

# Supplemental Literature Review of Binary Phase Diagrams: Au-Ce, B-Pr, Bi-Gd, Bi-Ho, Cd-Sr, Ga-Ti, Gd-Pb, Gd-Ti, Mg-Mn, Mn-Nd, Nd-Ni, and Ni-Ti

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## Introduction

*Binary Alloy Phase Diagrams, 2<sup>nd</sup> edition*, a comprehensive collection of alloy phase diagrams for 2159 binary systems, was published in 1990 (T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak., ASM International, Materials Park, OH [Massalski2]). This review intends to provide more recent information on the binary phase diagrams for the Au-Ce, B-Pr, Bi-Gd, Bi-Ho, Cd-Sr, Ga-Ti, Gd-Pb, Gd-Ti, Mg-Mn, Mn-Nd, Nd-Ni, and Ni-Ti systems that have become available after 1990. The criteria for selecting such information for inclusion in this review are (1) systems for which no phase diagram was given in [Massalski2], (2) complete diagrams that are substantially different from the earlier version, and (3) partial diagrams that alter or clarify the earlier version. Thermodynamic consistency of the new phase diagrams was checked based on phase rules and the diagrams were modified if necessary. However, each updated phase diagram has not gone through the ordinary evaluation process. Accordingly, a newer phase diagram is not always a better

diagram, especially when there is too little published data on a system. For convenience, reaction tables and crystal structure data have been added when new information was available.

## Au-Ce (Gold-Cerium)

The Au-Ce phase diagram in [1990Mas] was redrawn from [1987Gsc]. This phase diagram was thermodynamically analyzed by [2013Don]. The result is shown in Fig. 1. The Au<sub>4</sub>Ce<sub>3</sub> phase was added by [2013Don] by referring to the work of [2001Bou]. However, no information is found on this phase in [2001Bou]. Crystal structure data are not found either in [2007Vil] database. Therefore, this phase is tentatively shown with a dashed line in Fig. 1.

## References

**1987Gsc:** K.A. Gschneidner, Jr., F.W. Calderwood, H. Okamoto, and T.B. Massalski, The Au-Ce (Gold-Cerium)

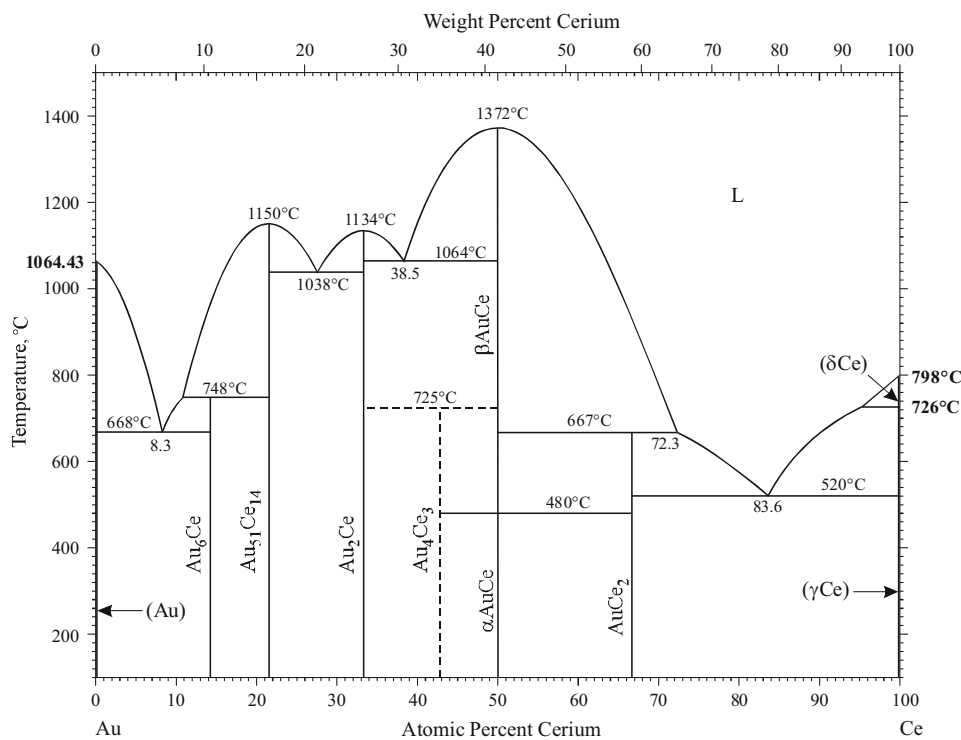


Fig. 1 Au-Ce phase diagram [2013Don]

System, *Phase Diagrams of Binary Gold Alloys*, H. Okamoto and T.B. Massalski, ed, Metals Park, OH, 1987, p 57-60

**1990Mas:** T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Au-Ce (Gold-Cerium), *Binary Alloy Phase Diagrams*, 2nd ed., ASM International, Materials Park, OH, 1990, p 352-353

**2001Bou:** P. Boulet, D. Mazzone, H. Noël, P. Rogl, and R. Ferro, Phase Equilibria and Magnetic Studies in the Ternary System Ce-Au-Sn, *J. Alloys Compd.*, 2001, **317-318**, p 350-356

**2007Vil:** P. Villars and K. Cenzual, *Pearson's Crystal Data CD-ROM*, Release 2007/8, ASM International, OH, 2007

**2013Don:** H.Q. Dong, X.M. Tao, T. Laurila, V. Vuorinen, and M. Paulasto-Kröckel, Thermodynamic Modeling of Au-Ce-Sn Ternary System, *Calphad*, 2013, **42**, p 38-50

## B-Pr (Boron-Praseodymium)

The B-Pr system was reviewed by [1990Lia]. Three intermediate phases,  $B_6Pr$  (13.5-15 at.% Pr),  $B_4Pr$  (20 at.% Pr), and  $B_xPr$  (28 at.% Pr) were shown in the assessed phase diagram. This system was thermodynamically analyzed by

[2013Wan]. Figure 2 shows the B-Pr phase diagram mostly based on [2013Wan]. According to the phase diagram shown by [2013Wan], the  $B_6Pr$  phase has a constant solubility range from 10 to 14.3 at.% Pr below 2027.2 °C. This feature is very unlikely. In the table showing the calculated result, [2013Wan] indicates that the composition of  $B_6Pr$  is the stoichiometric composition of 14.3 at.% Pr. No experimental data are available with regard to the solubility range of this phase.

$B_xPr$  in [1990Lia] was found later to be  $B_5Pr_2$  [2003Kuz]. B-Pr crystal structure data are summarized in Table 1.

## References

**1990Lia:** P.K. Liao and K.E. Spear, B-Pr (Boron-Praseodymium), *Binary Alloy Phase Diagrams*, 2nd ed., T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., ASM International, Materials Park, OH, 1990, p 519, 521-522

**2003Kuz:** Y.B. Kuz'ma, V.S. Babizhetskii, R. Guérin, and S.I. Mikhailenko, Crystal Structure of  $Pr_2B_5$  Boride, *Kristallografiya*, 2003, **48**, p 619-623 [in Russian]

**2013Wan:** C.P. Wang, Y. Shi, D. Wang, Y. Lu, D.L. Zhao, and X.J. Liu, Thermodynamic Assessment of the B-Ce and B-Pr Systems, *Calphad*, 2013, **41**, p 150-155

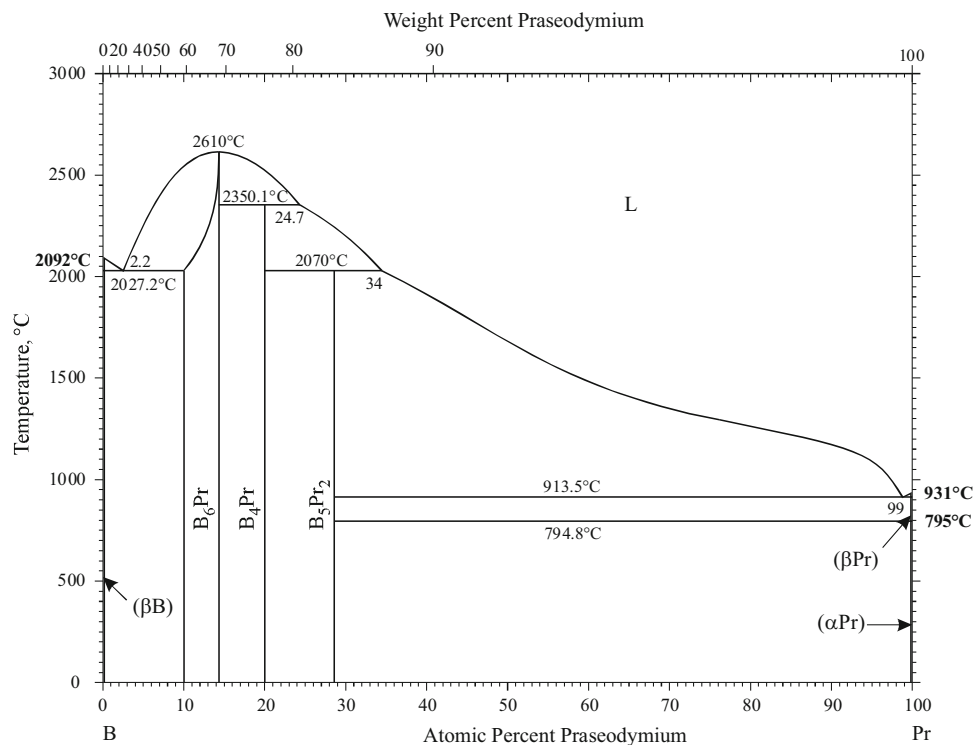


Fig. 2 B-Pr phase diagram

**Table 1 B-Pr crystal structure data**

Phase	Composition, at.% Pr	Pearson symbol	Space group	Strukturbericht designation	Prototype
(βB)	0	<i>hR108</i>	$R\bar{3}m$	...	...
B <sub>6</sub> Pr	14.3	<i>cP7</i>	$Pm\bar{3}m$	<i>D2</i> <sub>1</sub>	CaB <sub>6</sub>
B <sub>4</sub> Pr	20	<i>tP20</i>	$P4/mbm$	<i>D1</i> <sub>e</sub>	B <sub>4</sub> Th
B <sub>5</sub> Pr <sub>2</sub>	28.6	<i>mC56</i>	$C12/c1$	...	...
(βPr)	100	<i>cI2</i>	$Im\bar{3}m$	<i>A2</i>	W
(αPr)	100	<i>hP4</i>	$P6_3/mmc$	<i>A3'</i>	αLa

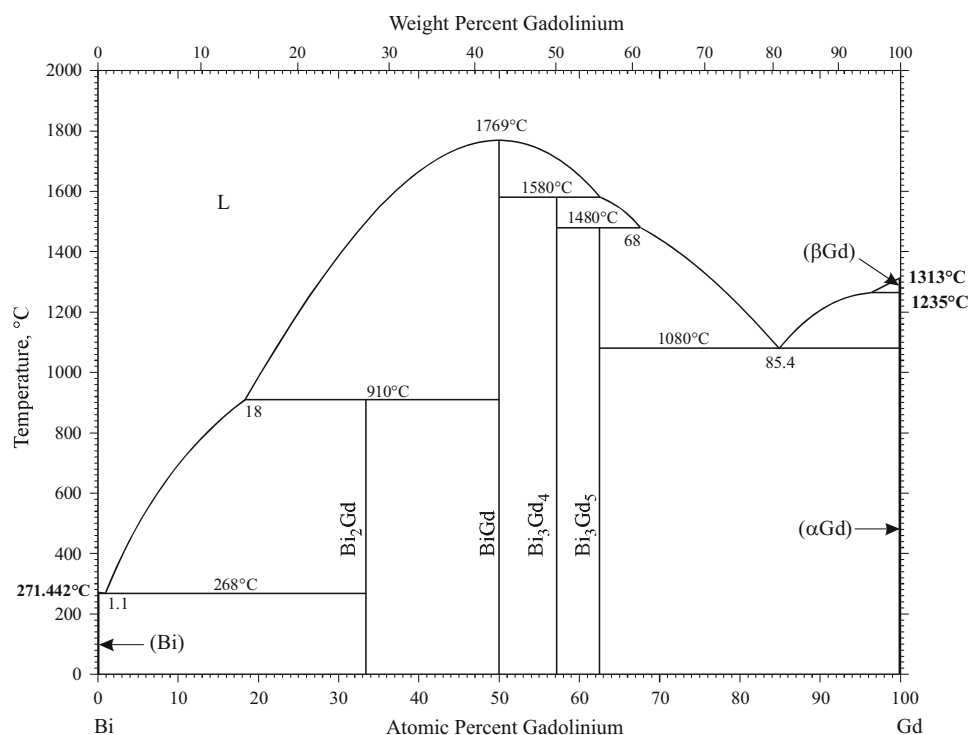
### Bi-Gd (Bismuth-Gadolinium)

The Bi-Gd phase diagram in [1990Mas] was adopted from [1989Gsc], which was primarily based on the work of [1967Gam].

This phase diagram was modified by [1993Abu], as a new phase Bi<sub>2</sub>Gd was discovered. [2013Wan] carried out thermodynamic assessment of this system and obtained a phase diagram shown in Fig. 3. The stability of Bi<sub>2</sub>Gd must be confirmed because [1993Abu] could not obtain this phase in a homogeneous form and could not determine its crystal structure, as already reviewed by [1994Oka].

### References

- 1967Gam:** R.J. Gambino, Rare-Earth-Sb and -Bi Compounds with the Gd<sub>4</sub>Bi<sub>3</sub> (anti-Th<sub>3</sub>P<sub>4</sub>) Structure, *J. Less-Common Met.*, 1967, **12**, p 344-352
- 1989Gsc:** K.A. Gschneidner Jr. and F.W. Calderwood, The Bi-Gd (Bismuth-Gadolinium) System, *Bull. Alloy Phase Diagrams*, 1989, **10**(4a), 436-438
- 1990Mas:** T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Bi-Gd (Bismuth-Gadolinium), *Binary Alloy Phase Diagrams*, 2nd ed., ASM International, Materials Park, OH, 1990, p 738, 740



**Fig. 3** Bi-Gd phase diagram [2013Wan]

**1993Abu:** V.D. Abulkhaev, Gd-Bi Phase Diagram, Russ. Metall., 1993, (1), p 152-155

**1994Oka:** H. Okamoto, "Comment on Bi-Gd (Bismuth-Gadolinium)," *J. Phase Equilib.*, 1994, **15**(6), p 650-651

**2013Wan:** J. Wang, C. Li, C. Guo, Z. Du, and B. Wu, Thermodynamic Assessment of the Gd-Bi and Ho-Bi Systems, *Calphad*, 2013, **41**, p 1-5

**1994Oka:** H. Okamoto, Comment on Bi-Ho (Bismuth-Holmium), *J. Phase Equilib.*, 1994, **15**(6), p 651-652

**2013Wan:** J. Wang, C. Li, C. Guo, Z. Du, and B. Wu, Thermodynamic Assessment of the Gd-Bi and Ho-Bi Systems, *Calphad*, 2013, **41**, p 1-5

## Bi-Ho (Bismuth-Holmium)

The original form of the Bi-Ho phase diagram in [1990Mas] was proposed by [1975Yos]. The existence of BiHo and  $\text{Bi}_3\text{Ho}_{5+x}$  was known, but the liquidus boundaries were speculative. [1994Abu] determined the Bi-Ho phase diagram based on DTA data, and [1994Oka] modified it into a more plausible form. Figure 4 shows the Bi-Ho phase diagram determined by thermodynamic analysis by [2013Wan]. The calculated result is in good agreement with [1994Oka].

## References

**1975Yos:** K. Yoshihara, J.B. Taylor, L.D. Calvert, and J.G. Despault, Rare-Earth Bismuthides, *J. Less-Common Met.*, 1975, **41**(2), p 329-337

**1990Mas:** T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Bi-Ho (Bismuth-Holmium), *Binary Alloy Phase Diagrams*, 2nd ed., ASM International, Materials Park, OH, 1990, p 744, 746

**1993Abu:** V.D. Abulkhaev, The Ho-Bi Phase Diagram, *Russ. Metall.*, 1993, (2), p 169-172

## Cd-Sr (Cadmium-Strontium)

The Cd-Sr phase diagram in [1990Mas] was based on [1965Kos] with  $\text{Cd}_3\text{Sr}_5$  modified from  $\text{CdSr}_2$  according to [1978Bru].

Figure 5 shows the Cd-Sr phase diagram thermodynamically assessed by [2013Zha].  $\text{Cd}_9\text{Sr}_2$  in [1990Mas] has been changed to  $\text{Cd}_{58}\text{Sr}_{13}$  according to [1972Bru].

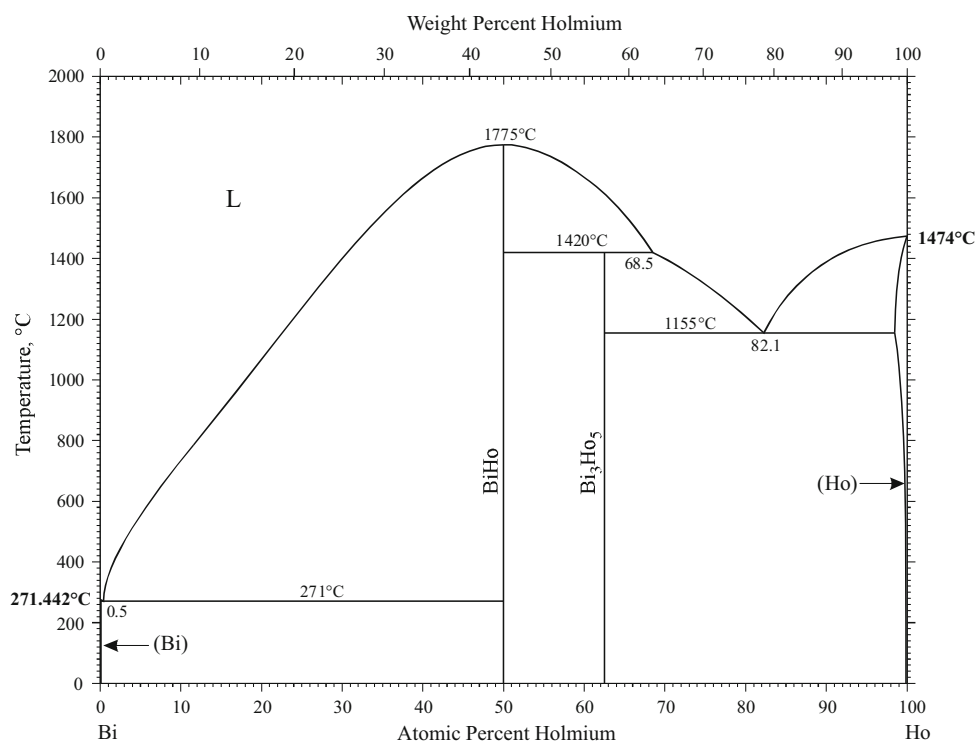
Cd-Sr crystal structure data shown in Table 2 have been updated according to [2007Vil].

## References

**1965Kos:** W. Köster and J. Meixner, Construction of the Systems of Europium with Silver, Cadmium, and Indium As Well As the Cadmium-Strontium System, *Z. Metallkd.*, 1965, **56**, p 695-703 [in German]

**1972Bru:** G. Bruzzone The Ca-Cd and Ba-Cd Systems, *Gazz. Chim. Ital.*, 1972, **102**, p 234-242 [in Italian]

**1978Bru:** G. Bruzzone, E. Franceschi, and F. Merlo,  $\text{M}_5\text{X}_3$  Intermediate Phases Formed by Ca, Sr, and Ba, *J. Less Common Met.*, 1978, **60**(1), p 59-63



**Fig. 4** Bi-Ho phase diagram [2013Wan]

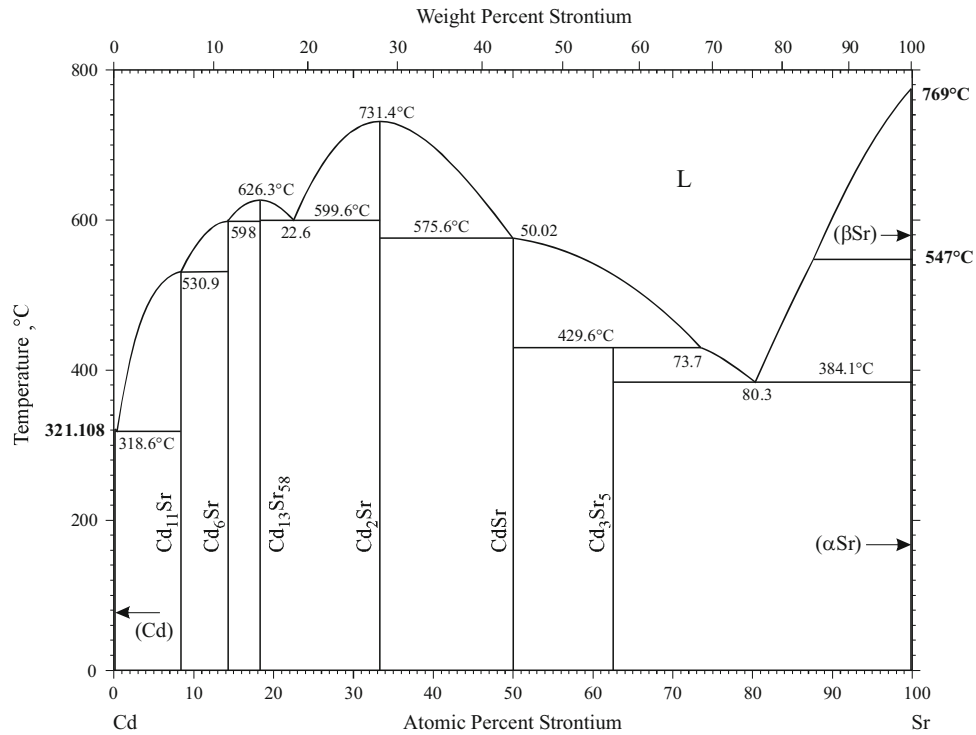


Fig. 5 Cd-Sr phase diagram [2013Zha]

Table 2 Cd-Sr crystal structure data

Phase	Composition, at.% Sr	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Cd)	0	<i>hP2</i>	<i>P6<sub>3</sub>/mmc</i>	<i>A3</i>	Mg
Cd <sub>11</sub> Sr	8.3	<i>tI48</i>	<i>I4<sub>1</sub>/amd</i>	...	BaCd <sub>11</sub>
Cd <sub>6</sub> Sr	14.3	<i>cI184</i>	<i>Im 3</i>	...	Cd <sub>6</sub> Y
Cd <sub>58</sub> Sr <sub>13</sub>	18.3	<i>hP142</i>	<i>P6<sub>3</sub>/mmc</i>	...	Gd <sub>13</sub> Zn <sub>58</sub>
Cd <sub>2</sub> Sr	33.3	<i>oI12</i>	<i>Imma</i>	...	KHg <sub>2</sub>
CdSr	50	<i>cP2</i>	<i>Pm 3m</i>	<i>B2</i>	CsCl
Cd <sub>3</sub> Sr <sub>5</sub>	62.5	<i>tI32</i>	<i>I4/mcm</i>	<i>D8<sub>1</sub></i>	Cr <sub>5</sub> B <sub>3</sub>
(βSr)	100	<i>cI2</i>	<i>Im 3m</i>	<i>A2</i>	W
(αSr)	100	<i>cF4</i>	<i>Fm 3m</i>	<i>A2</i>	Cu

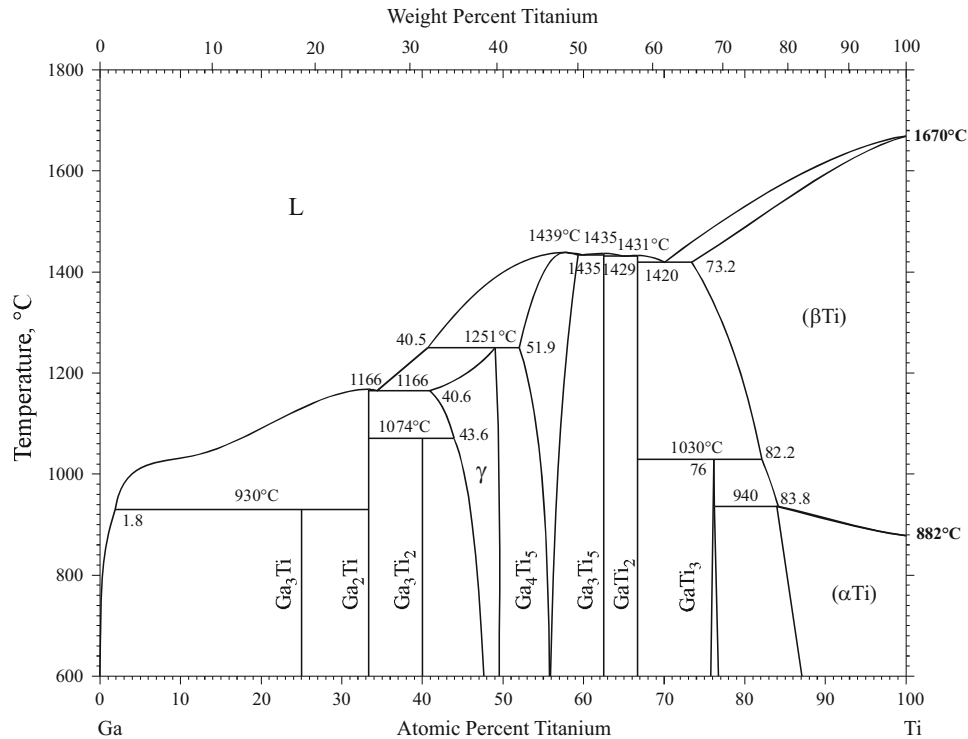
**1990Mas:** T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Cd-Sr (Cadmium-Strontium), *Binary Alloy Phase Diagrams*, 2nd ed., ASM International, Materials Park, OH, 1990, p 1030-1031

**2007Vil:** P. Villars and K. Cenzual, *Pearson's Crystal Data CD-ROM*, Release 2007/8, ASM International, OH, 2007

**2013Zha:** C. Zhang, K. Cheng, W. Wang, X. Li, B. Hu, S. Liu, and Y. Du, Thermodynamic Assessment of the Cd-X (X = Sr, Ti, B, V) Systems, *Calphad*, 2013, **42**, p 6-12

## Ga-Ti (Gallium-Titanium)

[2005Oka] compared two Ga-Ti phase diagrams reported by [2001Ant] and [2003Li]. The latter was preferred because problems in the diagram of [2001Ant] pointed out by [2002Oka] had been solved. Figure 6 shows the Ga-Ti phase diagram calculated by [2013Liu] using a more updated thermodynamic model. The diagram is in good agreement with [2003Li]. The only remarkable difference between [2003Li] and [2013Liu] is that the (βTi) shows a



**Fig. 6** Ga-Ti phase diagram [2013Liu]

maximum melting point according to the calculation of [2003Li], whereas the diagram of [2003Liu] (Fig. 6) does not show such a peak. No conclusive experimental data are available.

## References

- 2001Ant:** N.V. Antonova and L.A. Tretyachenko, Phase Diagram of the Ti-Ga System, *J. Alloys Compd.*, 2001, **317-318**, p 398-405
- 2002Oka:** H. Okamoto, Ga-Ti (Gallium-Titanium), *J. Phase Equilib.*, 2002, **23**(5), p 457-458
- 2003Li:** J.B. Li, J.C. Tedenac, M.C. Record, Thermodynamic Analysis of the Ga-Ti System, *J. Alloys Compd.*, 2003, **358**, p 133-141
- 2005Oka:** H. Okamoto, Ga-Ti (Gallium-Titanium), *J. Phase Equilib. Diffus.*, 2005, **26**(4), p 398
- 2013Liu:** Y. Liu, J.C. Tedenac, X.P. Su, C. Colinet, and J.H. Wang, An Updated Thermodynamic Modeling of the Ga-Ti System, *Calphad*, 2013, **41**, p 140-149

## Gd-Pb (Gadolinium-Lead)

The Gd-Pb phase diagram in [1990Mas] was adopted from [1991Pal]. [2013Cui] optimized the phase boundary data using a random solution model and an associate model for the liquid phase. They discovered that the phase diagram calculated with the associate model fits better with the experimental data of [1991Pal]. Figure 7 shows the calculated phase diagram.

## References

- 1990Mas:** T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Gd-Pb (Gadolinium-Lead), *Binary Alloy Phase Diagrams*, 2nd ed., ASM International, Materials Park, OH, 1990, p 1906-1907
- 1991Pal:** A. Palenzona and S. Cirafici, The Gd-Pb (Gadolinium-Lead) System, *J. Phase Equilib.*, 1991, **12**(6), p 686-690
- 2013Cui:** J. Cui, C. Guo, C. Li, and Z. Du, Thermodynamic Optimization of the Gd-Pb System Using Random Solution and Associate Models, *Calphad*, 2013, **42**, p 1-5

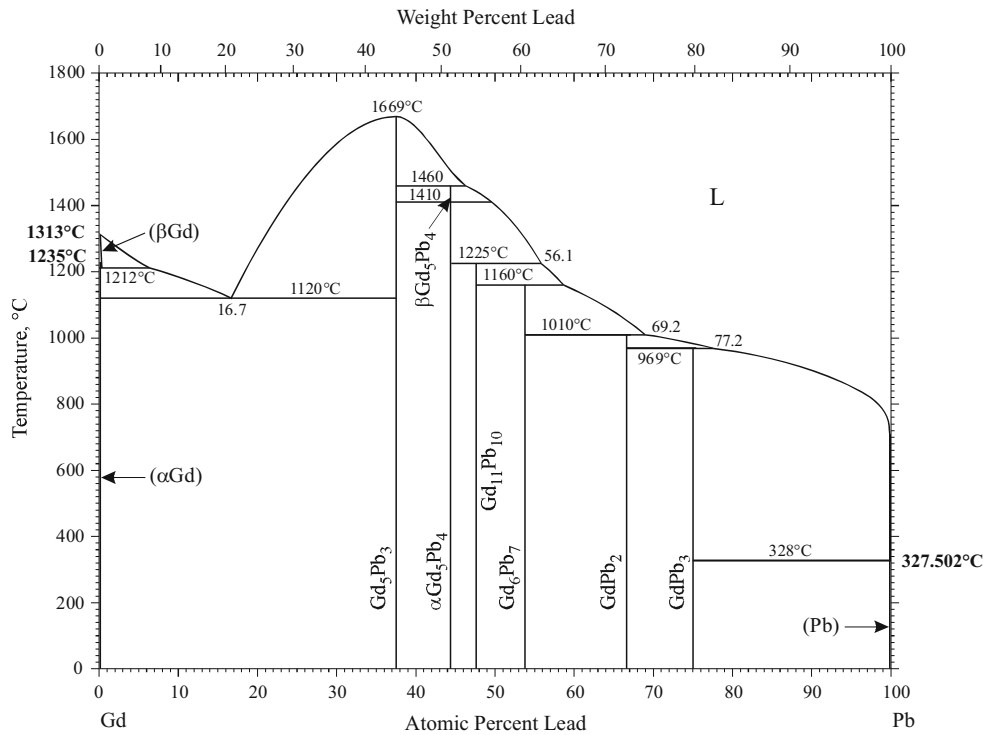


Fig. 7 Gd-Pb phase diagram [2013Cui]

## Gd-Ti (Gadolinium-Titanium)

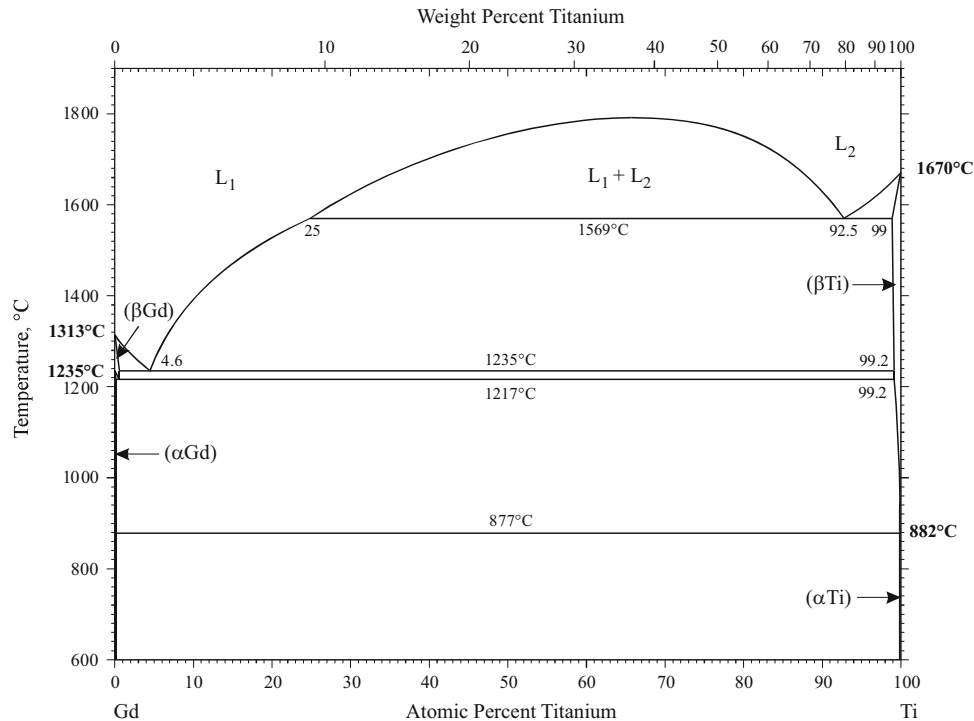
The Gd-Ti phase diagram in [1990Mas] was accepted from [1987Mur]. The assessed phase diagram was monotectic type based on thermodynamic consideration although [1961Cro] and [1962Sav] reported eutectic type phase diagrams.

The monotectic type Gd-Ti phase diagram was supported by [2010Sch], but [2012Oka] questioned the form of the miscibility gap as it is displaced far to the Ti rich side and noticed significant mismatch between [1987Mur] and [2010Sch].

In order to clarify these problems, [2013Mat] studied this system experimentally by combining electrostatic levitation of the melt with high energy synchrotron in situ x-ray diffraction at elevated temperatures. Figure 8 shows the Gd-Ti phase diagram obtained by thermodynamic calculation based on the experimental results. The critical temperature of the miscibility gap turned out to be much higher than that reported in earlier reports, i.e., 1515 °C [1987Mur] or ~1600 °C [2010Sch].

## References

- 1961Cro:** J.G. Croeni, S.C. Rhoads, C.E. Armantrout, and H. Kato, *Titanium-Gadolinium Phase Diagram*, U.S. Bur. Mines, Rep. Invest. 5796, 1961, 14 p
- 1962Sav:** E.M. Savitskii and G.S. Burkhanov, Equilibrium Diagram of the Gadolinium-Titanium System, *Russ. J. Inorg. Chem.*, 1962, 7, p 358-359
- 1987Mur:** J.L. Murray, The Gd-Ti (Gadolinium-Titanium) System. *Phase Diagrams of Binary Titanium Alloys*, J.L. Murray, ed., ASM International, Metals Park, OH, 1987, p 225-228
- 1990Mas:** T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Gd-Ti (Gadolinium-Titanium), *Binary Alloy Phase Diagrams*, 2nd ed., ASM International, Materials Park, OH, 1990, p 1935, 1937
- 2010Sch:** S. Schmitz, H.G. Lindenkreuz, N. Mattern, W. Loser, B. Buchner, Liquid Phase Separation in Gd-Ti and Gd-Zr Melts, *Intermetallics*, 2010, 18, p 1941-1945



**Fig. 8** Gd-Ti phase diagram [2013Mat]

**2012Oka:** H. Okamoto, Gd-Ti (Gadolinium-Titanium), *J. Phase Equilib. Diffus.*, 2012, **33**(5), p 422

**2013Mat:** N. Mattern, J.H. Han, O. Fabrichnaya, M. Zinkevich, W. Löser, J. Werner, R. Nowak, I. Kaban, O. Shuleshova, D. Holland-Moritz, J. Bednarčík, N. Sobczak, and J. Eckert, Experimental and Thermodynamic Assessment of the Gd-Ti System, *Calphad*, 2013, **42**, p 19-26

## Mg-Mn (Magnesium-Manganese)

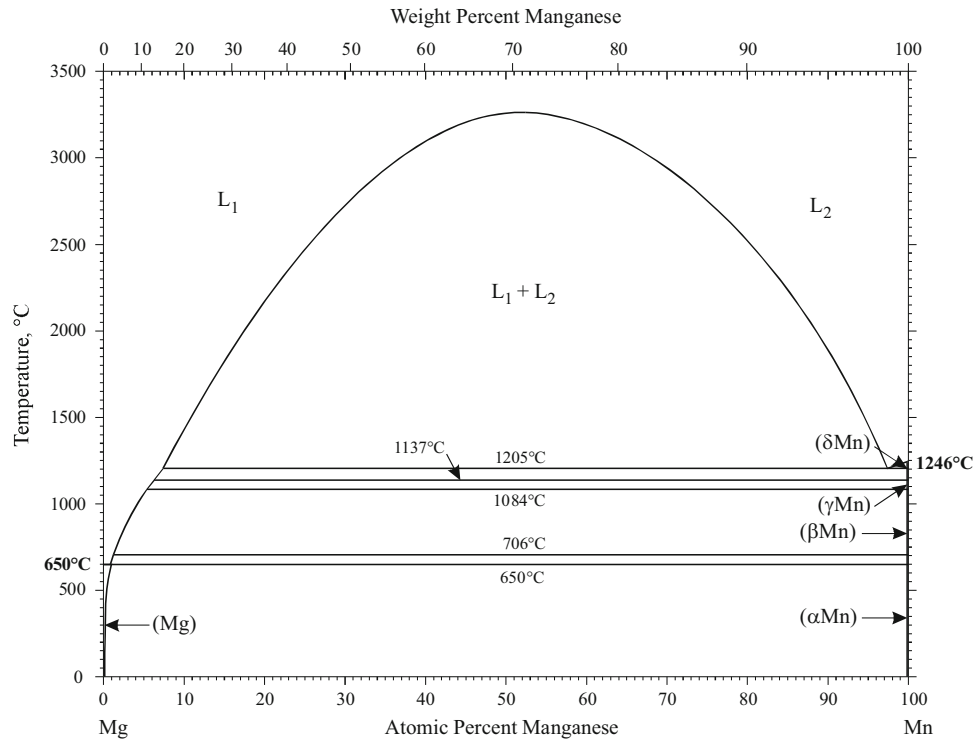
[2012Oka] introduced the Mg-Mn phase diagram reported by [2005Gro]. This phase diagram showed the miscibility gap of the liquid phase below 1400 °C. [2013Gho] re-optimized the data of [2005Gro] and calculated the

miscibility gap up to the critical temperature. The result is shown in Fig. 9.

## References

- 2005Gro:** J. Gröbner, D. Mirkovic, M. Ohno, R. Schmid-Fetzer, Experimental Investigation and Thermodynamic Calculation of Binary Mg-Mn Phase Equilibria, *J. Phase Equilib. Diffus.*, 2005, **26**(3), p 234-239
- 2012Oka:** H. Okamoto, Mg-Mn (Magnesium-Manganese), *J. Phase Equilib. Diffus.*, 2012, **33**(6), 496
- 2013Gho:** P. Ghosh and M. Medraj, Thermodynamic Calculation of the Mg-Mn-Zn and Mg-Mn-Ce Systems and Re-optimization of Their Constitutive Binaries, *Calphad*, 2013, **41**, p 89-107





**Fig. 9** Mg-Mn phase diagram [2013Gho]

## Mn-Nd (Manganese-Neodymium)

[2013Oka] introduced an updated phase diagram for the Mn-Nd system reported by [2012Kim]. This phase diagram is revised in Fig. 10, as [2013Mos] confirmed the existence of a new phase  $Mn_{17}Nd_2$  using EPMA and XRD.

Mn-Nd crystal structure data are summarized in Table 3.

## References

**2012Kim:** J. Kim and I.H. Jung, Critical Systematic Evaluation and Thermodynamic Optimiza-

tion of the Mn-RE System: RE = La, Ce, Pr, Nd, and Sm, *J. Alloys Compd.*, 2012, **552**, p 191-202

**2013Mos:** A.O. Mostafa, A.E. Gheribi, D. Kevorkov, Md. Mezbahul-Islam, and M. Medraj, Experimental Investigation and First-Principle Calculations Coupled with Thermodynamic Modeling of the Mn-Nd Phase Diagram, *Calphad*, 2013, **42**, p 27-37

**2013Oka:** H. Okamoto, Supplemental Literature Review of Binary Phase Diagrams: Cd-Se, Cu-Hg, Cu-Ho, Eu-Mg, H-Sr, Hf-Si, La-Mn, Mn-Nd, Nb-Y, Ni-Y, Pb-Se, and Sc-Sr, *J. Phase Equilib. Diffus.*, 2013, **34**(5), p 430-436

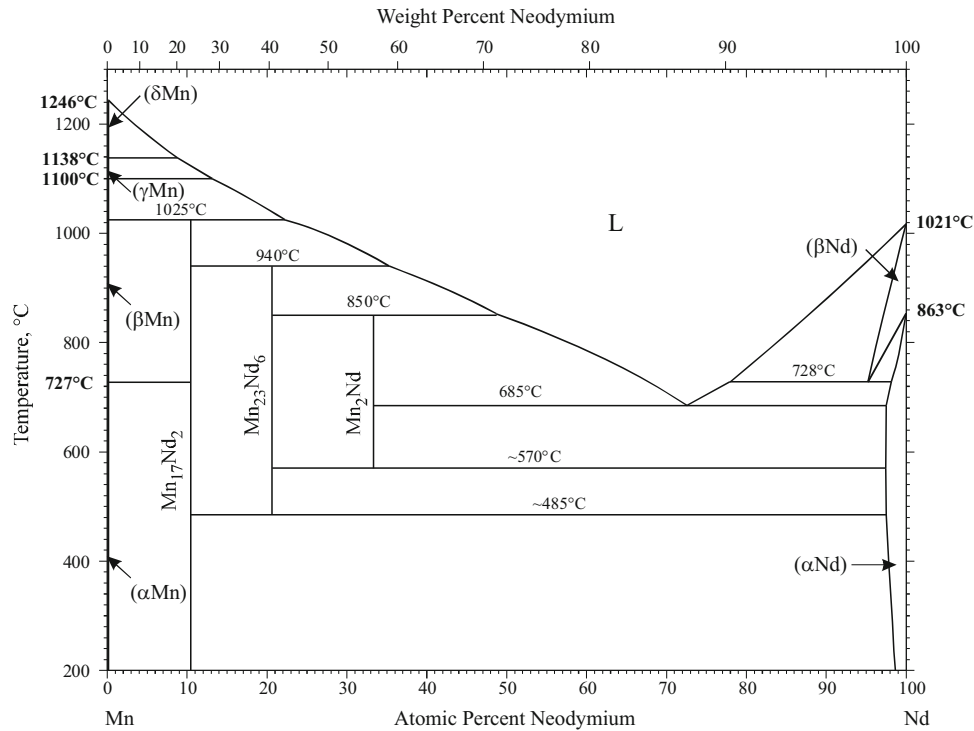


Fig. 10 Mn-Nd phase diagram [2013Mos]

Table 3 Mn-Nd crystal structure data

Phase	Composition, at.% Nd	Pearson symbol	Space group	Strukturbericht designation	Prototype
( $\delta$ Mn)	0	<i>cI2</i>	<i>Im</i> $\bar{3}m$	A2	W
( $\gamma$ Mn)	0	<i>cF4</i>	<i>Fm</i> $\bar{3}m$	A1	Cu
( $\beta$ Mn)	0	<i>cP20</i>	<i>P4</i> <sub>1</sub> 32	A13	$\beta$ Mn
( $\alpha$ Mn)	0	<i>cI58</i>	<i>I</i> 43 <i>m</i>	A12	$\alpha$ Mn
Mn <sub>17</sub> Nd <sub>2</sub>	10.5	<i>hP38</i>	<i>P6</i> <sub>3</sub> / <i>mmc</i>	...	Th <sub>2</sub> Ni <sub>17</sub>
Mn <sub>23</sub> Nd <sub>6</sub>	20.7	<i>cF116</i>	<i>Fm</i> $\bar{3}m$	D8 <sub>a</sub>	Mn <sub>23</sub> Th <sub>6</sub>
Mn <sub>2</sub> Nd	33.3	<i>hP12</i>	<i>P6</i> <sub>3</sub> / <i>mmc</i>	C14	MgZn <sub>2</sub>
( $\beta$ Nd)	95.3-100	<i>cI2</i>	<i>Im</i> $\bar{3}m$	A2	W
( $\alpha$ Nd)	97.5-100	<i>hP4</i>	<i>P6</i> <sub>3</sub> / <i>mmc</i>	A3'	$\alpha$ La

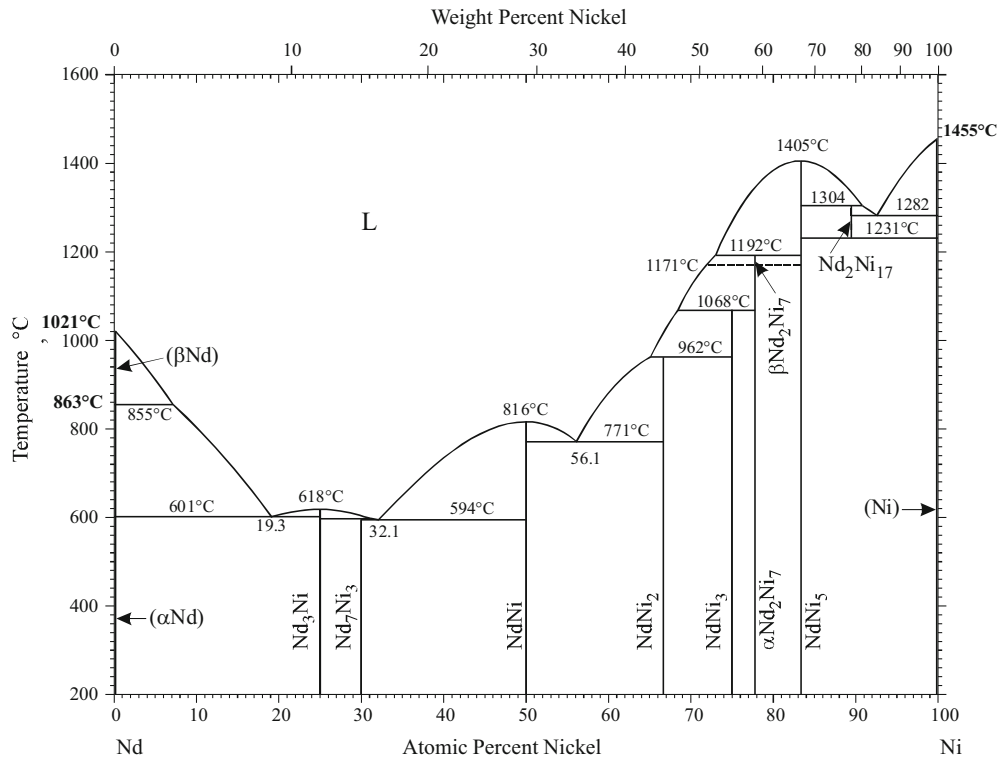
## Nd-Ni (Neodymium-Nickel)

According to the latest update on the Nd-Ni system by [2006Oka], invariant reaction temperatures in the Nd-Ni phase diagram reported by [2005Hua] are generally higher ( $\sim 50$  °C) than those reported by [1996Du]. [2013Hus] examined these two reports and derived a thermodynamic model more consistent with experimental thermodynamic data. The calculated phase diagram shown in Fig. 11 is generally consistent with [2005Hua].

The dimorphic transformation of Nd<sub>2</sub>Ni<sub>7</sub> at 1171 °C in Fig. 11 has been added based on the thermal effect observed by [2005Hua].

## References

- 1996Du:** Y. Du and N. Clavaguera, Thermodynamic Calculation of the Nd-Ni System, *Calphad*, 1996, **20**(3), p 289-296
- 2005Hua:** M. Huang, R.W. McCallum, and T.A. Lograsso, Experimental Investigation and Thermodynamic Modeling of the Nd-Ni System, *J. Alloys Compd.*, 2005, **398**, p 127-132
- 2006Oka:** H. Okamoto, Nd-Ni (Neodymium-Nickel), *J. Phase Equilib. Diffus.*, 2006, **27**(5), p 562
- 2013Hus:** A. Hussain, M.A. Van Ende, J. Kim, and I.H. Jung, Critical Thermodynamic Evaluation of the Co-Nd, Cu-Nd, and Nd-Ni Systems, *Calphad*, 2013, **41**, p 26-41



**Fig. 11** Nd-Ni phase diagram [2013Hus]

## Ni-Ti (Nickel-Titanium)

The Ni-Ti phase diagram in [1990Mas] was adopted from [1987Mur]. The high-temperature NiTi phase was shown to decompose into Ni<sub>3</sub>Ti and Ni<sub>2</sub>Ti at ~630 °C by a eutectoid reaction. However, the existence of a martensitic form of NiTi at room temperature was reported by [1981Mic] and confirmed by other investigators [2007Vil]. Figure 12 shows the Ni-Ti phase diagram calculated by [2013Pov] including the low-temperature phase. A similar phase diagram was reported by [1999Tan]. The β/α transition temperature of NiTi estimated by [1999Tan] was 93 °C. [1987Mur] viewed the αNiTi phase as metastable.

Table 4 shows Ni-Ti crystal structure data.

## References

- 1981Mic:** G.M. Michal and R. Sinclair, The Structure of TiNi Martensite, *Acta Crystallogr. B*, 1981, **37**, p 1803-1807
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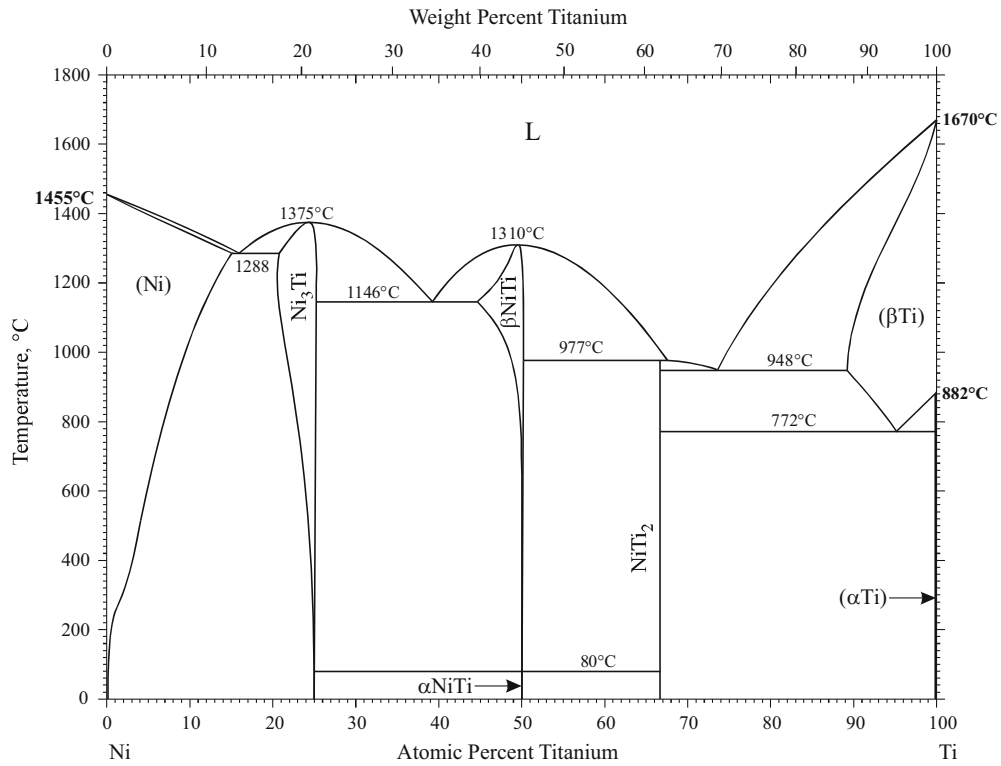


Fig. 12 Ni-Ti phase diagram [2013Pov]

Table 4 Ni-Ti crystal structure data

Phase	Composition, at.% Ti	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Ni)	0-15	<i>cF4</i>	<i>Fm</i> $\bar{3}m$	A1	Cu
Ni <sub>3</sub> Ti	20.5-25	<i>hP16</i>	<i>P6<sub>3</sub>/mmc</i>	<i>D0<sub>24</sub></i>	Ni <sub>3</sub> Ti
βNiTi	45-50	<i>cP2</i>	<i>Pm</i> $\bar{3}m$	B2	CsCl
αNiTi	50	<i>mP4</i>	<i>P12<sub>1</sub>/m1</i>	<i>B19'</i>	NiTi
NiTi <sub>2</sub>	66.7	<i>cF96</i>	<i>Fd</i> $\bar{3}m$	...	...
(βTi)	89-100	<i>cI2</i>	<i>Im</i> $\bar{3}m$	A2	W
(αTi)	100	<i>hP2</i>	<i>P6<sub>3</sub>/mmc</i>	A3	Mg