

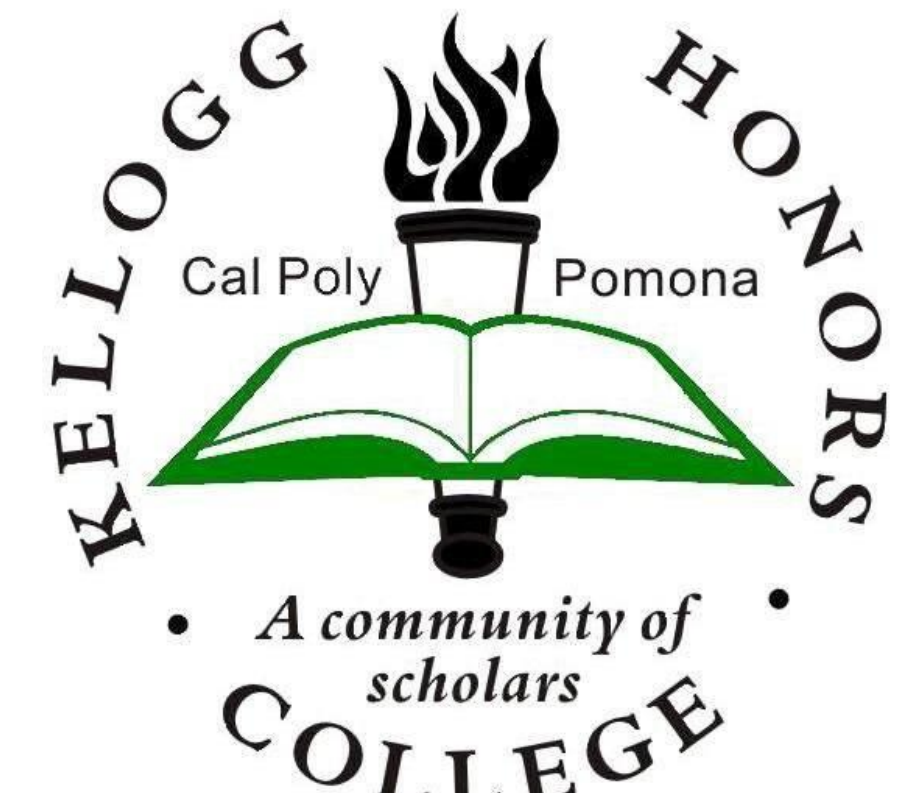
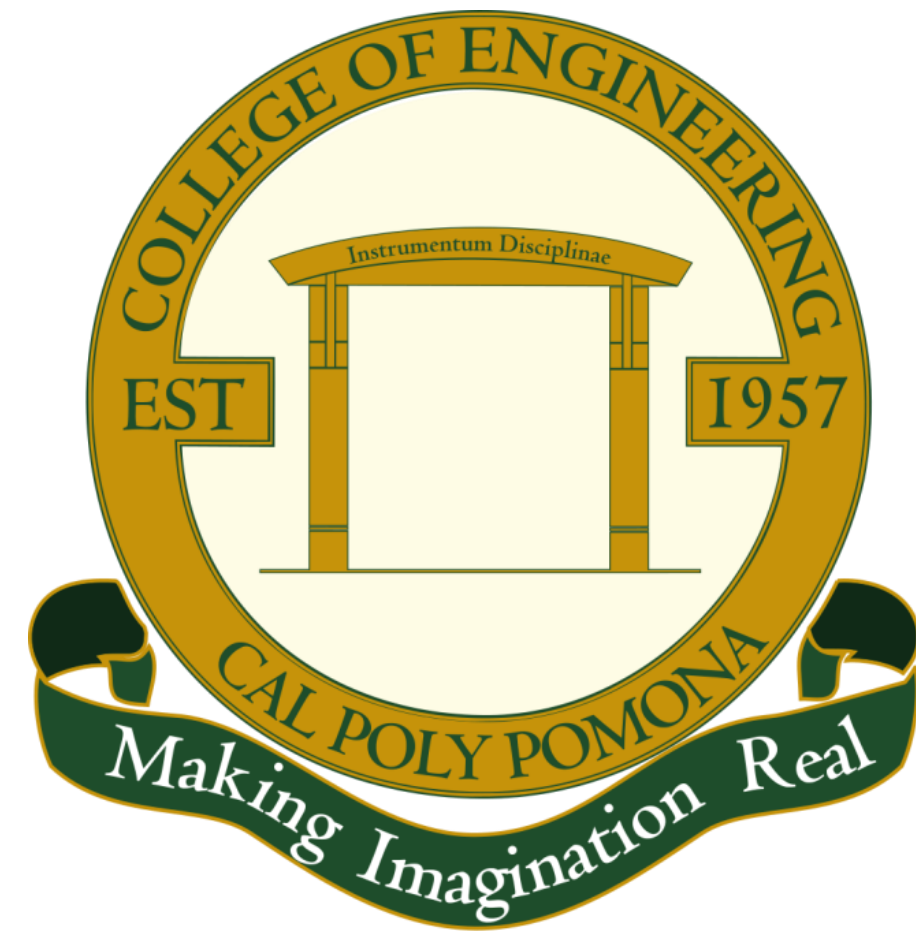
Thermodynamic Modeling of a Magnetic

Shape Memory Alloy System

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Kellogg Honors College Capstone Project



Objective: To model a complicated quaternary alloy system for alloy design purposes.

Background

Magnetic shape memory alloys (SMAs) are a class of metallic alloys that can sustain magnetically induced plastic deformation and then return to their original shape by mechanical deformation or upon heating via the pseudo-elastic effect (figure 1). These materials have the potential to become widespread in the next generation of mechanical actuators (figure 2) and biomedical implants.

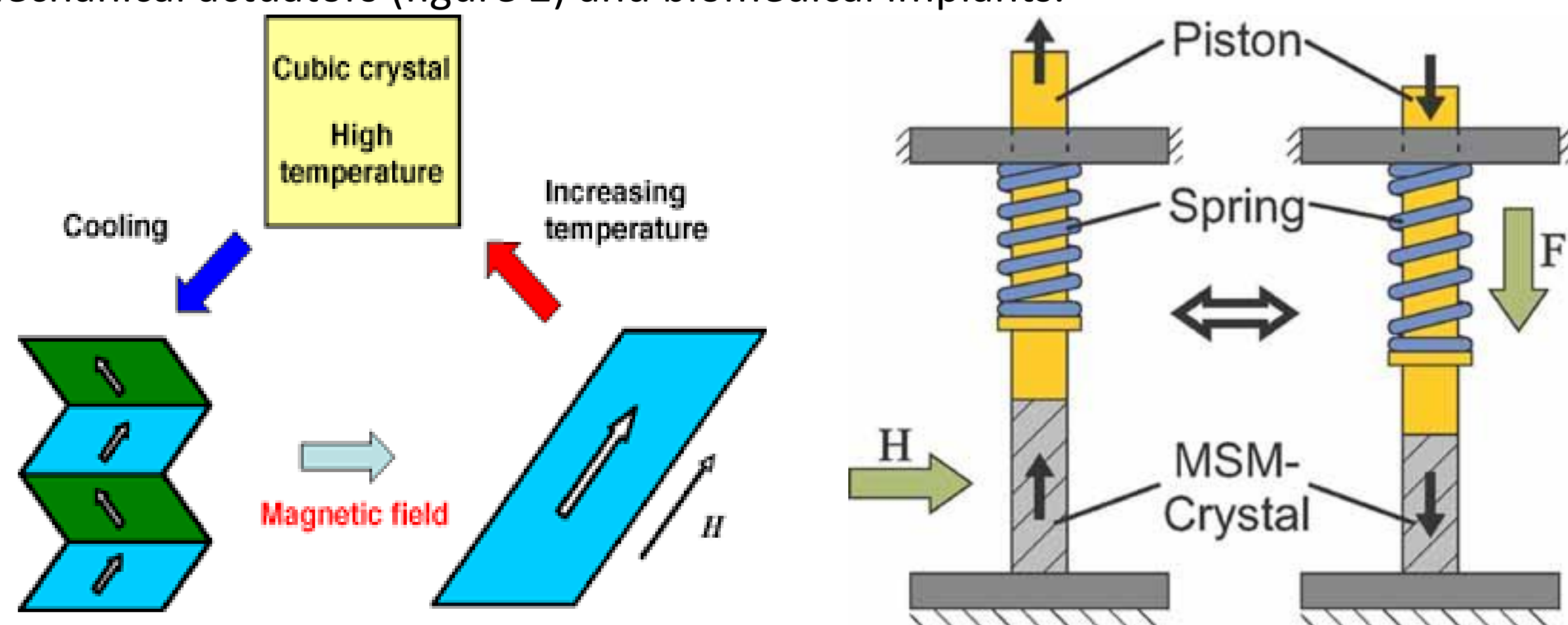


Figure 1. Magnetic shape-memory effect [8]

Figure 2. Example of Spring/MSM Actuator [9]

The mechanical and magnetic performance of these materials is to a large degree determined by the proportion of magnetic and reinforcing, shape-memory effect martensitic phases in the alloy microstructure.

In this study, we aggregated the thermodynamic data required to model the phase composition of alloys in the cobalt (Co) nickel (Ni) gallium (Ga) aluminum (Al) system. The phase diagrams produced using these data can be used to design alloys with finely tuned proportions of the crucial magnetic (β) and martensitic (γ) phases.

Method

Our modeling method utilizes standard computer calculation of phase diagram (CALPHAD) approaches (see figure 3). In this method, the behavior of different phases in multicomponent alloys can be predicted from the Gibbs energy associated with the different pure phases and the interactions between phases. The Gibbs energy functions G of a given phase α typically have a form

$$G^\alpha = G^\alpha(p, T, n_A, n_B, \dots) \quad (1)$$

where p is the system pressure, T is the temperature, and the n_i are the amounts of the different components in the phase. These functions (neglecting p) are typically expressed as the sums of individual G^α terms for the components (A, B, ...) and their interactions (A:B, ...):

$$G^\alpha = G_A^\alpha(T) + G_B^\alpha(T) + G_{A:B}^\alpha(T) + \dots \quad (2)$$

where the functions are typically linear in T . These functions are then solved using the principles of phase equilibria to determine the phases present across compositions and temperatures.

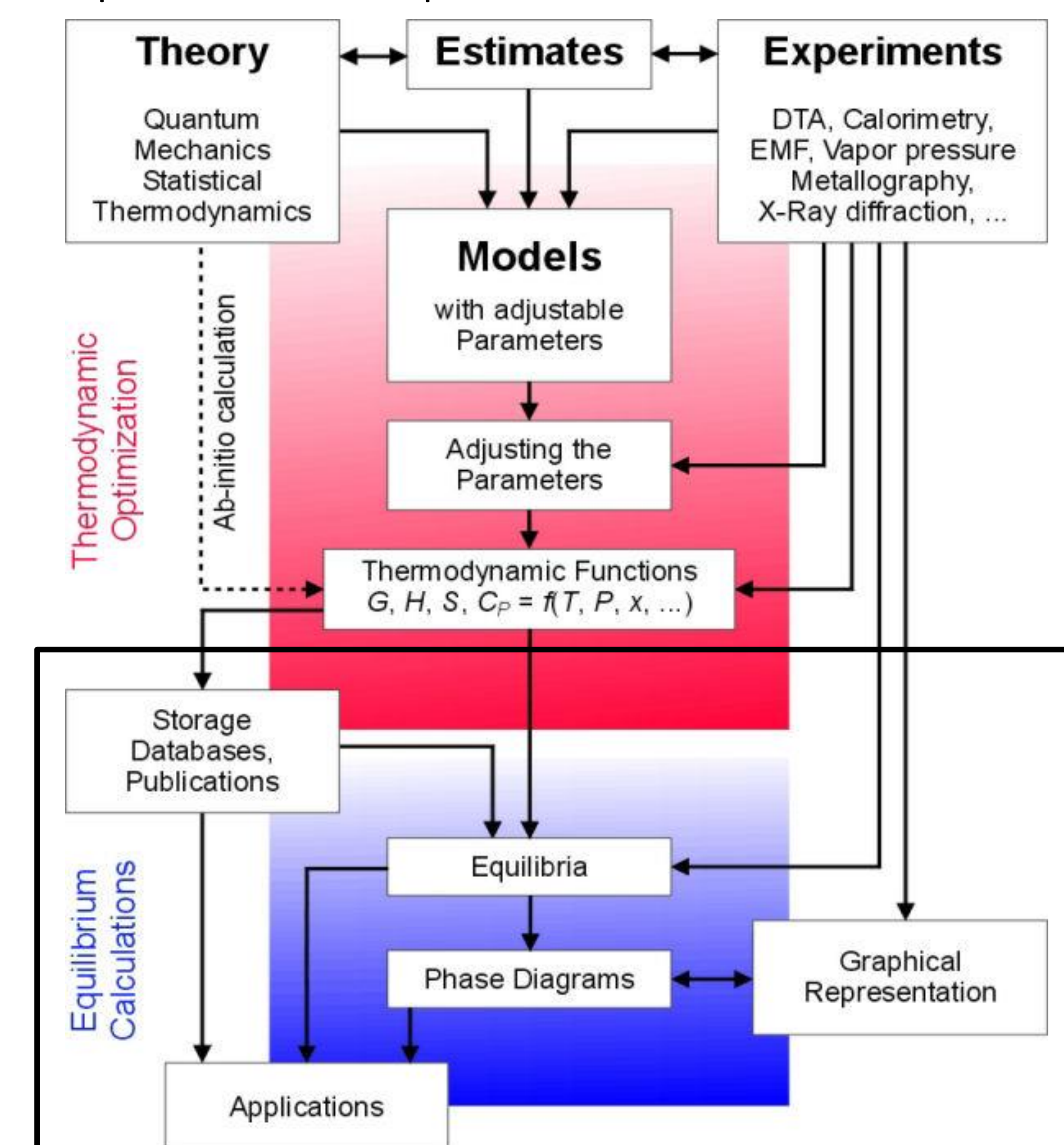


Figure 3: Focus of study within the CALPHAD approach [5]

We aggregated the Gibbs energy functions for the phases in the CoNiGaAl alloy system from literature sources [1–4] and published databases [5, 6], and then constructed a custom database containing the formatted functions. We then used the Thermo-Calc [7] CALPHAD software package to compute and generate the binary and ternary phase diagrams of interest.

Results

Examples of the results of the CALPHAD calculations are shown below.

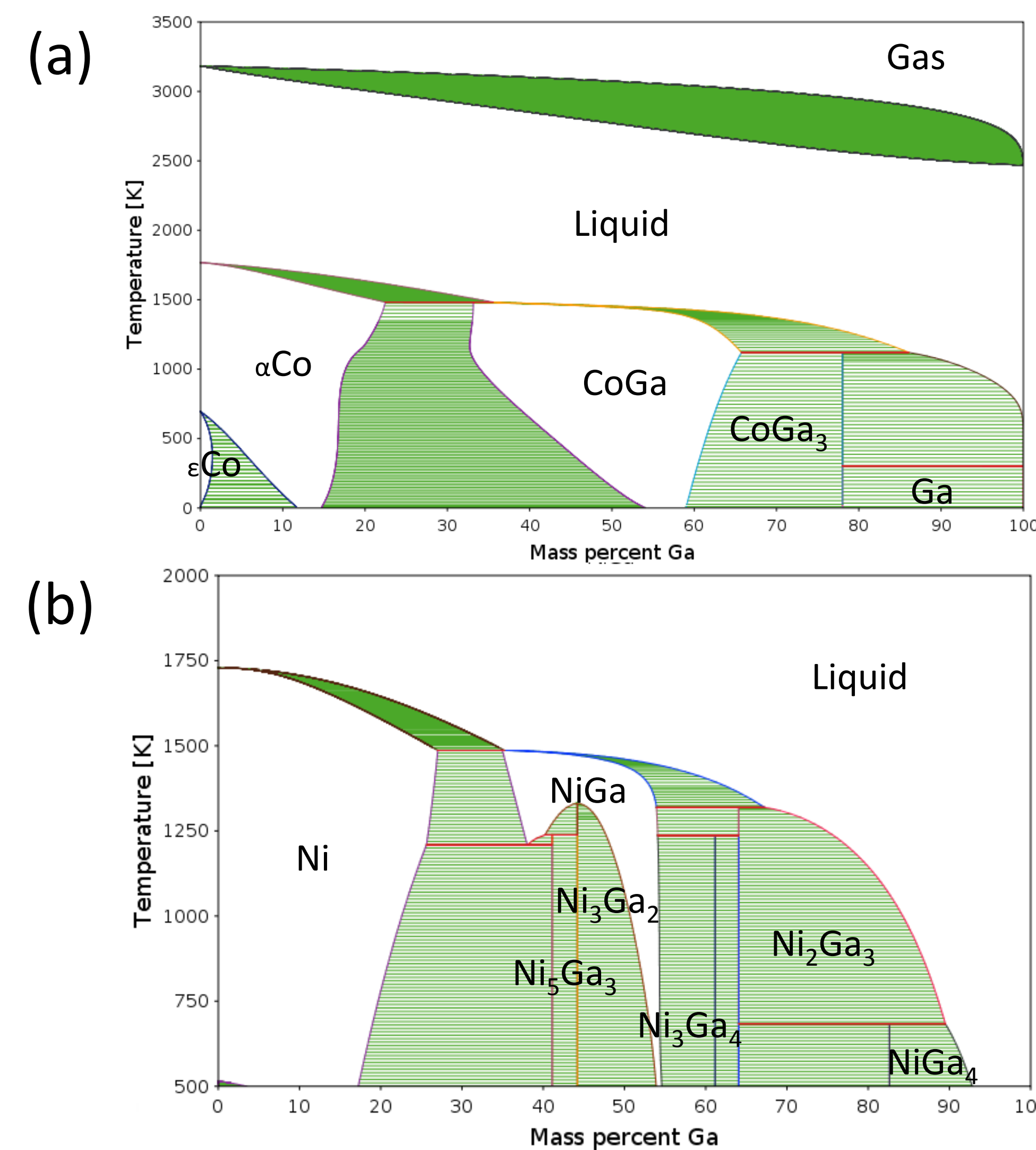


Figure 4. Binary phase diagrams for (a) CoGa and (b) NiGa.

Figure 4 shows two of the six constituent binary systems of the CoNiGaAl quaternary system, the CoNi and NiGa systems. By synthesizing the Gibbs energy functions of these systems, the CoNiGa ternary system database was created, as shown figure 5. Note the subtle differences caused the addition of a third constituent; for example, the presence of CoGa_3 phase in figure 4(a) and 5(a) at a temperature of 700° Celsius.

The CoNiGa ternary diagrams reveal that as you increase the temperature, the stoichiometric compounds begin to vanish as the magnetic β phase begins to grow. However, as the temperature continues to rise, the liquid phase begins to grow as well, decreasing the size of the desired β region. Therefore, an optimum temperature exists between 700°C and 1200°C, which would minimize the presence of stoichiometric compounds and promote the formation of the desired magnetic β phase.

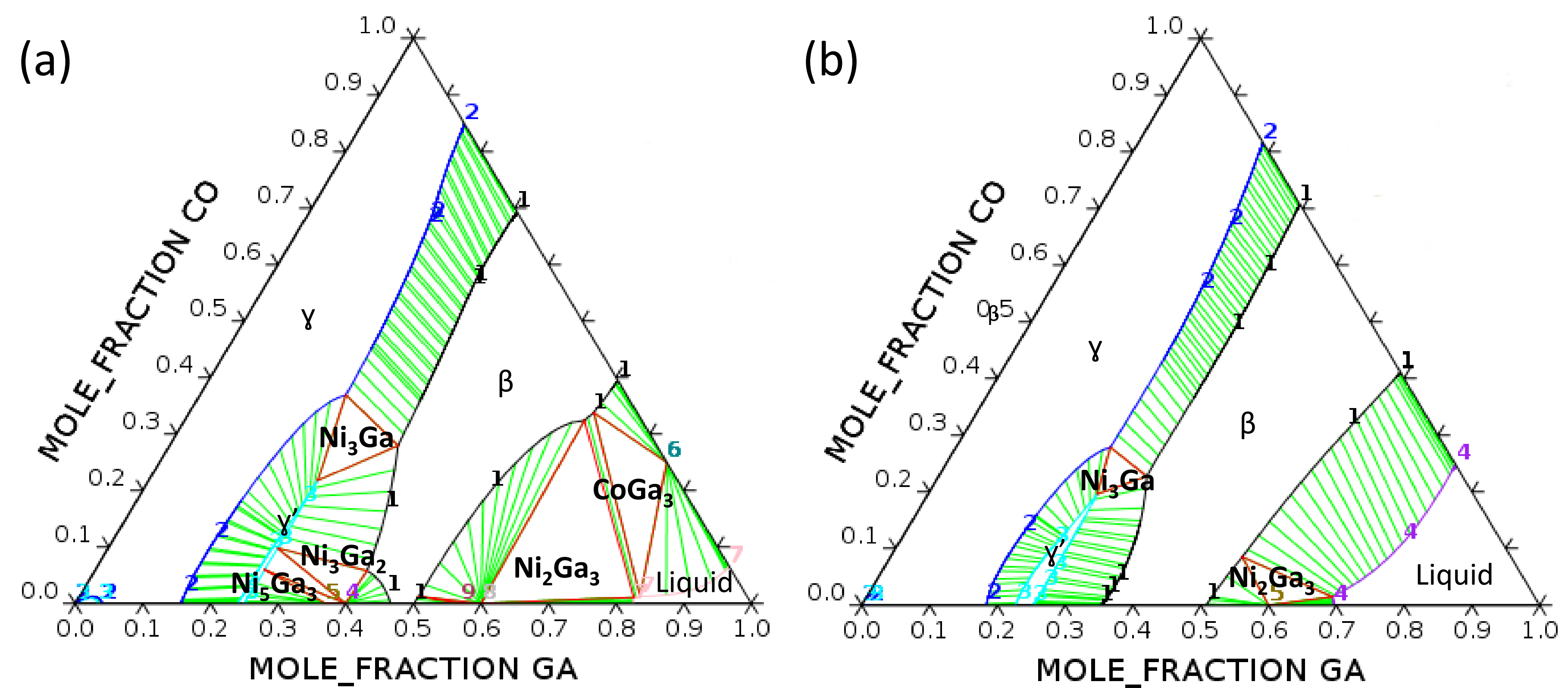


Figure 5. CoNiGa ternaries phase diagrams at (a) 700 °C and (b) 1000 °C.

There is a discrepancy in figure 5(b) when compared to published literature [1]. According to Chari, at 1000°C the liquid and the Ni_2Ga_3 regions should have receded and replaced by a larger β phase.

Conclusion

We created a database of thermodynamic data describing phases present in the CoNiGaAl quaternary alloy system. Using these data and the CALPHAD method, we constructed phase diagrams for the NiGa, CoGa, CoNi, NiAl, AlCo, GaAl, and CoNiGa subsystems. These phase diagrams can be used in the design of SMAs containing magnetic phases. We can trace the development of the different phases during alloy solidification and cooling, expanding our understanding of microstructure development for many alloy compositions in this important system. Future work involves the database compilation of the functions required for the NiGaAl, NiCoAl, and CoAlGa subsystems. Once this work is completed, all of the data required to model the full CoNiGaAl quaternary system will be available.

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Acknowledgements

I would like to thank Dr. Jonathan Puthoff and the Department of Chemical Engineering for their continued academic and financial support throughout this project. I would also like to acknowledge Mr. Paul Mason at Thermo-Calc Software Inc. for his assistance in learning the CALPHAD process, as well as the Kellogg Honors College for providing this research opportunity.