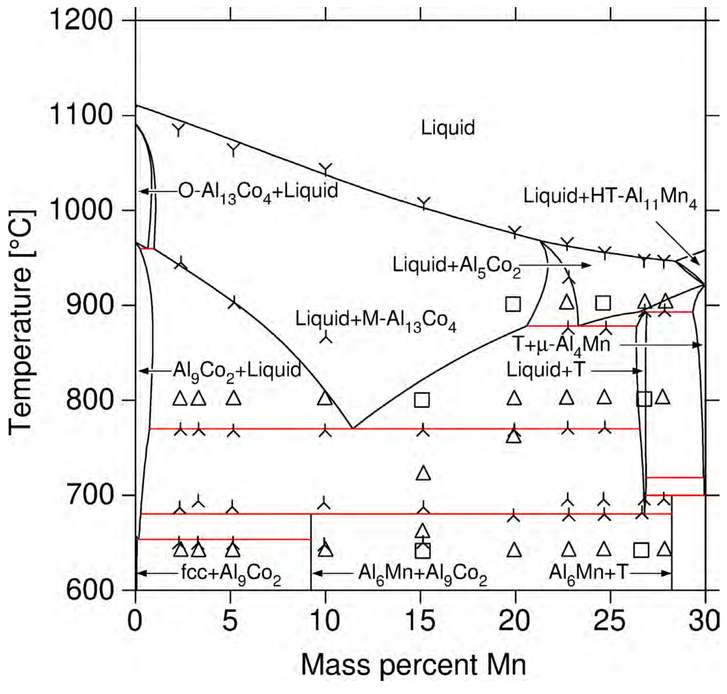

Figure 7: Isoplethal section of Al–Co–Mn at 70 wt.% Al with experimental data from Gödecke and Köster [5].

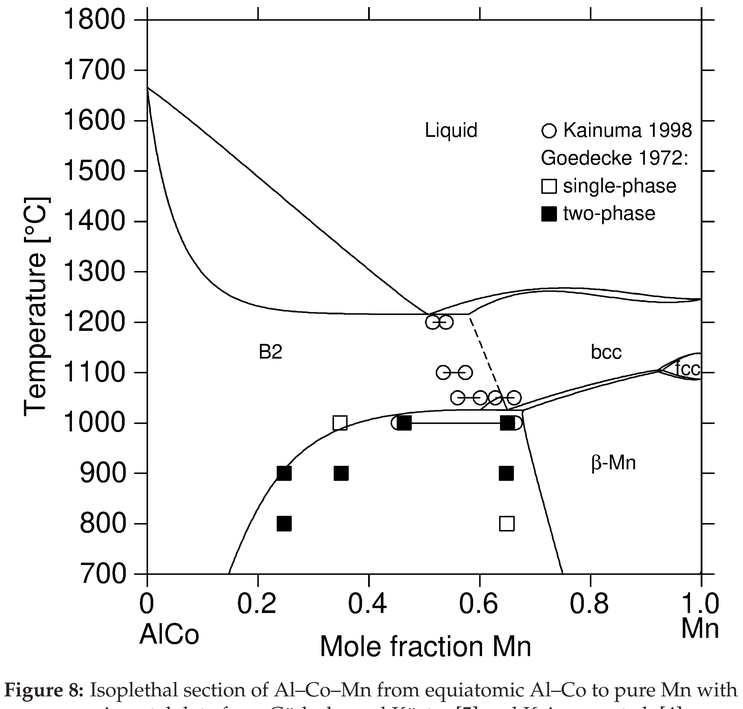

Figure 8: Isoplethal section of Al–Co–Mn from equiatomic Al–Co to pure Mn with experimental data from Gödecke and Köster [5] and Kainuma et al. [4].

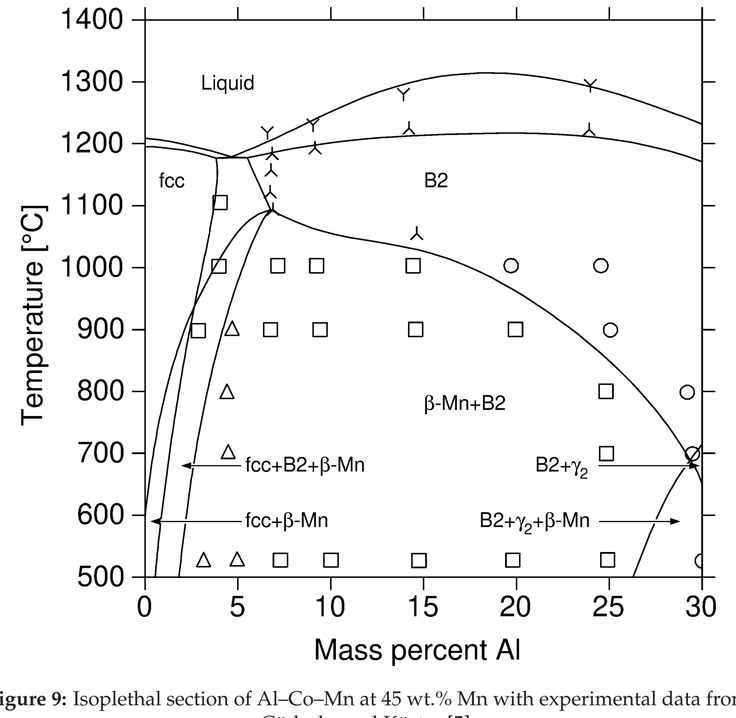

Figure 9: Isoplethal section of Al–Co–Mn at 45 wt.% Mn with experimental data from Gödecke and Köster [5].