Thermodynamic modelling of the Al–Co–Fe system

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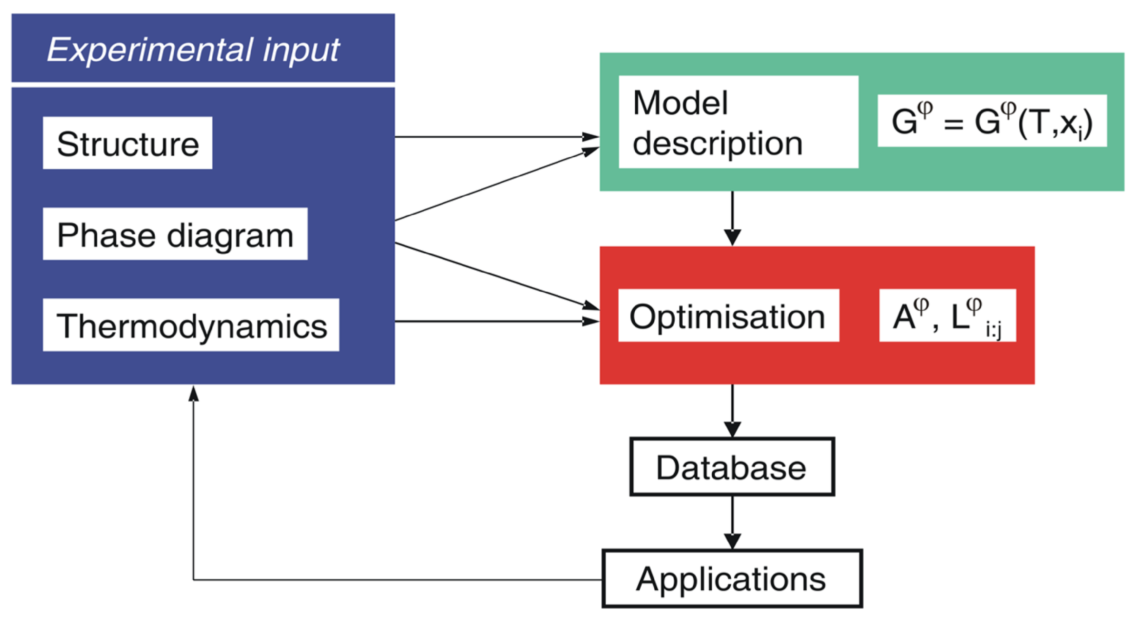
Objectives

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

Methodology



Crystal structure

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

Phase label 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	β	CsCl	$cP2$	$Pm\bar{3}m$ (221)	$B2$
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-$Al_{13}(Co,Fe)_4$		$Al_{13}Fe_4$	$mC102$	$C2/m$	
Al_9Co_2		Al_9Co_2	$mP22$	$P2_1/c$ (014)	
Al_3Co		Al_3Co			
Al_8Fe_5		Cu_5Zn_8	$cI52$	$I\bar{4}3m$ (217)	$D8_2$
Al_5Fe_2		$Al5_5Fe_2$	$oC24$	$Cmcm$ (063)	

Conclusion

- The Al–Co–Fe ternary system is modelled using Calphad method.
- Liquidus surface of the system over the whole composition is calculated.
- Various isothermal and vertical sections were calculated and compared with the literature. A good agreement between them is achieved.
- A thermodynamic description of the Al–Co–Fe is proposed.

Acknowledgment

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References

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Binaries: Al–Co, Al–Fe, and Co–Fe

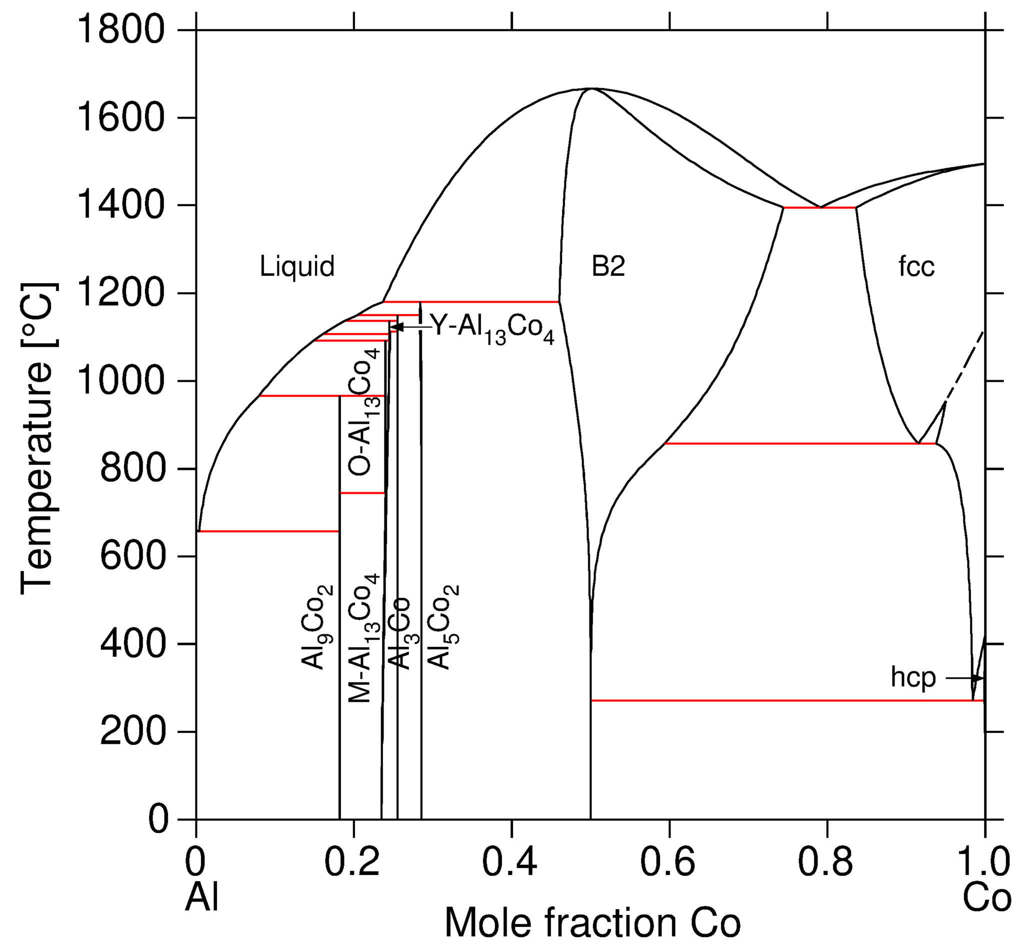

Figure 1: Calculated Al–Co phase diagram from Ostrowska and Cacciamani [1].

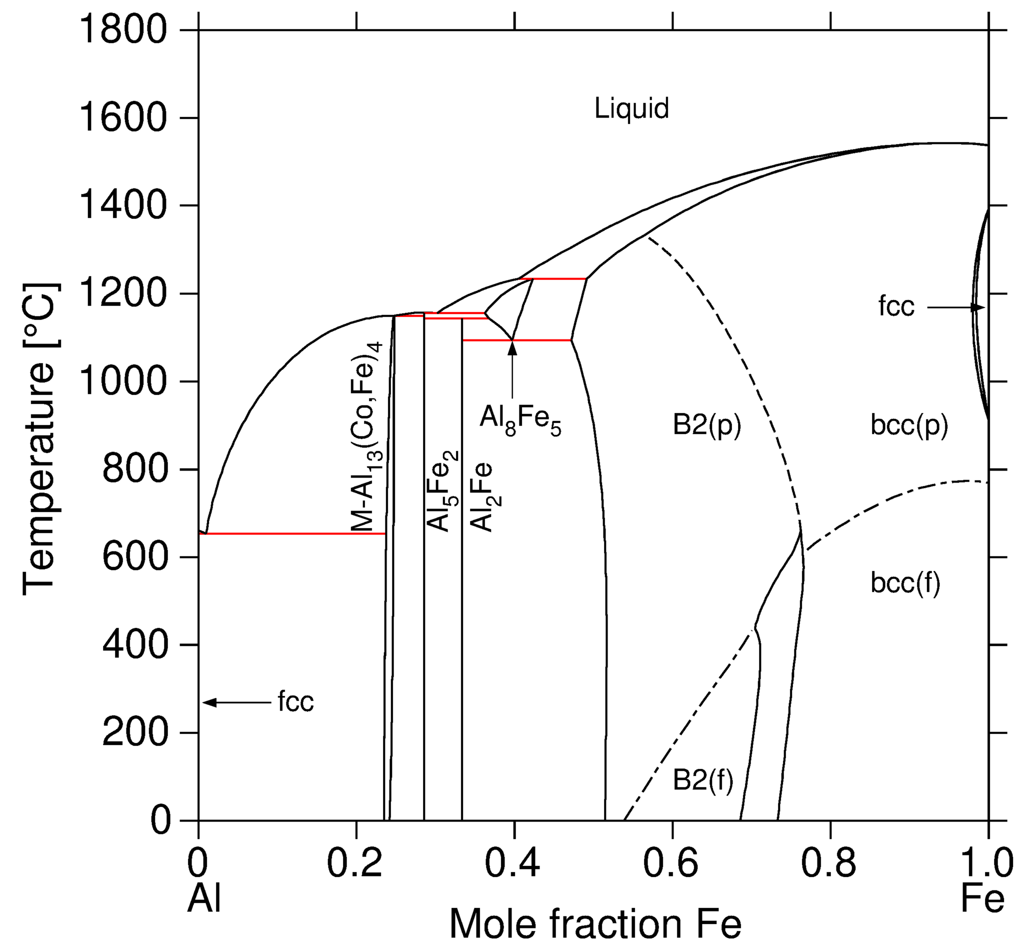

Figure 2: Calculated Al–Fe phase diagram from Zheng et al. [2].

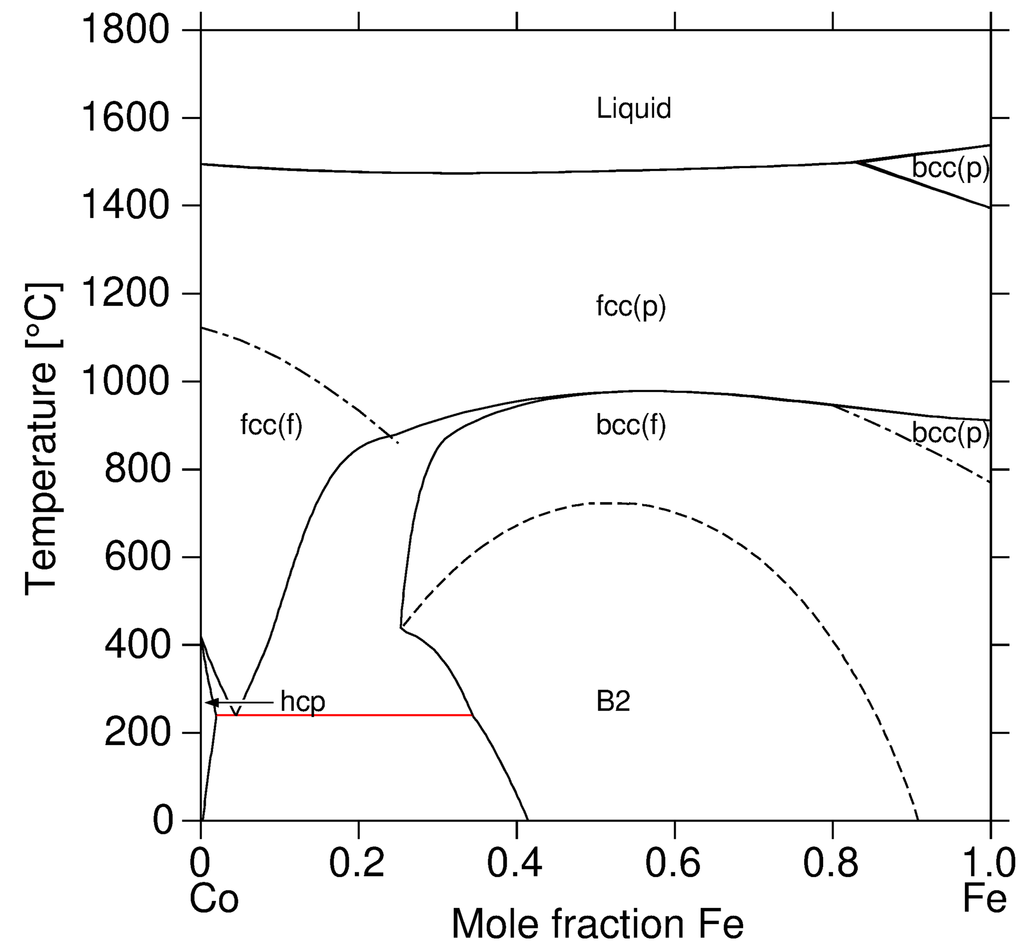

Figure 3: Calculated Co–Fe phase diagram from Ohnuma et al. [3].

Results: Liquidus surface of Al–Co–Fe

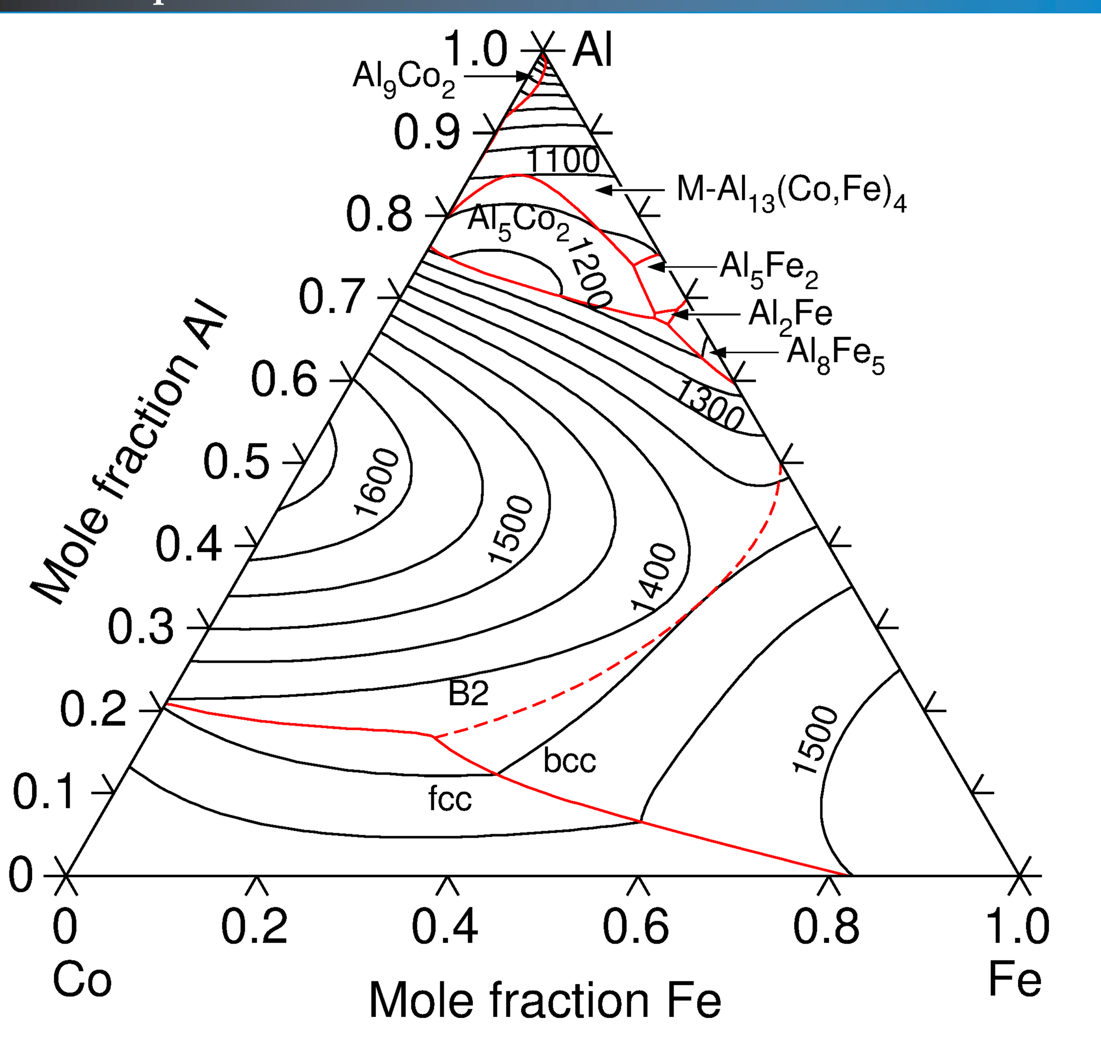

Figure 4: Liquidus projection over the whole composition range. All the temperatures are in °C.

Results: Isothermal sections of Al–Co–Fe

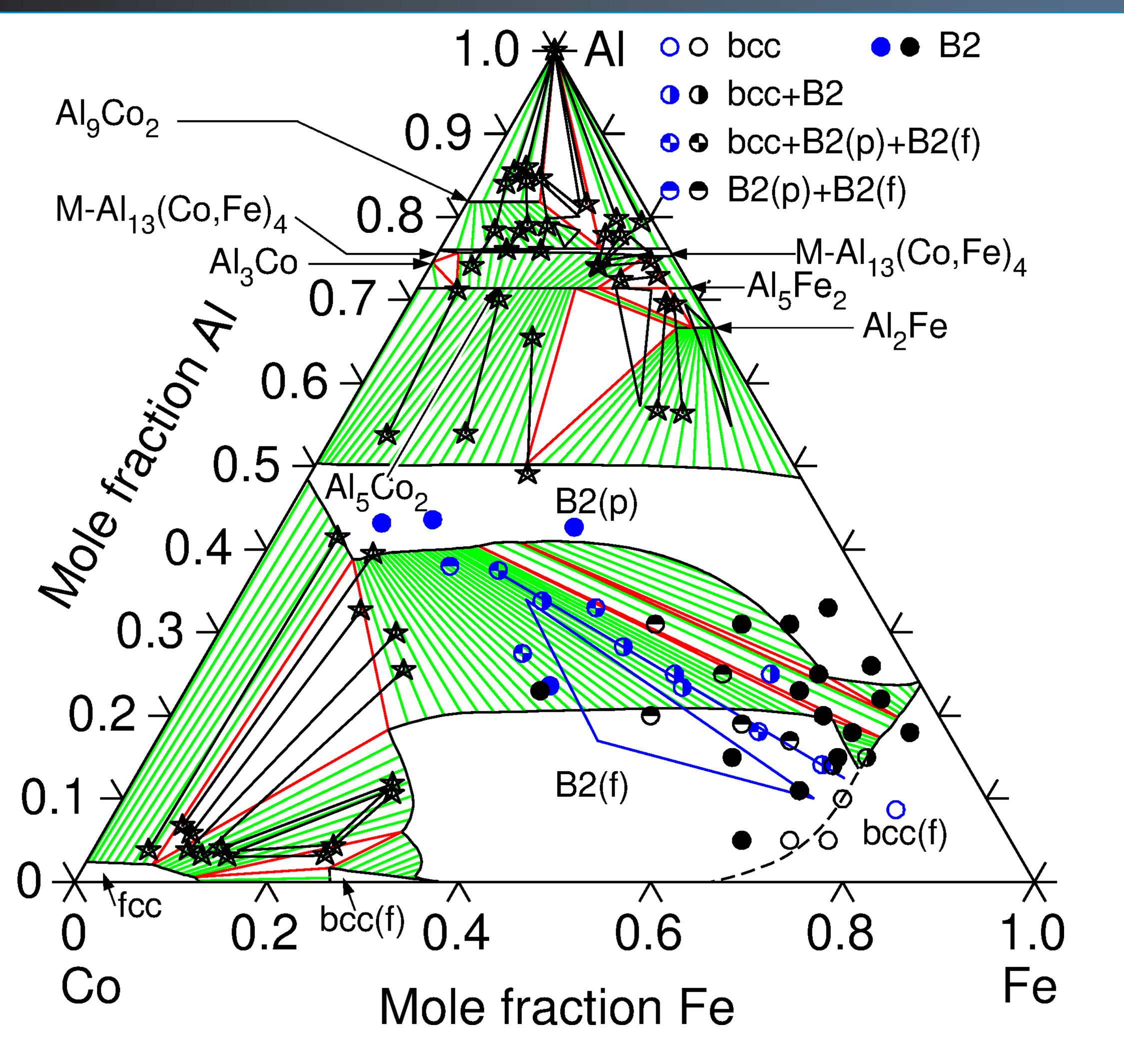

Figure 5: Isothermal section at 650 °C using experimental data from Kozakai et al. [4] (star symbols), Ackermann [5] (blue color), and Miyazaki et al. [6] (black circles).

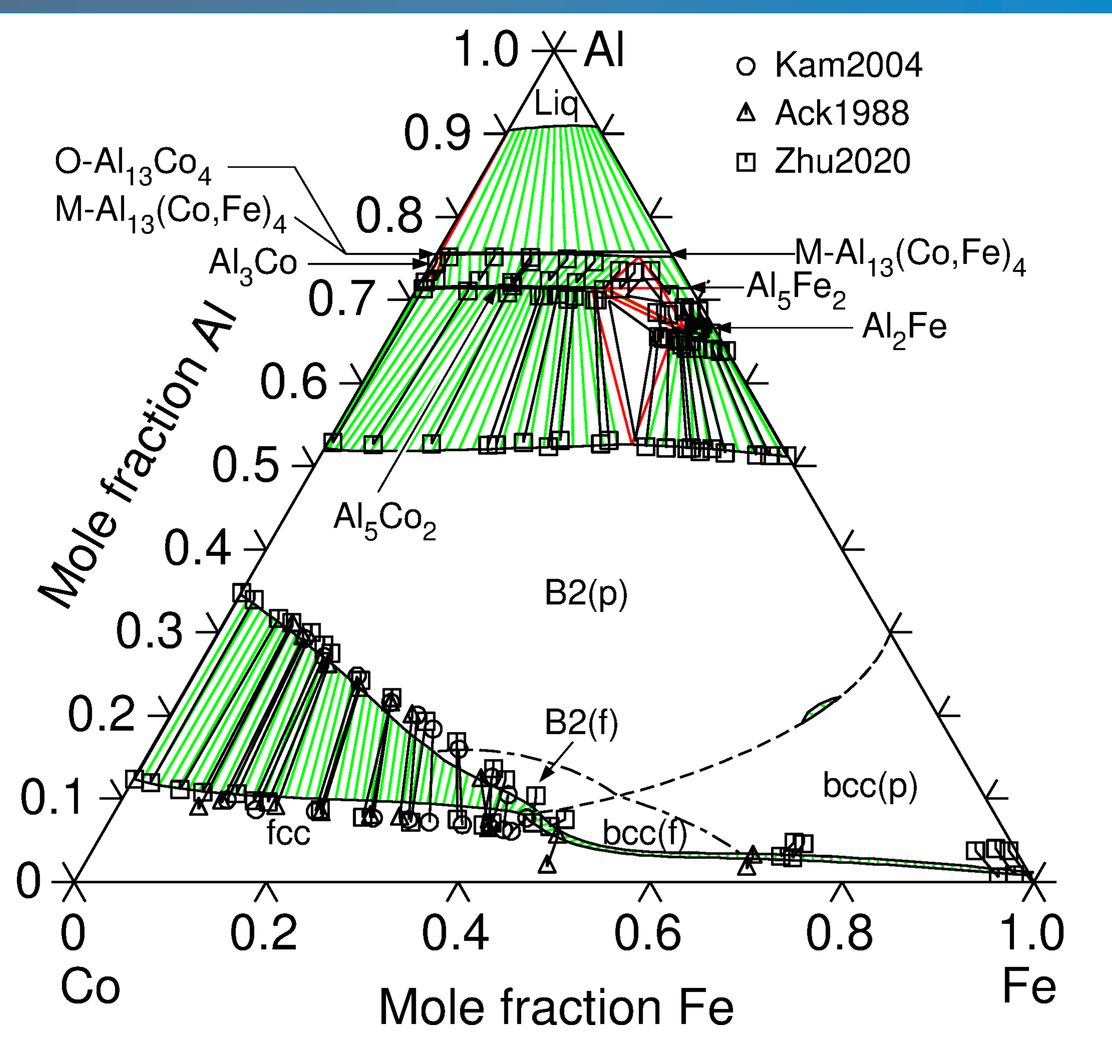

Figure 6: Isothermal section at 1000 °C using experimental data from Ackermann [5], kamiya et al. [7], and Zhu et al. [8].

Results: Vertical sections of Al–Co–Fe

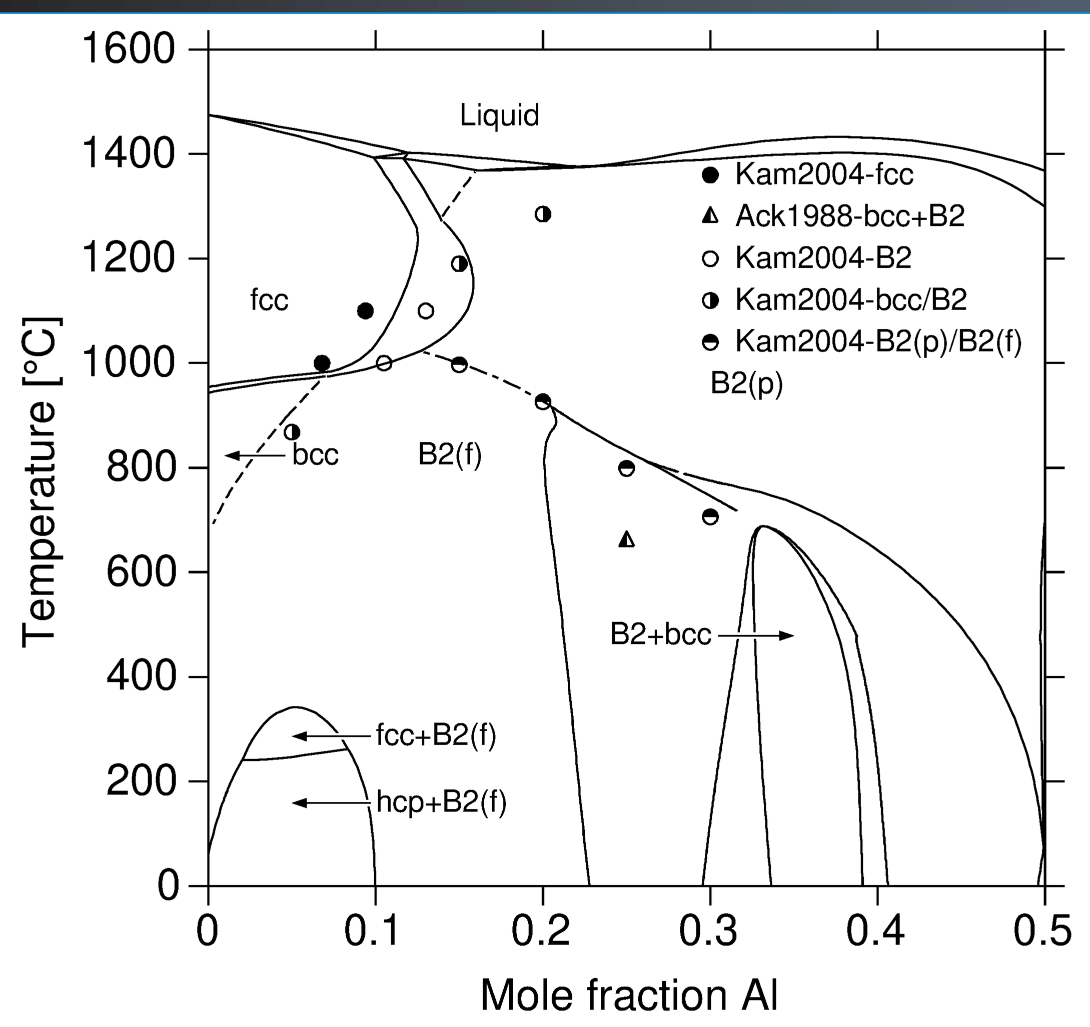

Figure 7: Vertical section at 40 at.% Fe with experimental data from Kamiya et al. [7] and Ackermann [5].

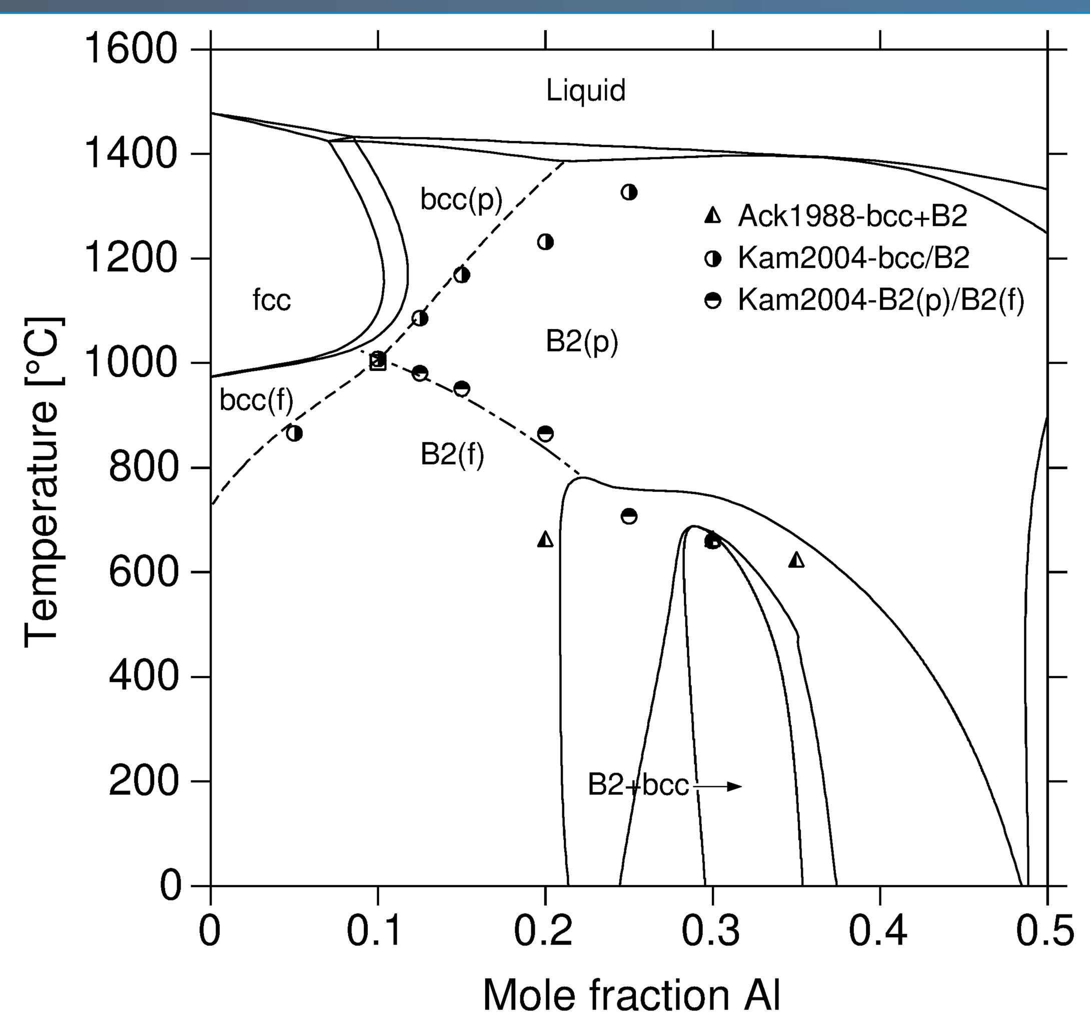

Figure 8: Vertical section at 50 at.% Fe with experimental data from Kamiya et al. [7] and Ackermann [5].

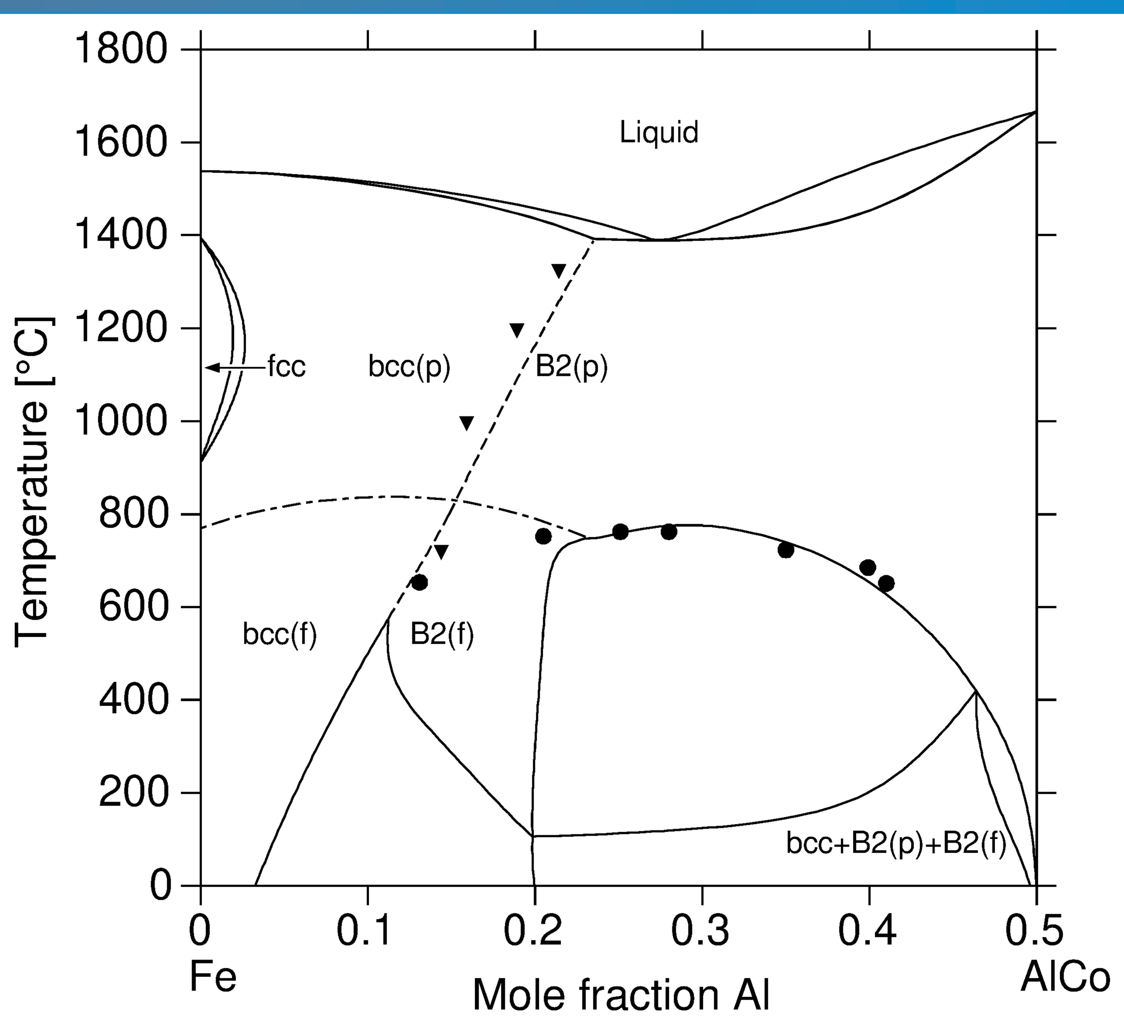

Figure 9: Vertical section from Fe to equiatomic AlCo with experimental data from Ackermann [5]. Triangle and circle indicate bcc/B2 transition and bcc+B2 miscibility gap.