Plotting Binary Phase Diagrams Using CALPHAD Software

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1. Introduction

Calculation of phase diagrams is central to the practice of materials thermodynamics. This study plots the binary phase diagram of the nickel-aluminum (Ni-Al) system and nickel-copper system (Ni-Cu) using CALPHAD software using thermodynamic database (.tdb) files publicly available in the SGTE collection of binary datasets [1]. This study demonstrates the ability to plot a .tdb file, which will ultimately be used to plot the binary phase diagram for the Ni-Be system, whose thermodynamic database is not publicly available in the SGTE collection.

This study is Part V of an ongoing materials thermodynamics project being completed for the Fall 2025 session of MTEN 6005 taught by Dr. Eric Payton. The overall objective of this project is to generate a thermodynamic database (i.e. a .tdb file) that can be used to calculate the phase diagram of a binary system not publicly available in the SGTE collection of binary datasets. Parts I through III focused on thermodynamic principles necessary to calculate unary phase diagrams and Part IV focused on selecting a binary system to generate a thermodynamic database for.

2. Methods

To plot the Ni-Al and Ni-Cu binary phase diagrams of interest, it was necessary to source .tdb files for each alloy system. The Ni-Al .tdb file used for plotting was generated based on the results of Dupin et al. during their re-assessment of the Al-Cr-Ni system [2]. The Ni-Cu .tdb file used for plotting was generated based on the results of Mey during their re-assessment of the Ni-Cu alloy system [3]. Both .tdb files were sourced from the SGTE collection of publicly available binary datasets.

In addition to sourcing a .tdb file, a CALPHAD software was selected to calculate the phase diagram based on the thermodynamic database. For this study, Pandat 2025 was selected as the CALPHAD software used for its straightforward user interface and ability to plot .tdb files within their free version of the software. Pandat's "Section Calculation" tool was specifically used to calculate the binary phase diagram of interest [4]. The Ni-Al binary phase diagram was calculated from 300–1700°C and from 0–100 at% Ni. To assess the phase diagram calculated within Pandat, the results are compared to the calculated phase diagram published by Dupin et al. The Ni-Cu binary phase diagram was calculated from 1000–1500°C and from 0–100 at% Ni. To assess the phase diagram calculated within Pandat, the results are compared to the calculated phase diagram published by Mey.

3. Results

Figure 1 and Figure 2 illustrate the Ni-Al and Ni-Cu binary phase diagrams, respectively, calculated using Pandat.

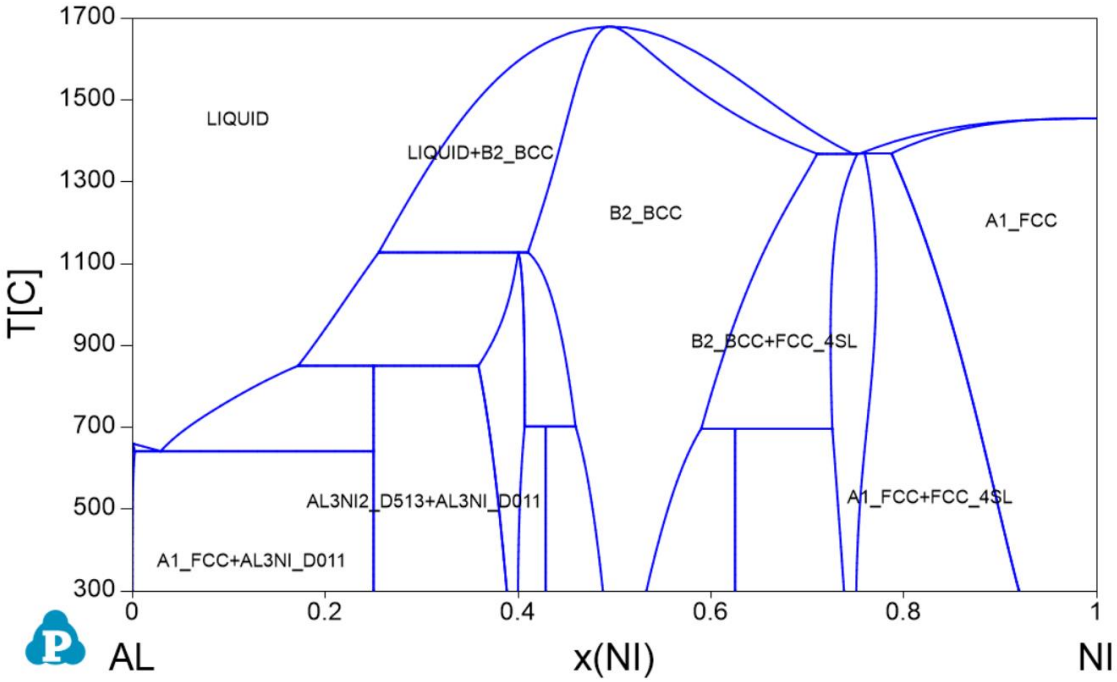

Figure 1. Calculated Ni-Al binary phase diagram.

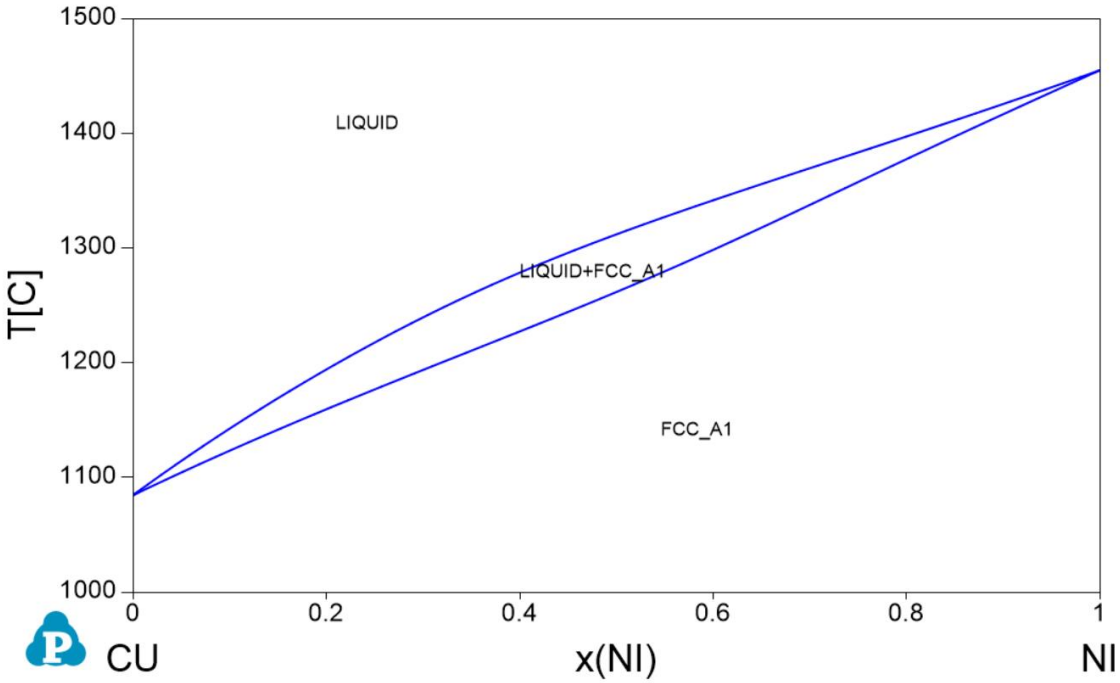

Figure 2. Calculated Ni-Cu binary phase diagram.

4. Discussion

Figure 3 illustrates the Ni-Al phase diagram calculated by Dupin et al. (solid lines) compared to the experimental data used to calibrate the calculated thermodynamic models (solid dots). Comparing Figure 3 to Figure 1, there is a clear agreement between the phase diagrams, which is expected because they are both calculated using the same thermodynamic models.

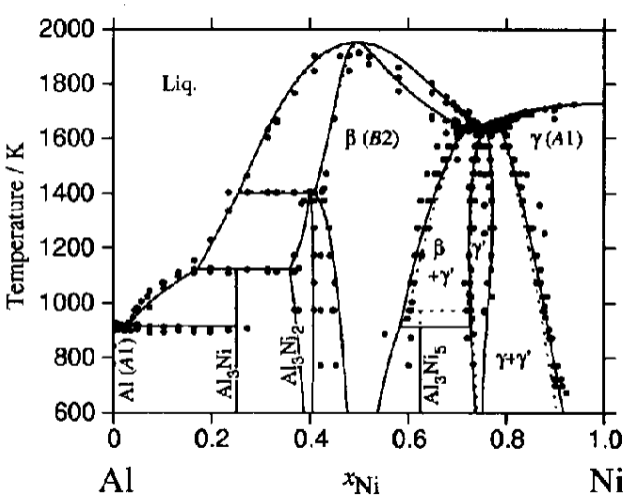

Figure 3. Ni-Al binary phase diagram calculated by Dupin et al. *Reproduced from Figure 1 of [2].*

Figure 4 illustrates the Ni-Cu phase diagram calculated by Mey (solid lines) compared to the experimental data used to calibrate the calculated thermodynamic models (points). Comparing Figure 4 to Figure 2, there is a clear agreement between the phase diagrams, like the Ni-Al system. The strong agreement between established phase diagrams and phase diagrams plotted in Pandat confirm that the phase diagrams calculated within Pandat are accurate and the software is being used correctly. Therefore, once a .tdb file is created for the Ni-Be system, the procedure implemented in this study can be used to produce the Ni-Be binary phase diagram.

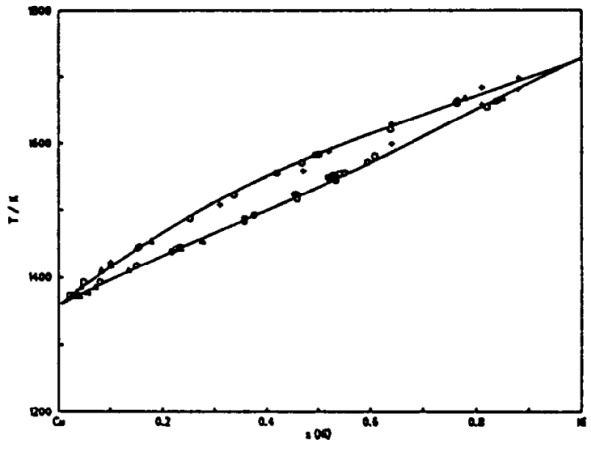

Figure 4. Ni-Cu binary phase diagram calculated by Mey. Phase diagram plotted from 1200-1800 K and 0-1 atomic fraction of Ni. *Reproduced from Figure 1 of [3].*

5. Conclusion

This study plotted the Ni-Al and Ni-Cu binary phase diagram to demonstrate calculating a binary phase diagram using a .tdb file and CALPHAD software. In this study, a binary systems whose thermodynamic databases are publicly available in the SGTE collection of binary datasets were selected. This procedure used to plot these binary phase diagrams using a .tdb file and CALPHAD software will ultimately be extended to plot the binary phase diagram for the Ni-Be system, whose thermodynamic database is not publicly available in the SGTE collection.

References

[1] B. Hallstedt, “The SGTE collection of binary datasets,” *Calphad*, vol. 89, p. 102833, Jun. 2025, doi: https://doi.org/10.1016/j.calphad.2025.102833.

[2] N. Dupin, I. Ansara, and B. Sundman, “Thermodynamic re-assessment of the ternary system Al-Cr-Ni,” *Calphad*, vol. 25, no. 2, pp. 279–298, Jun. 2001, doi: https://doi.org/10.1016/s0364-5916(01)00049-9.

[3] S. an Mey, “Thermodynamic re-evaluation of the Cu□Ni system,” *Calphad*, vol. 16, no. 3, pp. 255–260, Apr. 2003, doi: https://doi.org/10.1016/0364-5916(92)90022-P.

[4] “Section Calculation (2D),” *Computherm.com*, 2025. https://computherm.com/Pandat_OnlineHelp/Content/3-PanPhaseDiagram/3_Tutorial/3_Section%20Calculation%20(2D).htm (accessed Nov. 12, 2025).