Thermodynamic Assessment of a Hypothetical CrMnMo-based Ternary σ Phase

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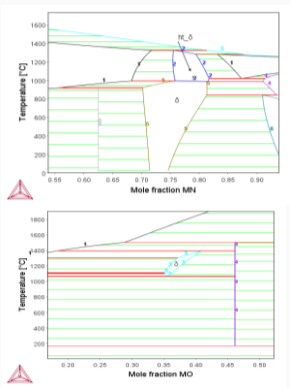
INTRODUCTION



The sigma phase has been of great interest to many scientist and engineers, owing this attention to its hard, brittle and thermally stable properties.

Although deleterious to stainless steel, they have become beneficial to enhancing the hardness of various HEA's. Especially ternary sigma phases as reported by [2].

From this perspective, we aim to model a ternary sigma phase to our Ti-Al based HEA which contains the following Pair Sigma-forming elements: Cr, Mn and Mo.

The forementioned PSFE components form a binary sigma phase in their sub-systems. However, the ternary system – CrMnMo has not yet been experimentally studied, or theoretically reported on.

It is the novelty of this work to predict a ternary hypothetical CrMnMo-based sigma phase. This objective is achieved by thermodynamic assessment of sub-binary systems of the CrMnMo and assessing the effects of Mn to the CrMo against an experimentally studied Fe-CrMo system.

MOTIVATION

- The sigma phase has shown superior properties in HEA systems by increasing hardness properties [2].
- The CrMnMo ternary sigma phase has not been reported or discussed either thermodynamically or experimentally in literature.
- The Cr, Mn and Mo elements fall within the Pair Sigma-forming Elements category, not different from the reported Fe-Cr-Mo ternary sigma phase.
- This work will provide one of the possible approaches to hypothetical phase modelling and further broadens the spectrum of the CALPHAD methodology to material's design.

FUTURE WORK

- Possible optimization of the CrMnMo system – Obtaining assessed thermodynamic parameters.
- Thermodynamic modelling/assessment of the Al-Cr-Mn-Mo quaternary system – to investigate the effects of Al to the stability of the CrMnMo sigma phase.

REFERENCES

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PRELIMINARY RESULTS

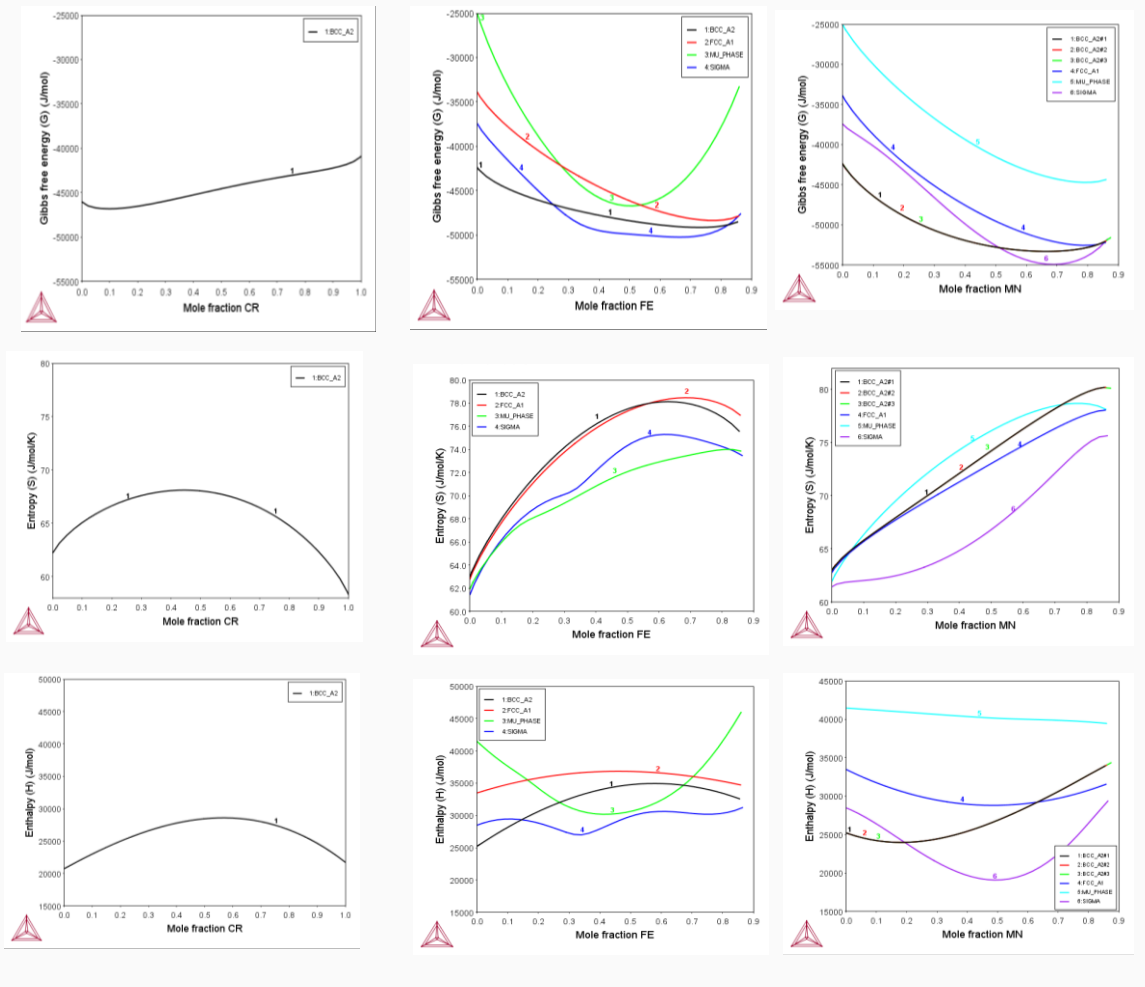
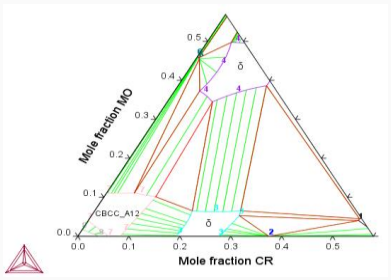


Fig. 1: Property diagrams comparing the effects of Fe and Mn addition to the CrMo binary system at 1073,15 K at 1atm. The left most diagrams show the Gibbs, Enthalpy and Entropy of the CrMo system. The middle diagrams show the thermodynamic properties of the Fe-CrMo system. The right most diagrams show the thermodynamic properties of the Mn-CrMo diagrams.

THERMODYNAMIC MODEL

- Full stoichiometric formula is for a sigma phase: $(A)_2^{12}(B)_4^{15}(C)_8^{12}(D)_8^{12}(E)_8^{14}$
- Three sublattice model which allows all elements to mix in each sublattice (SL1)10(SL2)4(SL3)16 [4].
- This three sublattice model covers the entire compositional range to yield: (A,D)10(B) 4(C,E)16 [5]
- CrMnMo sigma phase will be allowed to occupy each sublattice and the model is represented as: (Cr,Mn,Mo)10(Cr,Mn,Mo)4(Cr,Mn,Mo)16



Constitution	$(Cr,Mn,Mo)_{10}(Cr,Mn,Mo)_4(Cr,Mn,Mo)_{16}$	
	Constituent	*Site Fraction*
Sublattice 1:		
	Mn	0.88209
	Cr	0.11672
	Mo	0.00119
Sublattice 2:		
	Cr	0.74766
	Mn	0.13186
	Mo	0.12048
Sublattice 3:		
	Mn	0.82007
	Cr	0.15551
	Mo	0.02442

Fig. 2: Isothermal section of the hypothetical ternary sigma phase at 1073,15 K at 1atm on the left diagram. The diagram on the right shows the composition and thermodynamic model of the CrMnMo ternary sigma phase in this work