**Choosing a Binary System**

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## 1. Introduction

Calculation of phase diagrams is central to the practice of materials thermodynamics. This study evaluates several binary systems featuring nickel (Ni) to determine which Ni binary system to create a thermodynamic database for. A key requirement for the binary systems evaluated, and the binary system ultimately selected, is that the system's binary phase diagram is not already published in the SGTE collection of publicly available binary datasets [1].

This study is Part IV 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 that can be used to calculate the phase diagram of a binary system not publicly available in the SGTE collection of binary datasets [1]. Parts I through III focused on thermodynamic principles necessary to calculate unary phase diagrams. As mentioned, Part IV is focused on selecting a binary system that will be used for the remainder of the project.

## 2. Methods

The process of selecting a binary system began by identifying Ni binary systems that met the project requirements. The requirements are listed below:

(1) Element pair must not have a database already available from the SGTE collection of binary datasets.
(2) Element pair must not be normally immiscible in both the solid and liquid states.
(3) Both elements must be naturally occurring (atomic number less than or equal to 94).

Using requirements (1) and (3), an initial search space for Ni binary systems was established. To check for immiscibility, the ASM Handbook of Alloy Phase Diagrams was referenced [2]. From the phase diagrams included in ASM Handbook, solubility is confirmed based on the existence of phases made up of both elements in the element pair. Table 1 summarizes these results.

**Table 1.** Initial Search Space for Viable Ni-Binary System Element Pairs

| Not Available in SGTE Collection | Phase Diagram Published in ASM Handbook |
|---|---|
| Ni – Am | No |
| Ni – Be | Yes |
| Ni – Br | No |

**Table 1 continued.** Initial Search Space for Viable Ni-Binary System Element Pairs

| Not Available in SGTE Collection | Phase Diagram Published in ASM Handbook |
|---|---|
| Ni – Cd | Yes |
| Ni – Cl | No |
| Ni – Cs | No |
| Ni – F | No |
| Ni – Hg | No |
| Ni – I | No |
| Ni – K | No |
| Ni – Lu | No |
| Ni – Na | No |
| Ni – Np | No |
| Ni – Pu | Yes |
| Ni – Rb | No |
| Ni – S | Yes |
| Ni – Tl | No |
| Ni – Tm | No |

Of the eighteen Ni binary system element pairs not included in the SGTE collection, only four element pairs had published phase diagrams – beryllium (Be), cadmium (Cd), plutonium (Pu), and sulfur (S). All four elements exhibited solubility in Ni based on their phase diagrams.

For these four elements, their Ni binary phase diagram was found within the online Materials Platform for Data Science (MPDS) published by ASM International [3]. Using the references published within the MPDS database, the feasibility of generating a system's thermodynamic database was evaluated based on the experimental data published for each binary system.

## 3. Results

Figures 1-4 are the binary phase diagrams of the four element pairs not included in the SGTE collection and accessible within the MPDS database [4-7]. Each of these phase diagrams are a reproduction and digitization of phase diagrams originally published in the Bulletin of Alloy Phase Diagrams [4-6], or the International Journal of Materials Research [7], by ASM International for the MPDS database. All of the binary systems presented include predictions about the formation of several phases, indicating solubility between the two elements and, therefore, meet requirement (2) of the project.

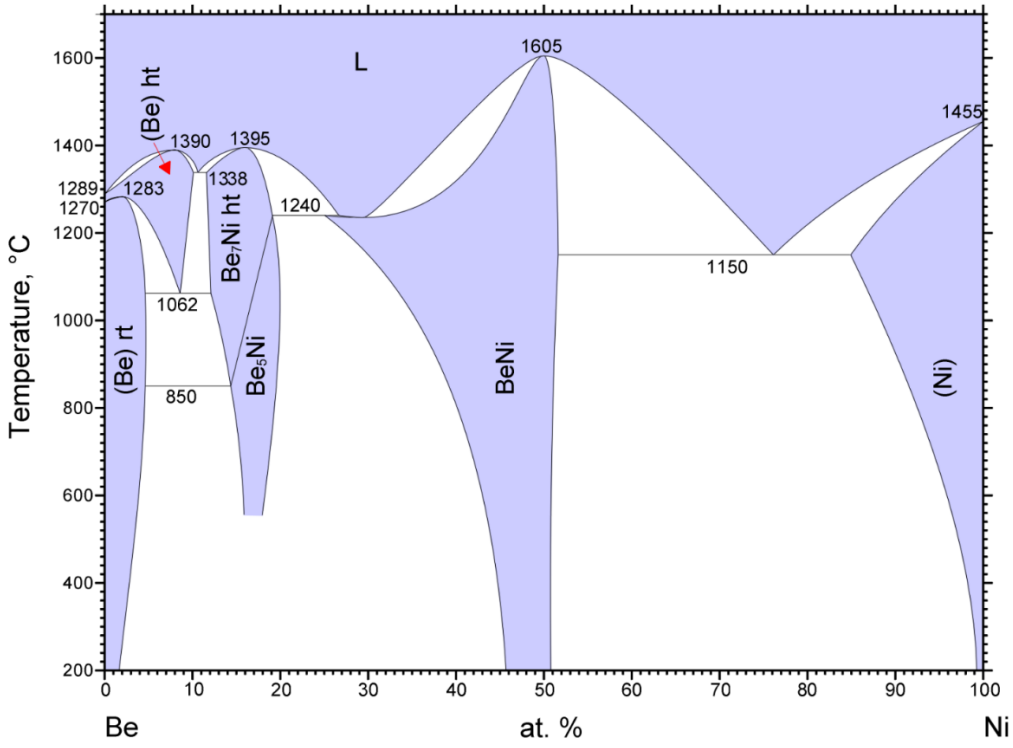


**Figure 1.** Be-Ni Phase Diagram. Reproduced from [4].

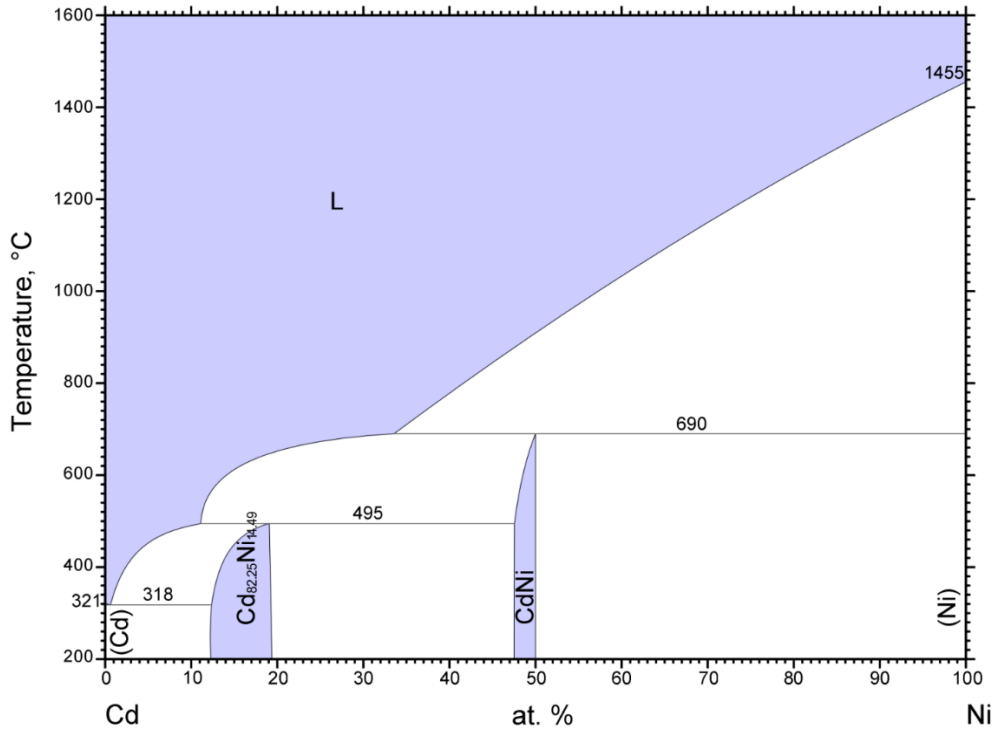


**Figure 2.** Cd-Ni Phase Diagram. Reproduced from [5].

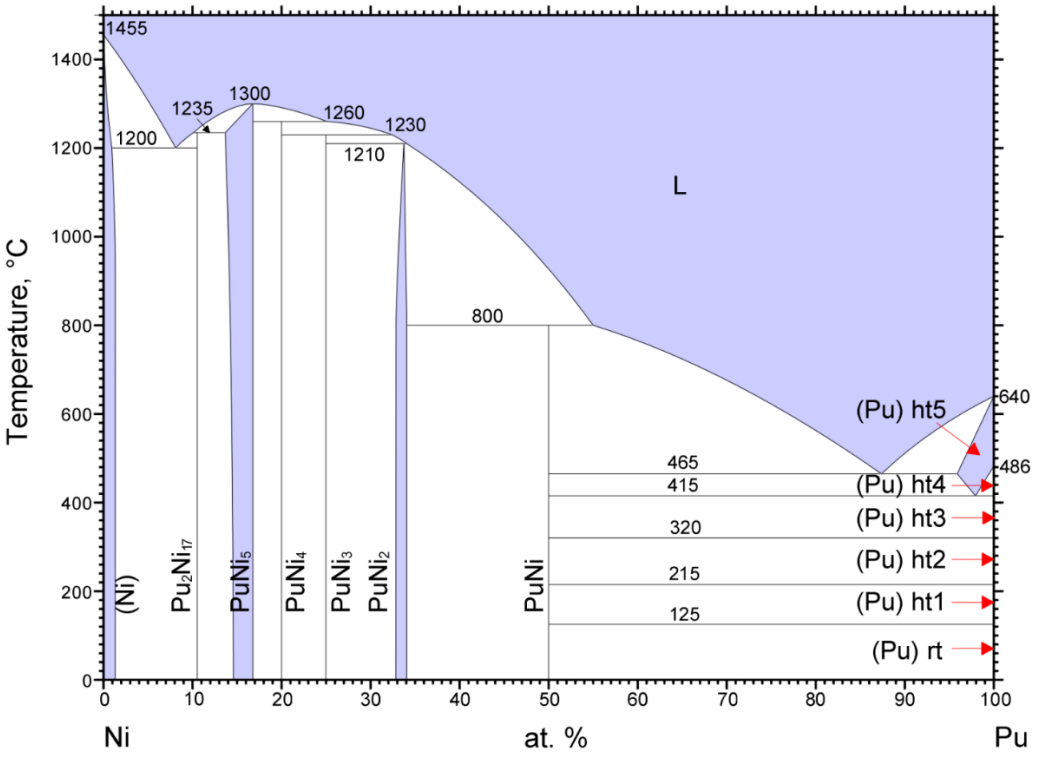


**Figure 3.** Ni-Pu Phase Diagram. Reproduced from [6].

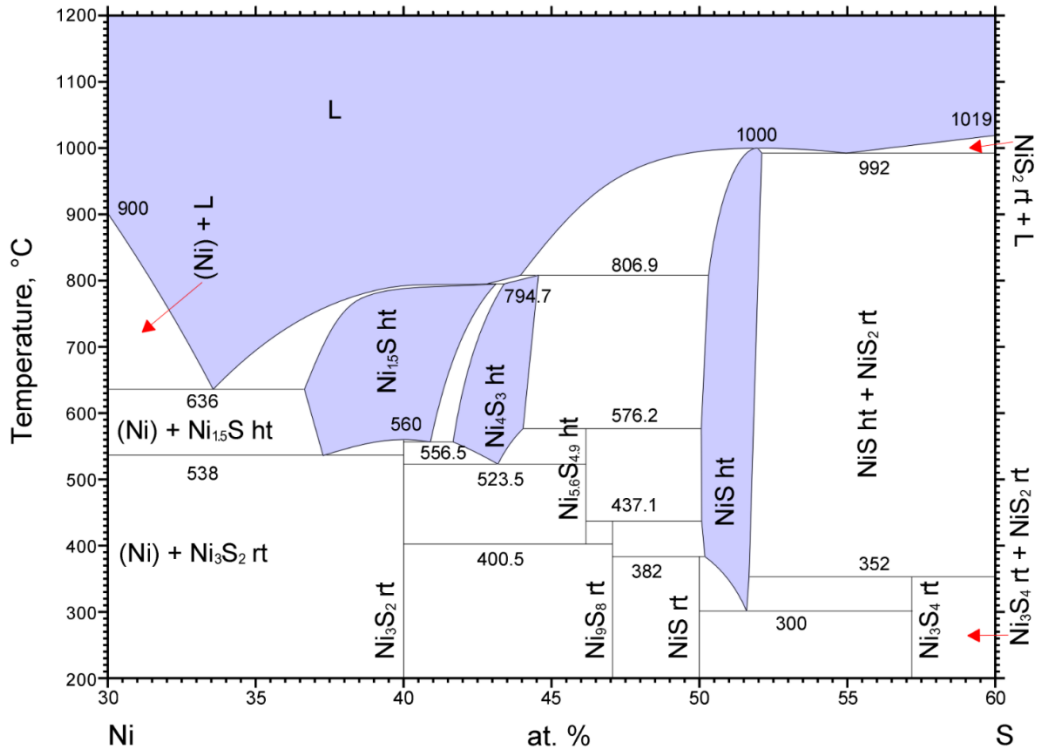


**Figure 4.** Ni-S Phase Diagram. Reproduced from [7].

Alongside the phase diagrams, the references used by MPDS have published additional thermodynamic data relevant to the evaluation of their respective phase diagrams. This data ranged from the crystal structure of each phase, lattice parameter data of each phase, the temperature and composition of special reactions in the phase diagram, and the temperature and composition of different phase boundaries [4-6]. This experimental data was used to evaluate the phase diagram by curve-fitting solution models to experimental data and then evaluating the phase diagram across the temperature and composition ranges of interest. Figure 5-7 provide examples of different forms of thermodynamic data published for the Be-Ni system used to calculate the Be-Ni phase diagram shown in Figure 1 [4].

**Table 2 Solvus Boundaries of Be-Ni (βBe), (αBe), γ, and β Phases**

| Reference | Temperature, °C | Composition, at.% Ni (αBe) | (βBe) | | γ | | β | Method |
|---|---|---|---|---|---|---|---|---|
| [50Kau] | 1050 | 1.3 to 1.7 | ... | ... | ... | ... | ... | Metallographic |
| [59Gel] | 1202 ± 2 | 3.74 ± 0.08 | ... | ... | ... | ... | ... | Diffusion couple |
| | 1162 | 4.10 | ... | ... | ... | ... | ... | |
| | 1103 ± 3 | 4.64 ± 0.08 | ... | ... | ... | ... | ... | |
| | 999 ± 1 | 4.62 ± 0.02 | ... | ... | ... | ... | ... | |
| | 900 | 4.43 ± 0.11 | ... | ... | ... | ... | ... | |
| | 1200 | ... | 5.78 | 9.18 | ... | ... | ... | |
| | 1102 | ... | 7.67 | 8.48 | ... | ... | ... | |
| [62Amo] | 300 | 0.23 | ... | ... | ... | ... | ... | Lattice parameter |
| [80Fri](a) | 1050 | 4.5 | ... | ... | 12.8 | 20 | 34 | Metallographic |
| | 750 | 4.2 | ... | ... | 15 | 18.5 | 41 | |

**Note:** See Table 1 for the data obtained by thermal analyses. (a) From graph.

**Figure 5.** Example Thermodynamic Data. Solvus Boundaries of the Be-Ni System. Reproduced from [4].

**Table 4 Special Points of the Assessed Be-Ni Phase Diagram**

| Reaction | Compositions of the respective phases, at.% Ni | | Temperature, °C | Reaction type |
|---|---|---|---|---|
| L ↔ βBe | 0 | | 1289 ± 5 | Melting |
| L ↔ (βBe) 8 | | | 1390 | Maximum melting |
| βBe ↔ αBe | 0 | | 1270 ± 6 | Allotropic |
| (βBe) ↔ (αBe) | 2 | | 1283 | Maximum transition |
| (βBe) ↔ (αBe) + γ 8.5 | 4.5 | 12 | 1062 | Eutectoid |
| L ↔ (βBe) + γ 10.5 | 10 | 11.5 | 1338 | Eutectic |
| L ↔ γ | 16 | | 1395 | Congruent |
| γ ↔ γ′ | 14 to ? | | ... | Order-disorder |
| L + γ ↔ β 26.5 | 19 | 25 | 1240 | Peritectic |
| L ↔ β | 29.5 | | 1236 | Minimum melting |
| L ↔ β | 50 | | 1605 | Maximum melting |
| L ↔ β + (Ni) 76.2 | 51.6 | 85 | 1150 | Eutectic |
| L ↔ Ni | 100 | | 1455 | Melting |

**Figure 6.** Example Thermodynamic Data. Special Reactions in the Be-Ni System. Reproduced from [4].

**Table 6 Be-Ni Crystal Structure Data**

| Phase | Composition, at.% Ni | Pearson symbol | Space group | Strukturbericht designation | Prototype |
|---|---|---|---|---|---|
| (βBe) | 0 to 4.9 | *cI*2 | $Im\bar{3}m$ | *A*2 | W |
| (αBe) | 0 to 10 | *hP*2 | $P6_3/mmc$ | *A*3 | Mg |
| γ | 11.5 to >14 | *cI*52 | $I\bar{4}3m$ | $D8_{1\text{-}3}$ | $Ni_5Zn_{21}$ |
| γ′ | 14 to 20 | *cF*416 | *F*23 | ... | ... |
| β | 25 to 51.6 | *cP*2 | $Pm\bar{3}m$ | *B*2 | CsCl |
| (Ni) | 85 to 100 | *cF*4 | $Fm\bar{3}m$ | *A*1 | Cu |
| **Metastable phases** | | | | | |
| ? | 64.5 to 68.5 | *o*** | ? | ... | |
| β′ | >50 to <75 | *tI** | ? | ... | ... |
| γ′ | 75 | ? | ? | ? | ? |

**Figure 7.** Example Thermodynamic Data. Be-Ni Crystal Structures. Reproduced from [4].

Table 2 summarizes the experimental data found published for the Be-Ni, Cd-Ni, Ni-Pu, and Ni-S binary systems.

**Table 2.** Experimental Data Found for Ni-Binary System Element Pairs

| Binary System | Experimental Data Found |
|---|---|
| Ni – Be [4] | • Liquidus and solidus temperature for varying at. % Ni<br>• Solvus boundaries of secondary phases<br>• Solubility of Be in Ni and different temperatures<br>• Temperature and composition of special reactions<br>• Crystal structure of phases<br>• Lattice parameters of phases<br>• Curie temperature of Ni phase<br>• Lattice stability parameter and excess Gibbs energy curve-fits |
| Ni – Cd [5] | • Lattice parameters of phases<br>• Crystal structure of phases |
| Ni – Pu [6] | • Temperature and composition of special reactions<br>• Crystal structure of phases<br>• Lattice parameters of phases |
| Ni – S [7] | • Crystal structure of phases<br>• Temperature and composition of special reactions |

## 4. Discussion

Based on the experimental thermodynamic data collected from the references published in the MPDS database, the Ni-Be system seems to be the most extensively investigated binary system of the four Ni systems not included in the SGTE database. The thermodynamic data necessary to curve-fit solution models used in the calculation of the phase diagram is published in detail by Tanner from Lawrence Livermore National Laboratory [4]. Secondly, Tanner has published the lattice stability and excess Gibbs energy models, derived from numerous sources, used to evaluate the published Ni-Be phase diagram. Visibility on the models used is highly advantageous as these models can be used as a reference to assess the accuracy of the models calculated for the MTEN 6005 project. Equivalent models for the Ni-Cd, Ni-Pu, and Ni-S binary systems were not found in the initial screening of published results.

## 5. Conclusion

This study investigated binary Ni systems that lack publicly available thermodynamic databases in the SGTE collection with the ultimate aim of selecting one binary system to produce a thermodynamic database for. After evaluating which binary Ni systems are not publicly available but have been evaluated, published research was screened to determine which Ni system is most suitable to produce a thermodynamic database for. The combination of rich

experimental data, lattice stability models, and excess Gibbs energy models available for the Ni-Be system makes this system the most suitable for producing a thermodynamic database. Therefore, this system will be pursued for the remainder of the MTEN 6005 project.

**References**


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[2] H. Okamoto, M. E. Schlesinger, and E. M. Mueller, Eds., *ASM Handbook Alloy Phase Diagrams*, vol. 3. Materials Park, OH: ASM International, 2016.

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[4] H. Okamoto and L. E. Tanner, "The Be-Ni (Beryllium-Nickel) System," *Bulletin of Alloy Phase Diagrams*, vol. 9, no. 5, pp. 563–573, 1988.

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[7] P. Waldner, "Thermodynamic analysis of high-temperature heazlewoodite," *International Journal of Materials Research (formerly Zeitschrift fuer Metallkunde)*, vol. 97, no. 1, pp. 17–21, Jan. 2006, doi: https://doi.org/10.1515/ijmr-2006-0003.