JPEDAV (2016) 37:621–634
DOI: 10.1007/s11669-016-0465-z
1547-7037 ©ASM International

Supplemental Literature Review of Binary Phase Diagrams: B-Fe, Cr-Zr, Fe-Np, Fe-W, Fe-Zn, Ge-Ni, La-Sn, La-Ti, La-Zr, Li-Sn, Mn-S, and Nb-Re

H. Okamoto

Introduction

Binary Alloy Phase Diagrams, 2nd 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 B-Fe, Cr-Zr, Fe-Np, Fe-W, Fe-Zn, Ge-Ni, La-Sn, La-Ti, La-Zr, Li-Sn, Mn-S, and Nb-Re 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.

B-Fe (Boron-Iron)

The information on the Fe-B system assessed by [1993Lia] was updated by [1995Oka] and then by [2004Oka]. According to these updates, the phase diagram could not be determined conclusively because the phase diagrams calculated by [1994Hal] and [2002Van] disagreed with the experimental data differently.

[2013Van] noticed inconsistencies or disagreements among thermodynamic models reported by [1984Kau], [1988Oht], [1994Hal], [2001Pal], [2002Van], and [2008Yos]. Figure 1 and 2 show the Fe-B phase diagram calculated by [2013Van] using an improved thermodynamic model. This result is in good agreement with the existing experimental data assembled by [1993Lia].

[2013Pol] also reported a calculated Fe-B phase diagram. The most noticeable difference of this diagram from others is that the (βB) liquidus shows a plateau at around 2000 °C, ~90 at.% B. Because no experimental phase boundary data exist in this region, this phenomenon cannot be denied. Confirmation is required.

References

1984Kau: L. Kaufman, B. Uhrenius, D. Birnie, and K. Taylor, Coupled Pair Potential, Thermochemical and Phase Diagram Data for Transition Metal Binary Systems-VII, CALPHAD, 1984, 8(1), p 25-66

1988Oht: H. Ohtani, M. Hasebe, K. Ishida, T. Nishizawa, Calculation of Fe-C-B Ternary Phase Diagram, Trans. ISIJ, 1988, 28, p 1043-1050

1993Lia: P.K. Liao and K.E. Spear, B-Fe (Boron Iron), Phase Diagrams of Binary Iron Alloys, H. Okamoto, ed., ASM International, Materials Park, OH, 1993, p 41-47

1994Hal: B. Hallemans, P. Wollants, and J.R. Roos, Thermodynamic Reassessment and Calculation of the Fe-B Phase Diagram, Z. Metallkd., 1994, 85(10), p 676-682

1995Oka: H. Okamoto, B-Fe (Boron-Iron), J. Phase Equilib., 1995, *16*(4), p 364-365

2001Pal: M. Palumbo, G. Cacciamani, E. Bosco, and M. Baricco, Thermodynamic Analysis of Glass Formation in Fe-B System, CALPHAD, 2001, 25(4), p 625-637

2002Van: T. Van Rompaey, K.C. Hari Kumar, and P. Wollants, Thermodynamic Optimization of the B-Fe System, J. Alloys Compd., 2002, 334, p 173-181

2004Oka: H. Okamoto, B-Fe (Boron Iron), J. Phase Equilib. Diffus., 2004, 25(3), p 297-298

2008Yos: K. Yoshitomi, Y. Nakama, H. Ohtani, and M. Hasebe, Thermodynamic Analysis of the Fe-Nb-B Ternary System, ISIJ Int., 2008, 48, p 835-844

2013Pol: M.G. Poletti and L. Battezzati, Assessment of the Ternary Fe-Si-B Phase Diagram, CALPHAD, 2013, 43, p 40-47

2013Van: M.A. Van Ende and I.H. Jung, Critical Thermodynamic Evaluation and Optimization of the Fe-B, Fe-Nd, B-Nd, and Nd-Fe-B Systems, J. Alloys Compd., 2013, 548, p 133-154

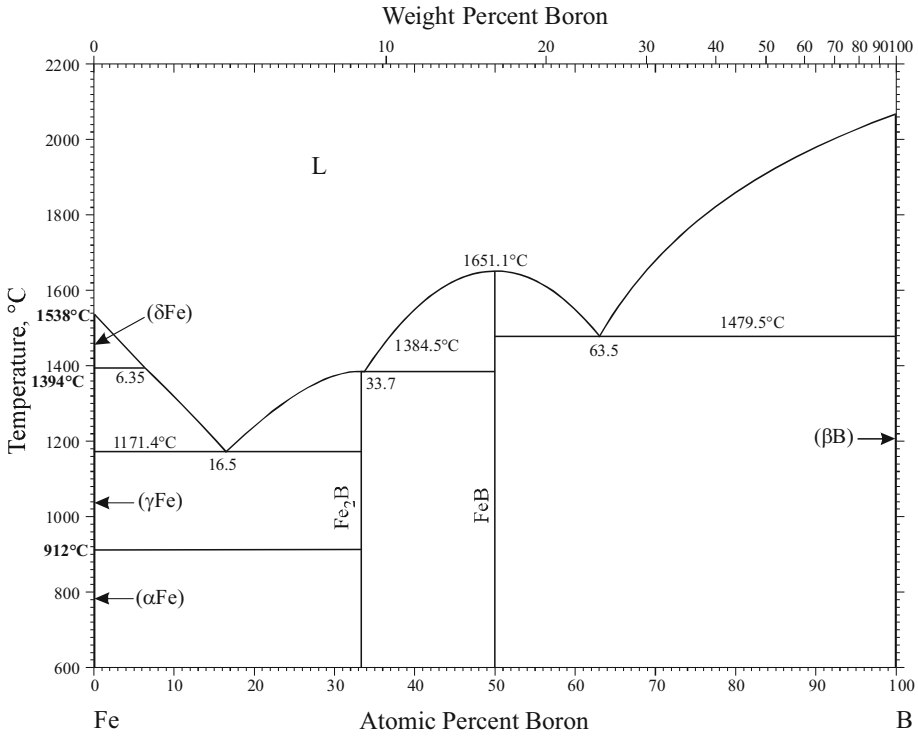

Fig. 1 Fe-B phase diagram [2013Van]

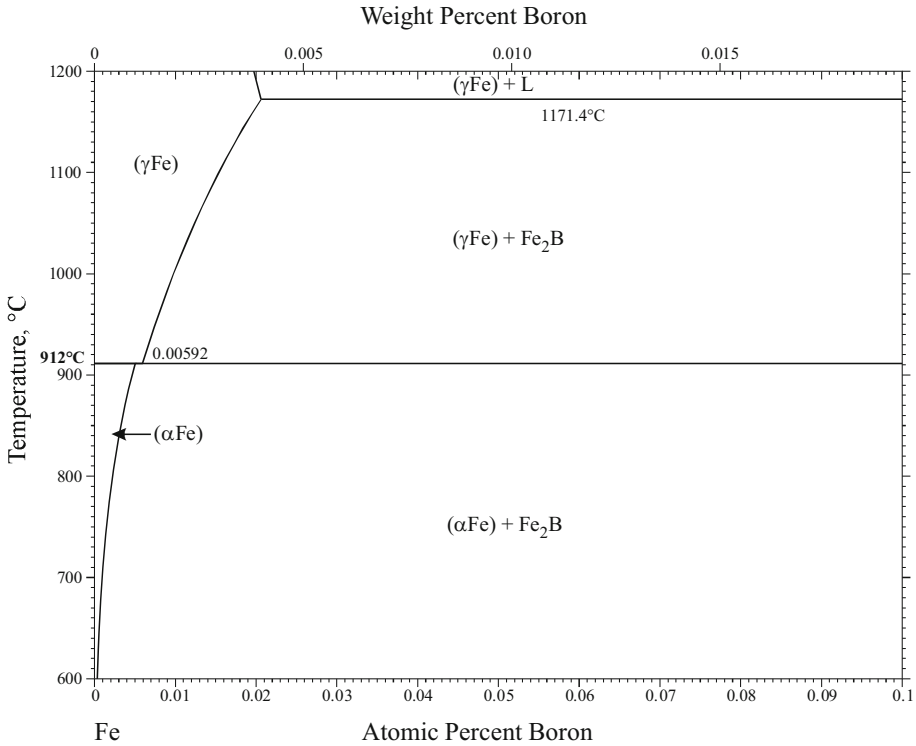

Fig. 2 Fe-rich corner of the Fe-B phase diagram [2013Van]

Cr-Zr (Chromium-Zirconium)

[1993Oka] updated the Cr-Zr phase diagram of [1990Mas] by introducing the thermodynamic modeling performed by [1993Zen2]. The information on this work is available in [1993Zen1] as well. Since then, [2009Pav] attempted thermodynamic modeling of this system based on the same experimental data as those used for determining the phase diagram of [1990Mas]. More recently, [2015Lu] reexamined the solvus boundaries of (Cr), αCr_2Zr, and (βZr) by EPMA measurements of annealed samples and then redetermined the Cr-Zr phase diagram by thermodynamic modeling. The result is shown in Fig. 3.

References

1990Mas: T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Cr-Zr (Chromium-Zirconium), *Binary Alloy Phase Diagrams*, *2nd ed*., ASM International, Materials Park, OH, 1990, p 1359-1360

1993Oka: H. Okamoto, Cr-Zr (Chromium-Zirconium), J. Phase Equilib., 1993, *14*(6), p 768

1993Zen1: K. Zeng, M. Hämäläinen, and K. Lilius, Thermodynamic Modeling of the Laves Phases in the Cr-Zr System, CALPHAD, 1993, 17, p 101-107

1993Zen2: K. Zeng, M. Hämäläinen, and R. Luoma, A Thermodynamic Assessment of the Cr-Zr System, Z. Metallkd., 1993, 84, p 23-28

2009Pav: J. Pavlů, J. Vřešt'ál, and M. Šob, Stability of Laves Phases in the Cr-Zr System, CALPHAD, 2009, 33, p. 382-387

2015Lu: H.J. Lu, W.B. Wang, N. Zou, J.Y. Shen, X.G. Lu, and Y.L. He, Thermodynamic Modeling of Cr-Nb and Zr-Cr with Extension to the Ternary Zr-Nb-Cr System, CALPHAD, 2015, 50, p 134-143

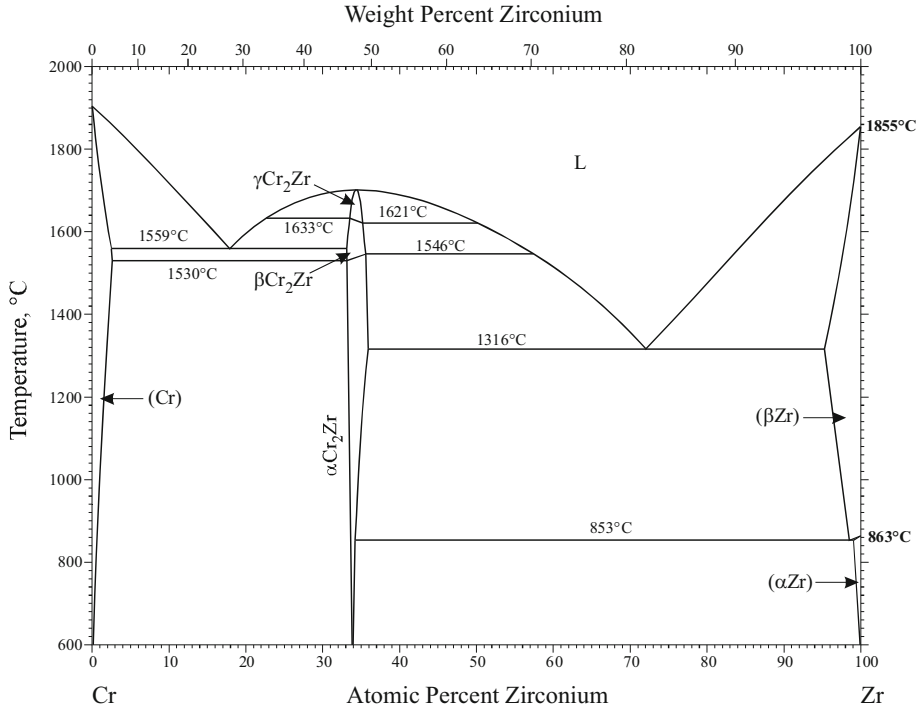

Fig. 3 Cr-Zr phase diagram [2015Lu]

Fe-Np (Iron-Neptunium)

[1995Oka] introduced the Fe-Np phase diagram reported by [1994Gib]. [2010Kur] updated this phase diagram by thermodynamic modeling, as shown in Fig. 4.

References

1994Gib: J.K. Gibson, R.G. Haire, E.C. Beahm, M.M. Gensini, A. Maeda, and T. Ogawa, The Neptunium-Iron Phase Diagram, J. Nucl. Mater., 1994, 211, p 215-222

1995Oka: H. Okamoto, Comment on Fe-Np (Iron-Neptunium), J. Phase Equilib., 1995, *16*(6), p 533-534

2010Kur: K. Kurata, Thermodynamic Database on U-Pu-Zr-Np-Am-Fe Alloy System II—Evaluation of Np, Am, and Fe Containing Systems, IOP Conf. Series: Mater. Sci. Eng., 2010, 9, 12023, 8 pp

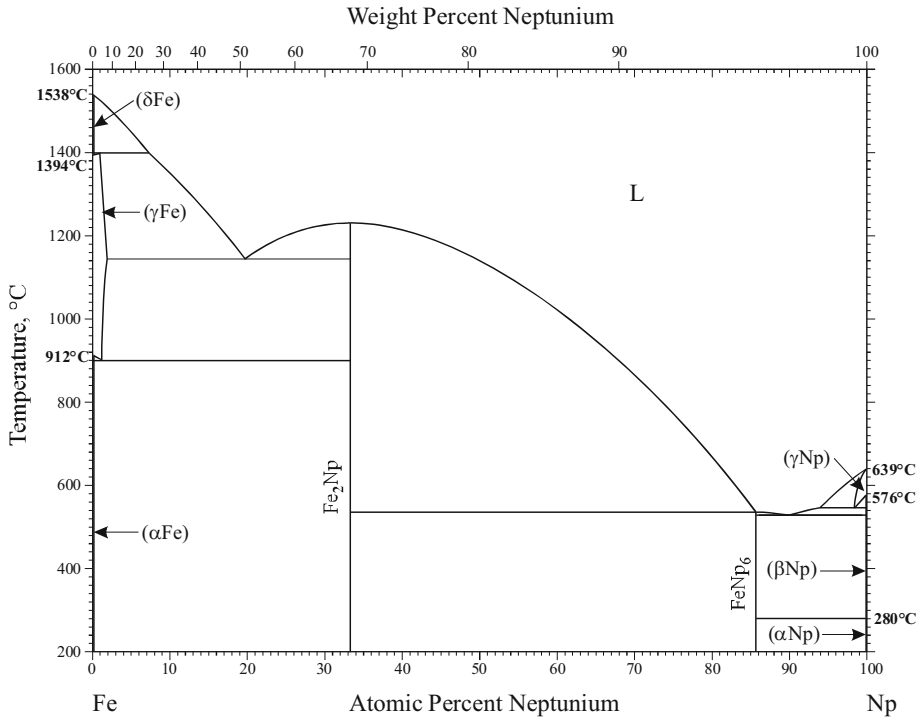

Fig. 4 Fe-Np phase diagram [2010Kur]

Fe-W (Iron-Tungsten)

The Fe-W phase diagram in [1990Mas] was adopted from the assessment done by [1986Nag]. This phase diagram was characterized by the existence of two intermediate phases Fe_7W_6 (1637-1190 °C) and FeW (< 1215 °C). The Fe_2W phase observed by many investigators [2007Vil] was regarded as metastable. These features were based on the report of [1981Hen].

There have been many other experimental and theoretical reports on the Fe-W system, and the general consensus was that only Fe_2W and Fe_7W_6 exist in the stable state in this system. There is no report on FeW in [2007Vil]. Figure 5 shows one of the two Fe-W phase diagrams calculated by [2015Jac] by using two different thermodynamic models. This phase diagram is in good agreement with the experimental data reported by [1967Hil], [1967Sin], [1970Fis], [1973Kir], [1981Tak], [1986Ich], and [2013Ant]. The other model of [2015Jac] is also in good agreement, but there is no experimental thermodynamic data to support either one of the models. Experimental confirmation of the stability/instability of Fe_2W and FeW may be difficult due to slow kinetics of the formation reaction of these compounds.

More information on the Fe-W phase diagram is available in [1987Gus], [1988Gus1], [1988Gus2], and [1995Yam].

References

1967Hil: M. Hillert, T. Wada, and H. Wada, The α-γ Equilibrium in Fe-Mn, Fe-Mo, Fe-Ni, Fe-Sb, Fe-Sn and Fe-W Systems, J. Iron Steel Inst., 1967, 205, p 539-546

1967Sin: A.K. Sinha and W. Hume-Rothery, The Iron-Tungsten System, J. Iron Steel Inst., 1967, 205, p 1145-1149

1970Fis: W.A. Fisher, K. Lorenz, H. Fabritius, and D. Schlegel, Study of Alpha-Gamma Transformation in High Purity Binary Alloys of Iron with Molybdenum, Vanadium, Tungsten, Niobium, Tantalum, Zirconium, and Cobalt, Arch. Eisenhuttenwes., 1970, 41, p 489-498 in Germen

1973Kir: G. Kirchner, H. Harvig, and B. Uhrenius, Experimental and Thermodynamic Study of the Equilibria between Ferrite, Austenite, and Intermediate Phases in the Fe-Mo, Fe-W, and Fe-Mo-S Systems, Metall. Trans, 1973, 4, p 1059-1067

1981Hen: E.T. Henig, H. Hofmann, and G. Petzow, The Constitution of W-Fe-Ni Refractory Metal Alloys and The Influence on the Mechanical Properties, Plansee Seminar 1981, H.M. Ortner, ed., Reuette, Austria, Metallwork Plansee, 1981, p 335-359

1981Tak: T. Takayama, M.Y. Wey, and T. Nishizawa, Effect of Magnetic Transition on the Solubility of Alloying Elements in BCC Iron and FCC Cobalt, Trans. Jpn. Inst. Met., Vol. 22, 1981, p 315-325

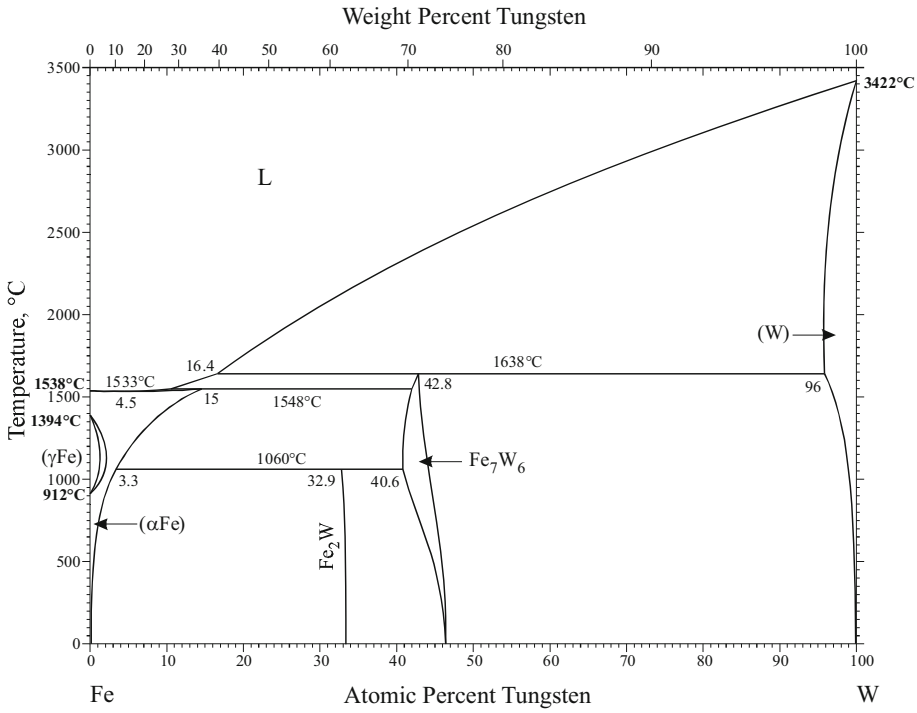

Fig. 5 Fe-W phase diagram [2015Jac]

1986Ich: E. Ichise, Y. Ueshima, and S. Miyagawa, Reexamination of the High Temperature Region of Fe-W Binary Alloy Phase Diagram, Tetsu to Hagane, Vol. 72, 1986, p 791-798 (in Japanese)
1986Nag: S.V. Nagender Naidu, A.M. Sriramamurthy, and P. Rama Rao, The Iron-Tungsten System, J. Alloy Phase Diagrams, 1986, 2, p 176-188
1987Gus: P. Gustafson, A Thermodynamic Evaluation of the C-Fe-W System, Metall. Trans. A, 18, 1987, p 175-188
1988Gus1: P. Gustafson, An Experimental Study and a Thermodynamic Evaluation of the Fe-Mo-W System, Z. Metallkd., Vol. 79, 1988, p 388-396
1988Gus2: P. Gustafson, An Experimental Study and a Thermodynamic Evaluation of the Cr-Fe-W System, Metall. Trans. A, Vol. 19, 1988, p 2531-2546
1990Mas: T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Fe-W (Iron-Tungsten), *Binary Alloy Phase Diagrams*, *2nd ed*., ASM International, Materials Park, OH, 1990, p 1791-1793
1995Yam: T. Yamane, Y.S. Kang, Y. Minamino, H. Araki, A. Hiraki, and Y. Miyamoto, Phase Diagrams of the Fe-rich Part of the Fe-W System under High Pressure, Z. Metallkd., Vol. 86, 1995, p 453-456
2007Vil: P. Villars and K. Cenzual, *Pearson's Crystal Data CD-ROM*, Release 2007/8, ASM International, OH, 2007
2013Ant: A. Antoni-Zdziobek, T. Commeau, and J.M. Joubert, Partial Redetermination of the Fe-W Phase Diagram, Metall. Mater. Trans. A, 2013, 44, p 2996-3003
2015Jac: A. Jacob, C. Schmetterer, L. Singheiser, A. Gray-Weale, B. Hallstedt, and A. Watson, Modeling of Fe-W Phase Diagram Using First Principles and Phonons Calculations, CALPHAD, 2015, 50, p 92-104

Fe-Zn (Iron-Zinc)

[2007Oka] introduced the Fe-Zn phase diagram calculated by [2005Nak] as possible refinement of the phase diagram evaluated by [1993Bur]. However, [2009Xio] found that the thermodynamic model used by [2005Nak] was inappropriate because an inversed miscibility gap would form in the liquid phase above about the melting temperature of Fe. The same problem occurs for the thermodynamic model used by [2001Su], which was also quoted in [2007Oka].

Figure 6 shows the Fe-Zn phase diagram calculated by [2009Xio] using a problem-free thermodynamic model.

References

1993Bur: B. Burton and P. Perrot, Fe-Zn (Iron-Zinc), Phase Diagrams of Binary Iron Alloys, H. Okamoto, ed., ASM International, Materials Park, OH, 1993, p 459-466
2001Su: X. Su, N.Y. Tang, and J.M. Toguri, Thermodynamic Evaluation of the Fe-Zn System, J. Alloys Compd., 2001, 325, p 129-136
2005Nak: J. Nakano, D.V. Malakhov, and G.R. Purdy, A Crystallographically Consistent Optimization of the Zn-Fe System, CALPHAD, 2005, 29, 276-288
2007Oka: H. Okamoto, Fe-Zn (Iron-Zinc), J. Phase Equilib. Diffus., 28(3), 2007, p 317-318

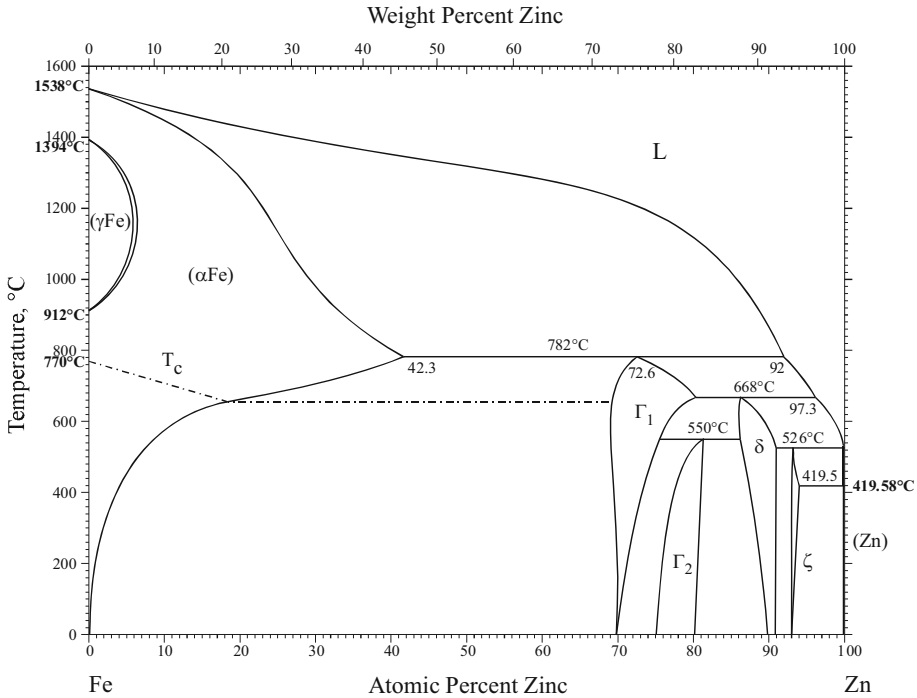

Fig. 6 Fe-Zn phase diagram [2009Xio]

2009Xio: W. Xiong, Y. Kong, Y. Du, Z.K. Liu, M. Selleby, and W.H. Sun, Thermodynamic Investigation of the Galvanizing Systems, I: Refinement of the Thermodynamic Description for the Fe-Zn System, CALPHAD, 2009, 33, p. 433-440

Ge-Ni (Germanium-Nickel)

[2014Oka] introduced a Ge-Ni phase diagram calculated by [2012Jin]. The Ge-Ni phase diagram shown in Fig. 7, calculated by [2010Liu], should have also been introduced for comparison. According to [2012Jin], three phases Ge_2Ni_3, $Ge_{12}Ni_{19}$, and ε shown in Fig. 7 form a single-phase region.

The phase diagram of [2010Liu] reproduced the diagram assessed by [1991Nas]. On the other hand, the phase diagram of [2012Jin] was partly based on more recent experimental data. Clarification is required by taking into account these contradictory reports.

Table 1 shows Ge-Ni crystal structure data for the Fig. 7 type phase diagram, revised by referring to [2006Vil].

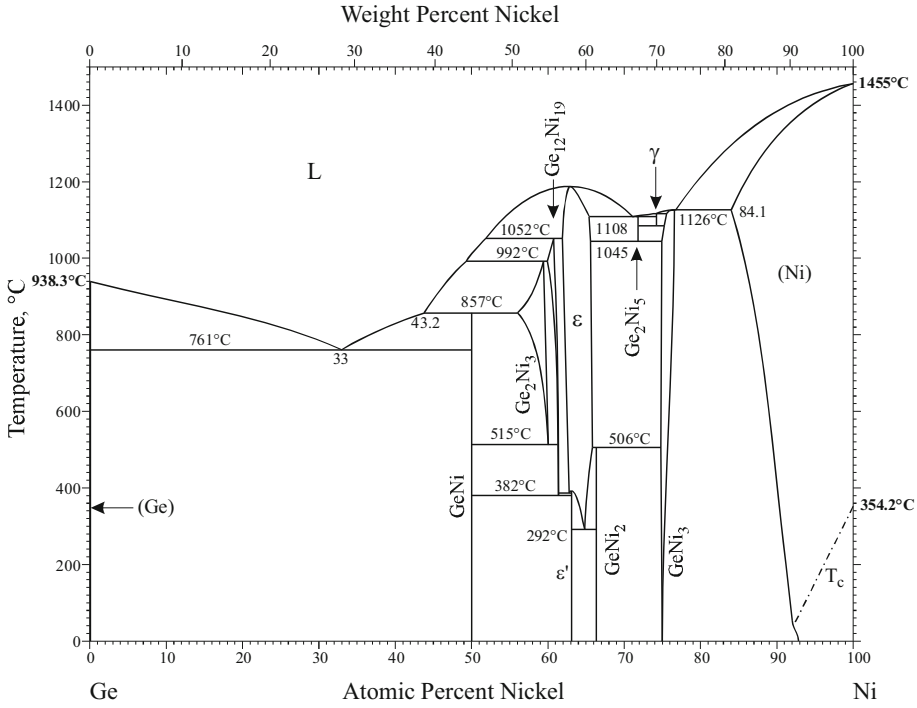

Fig. 7 Ge-Ni phase diagram [2010Liu]

Table 1 Ge-Ni crystal structure data

Phase	Composition, at.% Ni	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Ge)	0	*cF*8	$Fd\bar{3}m$	*A*4	C (diamond)
GeNi	50	*oP*8	*Pnma*	*B*31	MnP
Ge_2Ni_3	55.9 to 59.9	*hP*4	$P6_3/mmc$	$B8_1$	NiAs
$Ge_{12}Ni_{19}$	59.9 to 61.3	*mC*62	*C*121	…	…
ε	62 to 66.1	*mC*32	*C*121	…	…
ε'	63	*hP*6	$P6_3/mmc$	…	…
$GeNi_2$	66.7	*oP*12	*Pnma*	*C*23	Co_2Si
Ge_2Ni_5	72	*hP*42	$P6_3cm$	…	Pd_5Sb_2
γ	74.4	*cF*16	$Fd\bar{3}m$	*B*32	NaTl
$GeNi_3$	75 to 77	*cP*4	$Pm\bar{3}m$	$L1_2$	$AuCu_3$
(Ni)	84.1 to 100	*cF*4	$Fm\bar{3}m$	*A*1	Cu

References

1991Nas: A. Nash and P. Nash, *Phase Diagrams of Binary Nickel Alloys*, P. Nash, ed., ASM International, Materials Park, OH, 145-153 (1991)

2006Vil: P. Villars, H. Okamoto, and K. Cenzual, ASM Alloy Phase Diagrams Center, http://www1.asminternational.org/AsmEnterprise/APD, ASM International, Materials Park, OH, 2006

2010Liu: Y.Q. Liu, D.J. Ma, and Y. Du, Thermodynamic Modeling of the Germanium-Nickel System, J. Alloys Compd., 2010, 491, p 63-71

2012Jin: S. Jin, C. Leinenbach, J. Wang, L.L. Duarte, S. Delsante, G. Borzone, A. Scott, and A. Watson, Thermodynamic Study and Re-assessment of the Ge-Ni System, CALPHAD, 2012, 38, p 23-34

2014Oka: H. Okamoto, Supplemental Literature Review of Binary Phase Diagrams: Al-Br, B-Cd, Cd-Mg, Cd-Ti, Er-Fe, Fe-Nd, Ge-Na, Ge-Ni, Ge-Sc, Hf-W, Pb-Yb, and Re-Ti, J. Phase Equilib. Diffus., 2014, 35(2), p 195-207

La-Sn (Lanthanum-Tin)

The La-Sn system was reviewed by [1992Pal]. [2002Oka] introduced a thermodynamic assessment of this system reported by [2000Hua]. Substantial disagreement was observed between [1992Pal] and [2000Hua] with regard to the $LaSn_3$ liquidus temperatures.

[2009Idb] disclosed that the thermodynamic model used by [2000Hua] was inadequate, as it would cause formation of an inverted miscibility gap in the liquid phase at high temperatures. Figure 8 shows the La-Sn phase diagram calculated by [2009Idb] using an improved thermodynamic model. The form of the $LaSn_3$ liquidus was reproduced in good agreement with the experimental phase diagram of [1992Pal].

References

1992Pal: A. Palenzona and S. Cirafici, The La-Sn (Lanthanum-Tin) System, J. Phase Equilib., 1992, *13*(1), p 42-49

2000Hua: M. Huang, X. Su, F. Yin, P. Zhang, Z. Li, and C. Chen, A Thermodynamic Assessment of the La-Sn System, J. Alloys Compd., 2000, *309*, p 147-153

2002Oka: H. Okamoto, La-Sn (Lanthanum-Tin), J. Phase Equilib., 2002, *23*(3), p 289

2009Idb: M. Idbenali, C. Servant, N, Selhaoui, and L. Bouirden, A Thermodynamic Reassessment of the La-Sn System, CALPHAD, 2009, 33, p 398-404

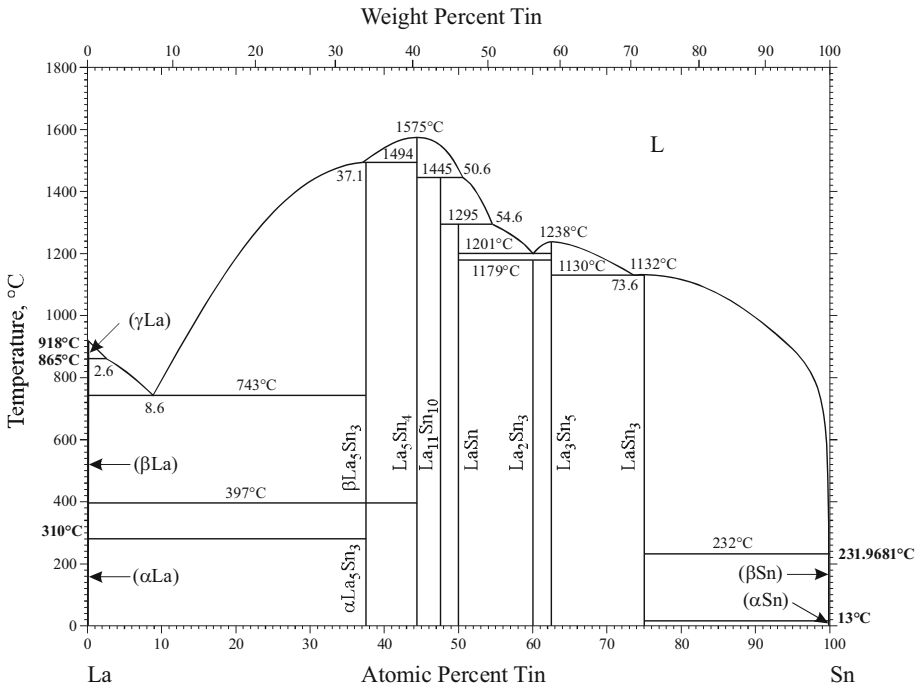

Fig. 8 La-Sn phase diagram [2009Idb]

La-Ti (Lanthanum-Titanium)

The La-Ti phase diagram in [1990Mas] was adopted from [1987Mur]. The assessed phase diagram was calculated based on very limited data of La solubility in (βTi) and (αTi) reported by [1957Sav] and [1962Sav]. Accordingly, [1987Mur] needed experimental determination of Ti solubility in (La) for reliable determination of the phase diagram.

Since then, [1988Cou] and [2016Mat] reported the La-Ti phase diagram. Figure 9 shows the phase diagram calculated by the latter based on experimental data obtained by in situ high-energy synchrotron x-ray diffraction. The phase diagram reported by [1988Cou] is also a monotectic type, but with a large (~20 at.%) solubility of Ti in (γLa). The phase diagram suggests a trend of forming continuous liquidus between W-type (γLa) and (βTi), in contradiction with the existence of the monotectic reaction. This problem does not exist in the phase diagram shown in Fig. 9.

References

1957Sav: E.M. Savitskii and G.S. Burkhanov, Diagrams of Titanium-Lanthanum and Titanium-Cerium Alloys, Zh. Neorg. Khim., 1957, 2, p 2609-2616 in Russian

1962Sav: E.M. Savitski and G.S. Burkhanov, Phase Diagrams of Alloys of Titanium with Rare-Earth Metals, Titan Ego Splavy, 1962, p 51-60 in Russian

1987Mur: J.L. Murray, The La-Ti (Lanthanum-Titanium) System, Phase Diagrams of Binary Titanium Alloys, J.L. Murray, ed., ASM International, Metals Park, OH, 1987, p 151-153

1990Mas: T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., La-Ti (Lanthanum-Titanium), *Binary Alloy Phase Diagrams*, *2nd ed*., ASM International, Materials Park, OH, 1990, p 2432, 2434

1988Cou: S.A. Court, J.W. Sears, M.H. Loretto, and H.L. Eraser, The Effect of Liquid Phase Separation on the Microstructure of Rapidly Solidified Titanium-Rare

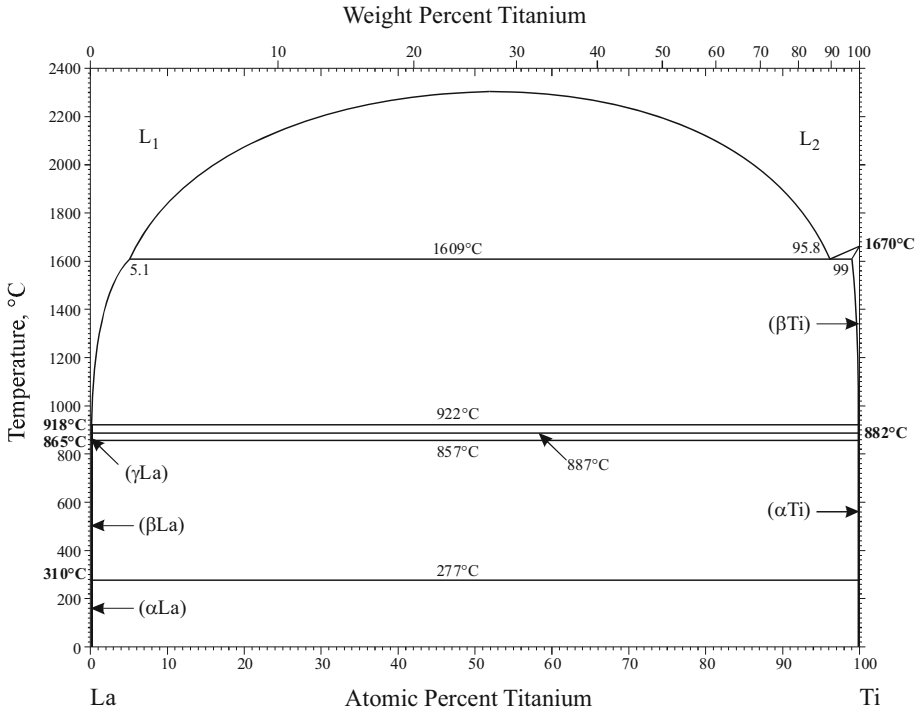

Fig. 9 La-Ti phase diagram [2016Mat]

Earth Alloys, Mater. Sci. Eng., 1988, 98, p 243-249
2016Mat: N. Mattern, Y. Yokoyama, A. Mizuno, J.H. Han, O. Fabrichnaya, M. Richter, and S. Kohara, Experimental and Thermodynamic Assessment of the La-Ti and La-Zr Systems, CALPHAD, 2016, 52, p 8-20

La-Zr (Lanthanum-Zirconium)

The La-Zr phase diagram was unknown in [1990Mas].

[2016Mat] investigated the La-Zr phase diagram by in situ high-energy synchrotron x-ray diffraction. Figure 10 shows the phase diagram calculated by [2016Mat] based on the experimental data.

Table 2 shows La-Zr crystal structure data.

References

1990Mas: T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., La-Zr (Lanthanum-Zirconium), *Binary Alloy Phase Diagrams*, *2nd ed.*, ASM International, Materials Park, OH, 1990, p 2444
2016Mat: N. Mattern, Y. Yokoyama, A. Mizuno, J.H. Han, O. Fabrichnaya, M. Richter, and S. Kohara, Experimen-

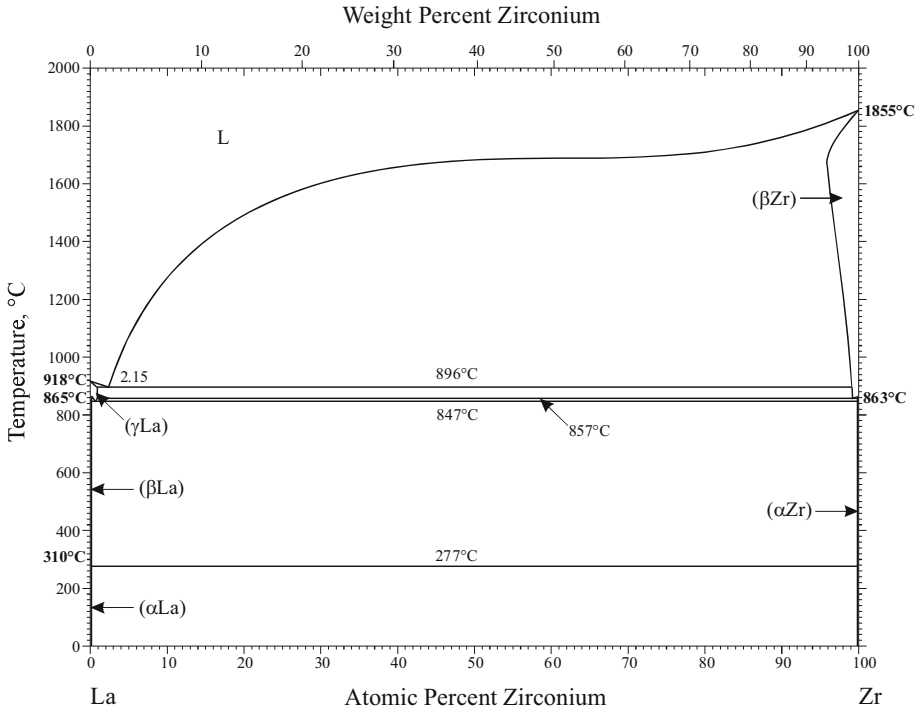

Fig. 10 La-Zr phase diagram [2016Mat]

Table 2 La-Zr crystal structure data

Phase	Composition, at.% Zr	Pearson symbol	Space group	Strukturbericht designation	Prototype
(γLa)	0 to 0.8	*cI*2	$Im\bar{3}m$	*A*2	W
(βLa)	0 to 0.08	*cF*4	$Fm\bar{3}m$	*A*1	Cu
(αLa)	0	*hP*4	$P6_3/mmc$	*A*3′	αLa
(βZr)	96 to 100	*cI*2	$Im\bar{3}m$	*A*2	W
(αZr)	99.71 to 100	*hP*2	$P6_3/mmc$	*A*3	Mg

tal and Thermodynamic Assessment of the La-Ti and La-Zr Systems, CALPHAD, 2016, 52, p 8-20

Li-Sn (Lithium-Tin)

The Li-Sn phase diagram in [1990Mas] was copied from [1976Mof]. It was constructed based on [1934Gru] with modification for the composition range from Li_7Sn_2 to LiSn according to [1979Bai]. Subsequently, this system was assessed by [1998San].

Thermodynamic modeling of the phase diagram was attempted by [1996Gas], [2005Yin], [2006Du], and [2014Wan] based on the same experimental data as used by [1998San] for assessment.

Further improvement of the Li-Sn phase diagram was achieved by [2014Li]. DTA measurements were carried out in order to clarify reactions involving L, $Li_{17}Sn_4$, Li_7Sn_2, and $Li_{13}Sn_5$. Figure 11 shows the Li-Sn phase diagram calculated by [2014Li] based on the new experimental data. $Li_{22}Sn_5$ in [1998San] was replaced by $Li_{17}Sn_4$. Table 3 shows Li-Sn crystal structure data copied from [1998San] with changes for $Li_{17}Sn_4$ according to [2003Lup]. This editor suspects the stability of $Li_{13}Sn_5$ at low temperatures because of its extreme proximity to Li_5Sn_2, as suggested by [1993Oka].

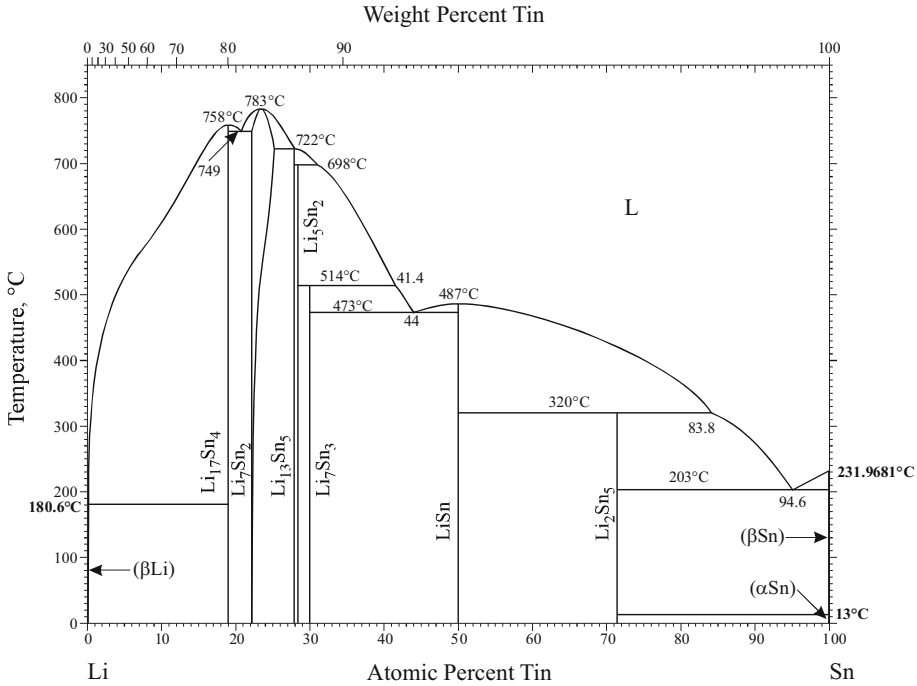

Fig. 11 Li-Sn phase diagram [2014Li]

Table 3 Li-Sn crystal structure data

Phase	Composition, at.% Sn	Pearson symbol	Space group	Strukturbericht designation	Prototype
(βLi)	0	*cI*2	$Im\bar{3}m$	*A*2	W
$Li_{17}Sn_4$	19.0	*cF*420	$F\bar{4}3m$	…	…
Li_7Sn_2	22.2	*oC*36	*Cmmm*	…	…
$Li_{13}Sn_5$	27.8	*hP*18	$P\bar{3}m1$	…	…
Li_5Sn_2	28.6	*hR*7	$R\bar{3}m$	$D8_i$	Mo_2B_5
Li_7Sn_3	30	*mP*20	$P2_1/m$	…	…
LiSn	50	*mP*6	*P*2/*m*	…	…
Li_2Sn_5	71.4	*tP*14	*P*4/*mbm*	…	…
(βSn)	100	*tI*4	$I4_1/amd$	*A*5	βSn
(αSn)	100	*cF*8	$Fd\bar{3}m$	*A*4	C (diamond)

References

1934Gru: G. Grube and E. Meyer, Electrical Conductivity and Phase Diagram of Binary Alloys, The Li-Sn System, Z. Elektrochem., 1934, 40(11), p 771-777 in German

1976Mof: W.G. Moffatt, ed, *Handbook of Binary Phase Diagrams*, General Electric Co., Schenectady, NY, 1976 and annual update

1979Bai: D.M. Bailey, W.H. Skelton, and J.F. Smith, Li-Sn Phase Relationships between Li_7Sn_2 and LiSn, J. Less-Common Met., 1979, 64(2), p 233-240

1990Mas: T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Li-Sn (Lithium-Tin), *Binary Alloy Phase Diagrams*, *2nd ed*., ASM International, Materials Park, OH, 1990, p 2469-2470

1993Oka: H. Okamoto and T.B. Massalski, Guidelines for Binary Phase Diagram Assessment, *J. Phase Equilib.,* 1993, *14*(3), p 316-335

1996Gas: W. Gasior, Z. Moser, and W. Zakulski, Thermodynamic Studies and the Phase Diagram of the Li-Sn System, J. Non-Cryst. Solids, 1996, 205/207, p 379-382

1998San: J. Sangster and C.W. Bale, The Li-Sn (Lithium-Tin) System, J. Phase Equilib., 1998, 19(1), p 70-75

2003Lup: C. Lupu, J.G. Mao, J.W. Rabalais, A.M. Guloy, and J.W. Richardson, X-Ray and Neutron Studies on $Li_{4.4}Sn$, Inorg. Chem., 2003, 4, p 3765-3771

2005Yin: F. Yin, X. Su, Z. Li, and J. Wang, Thermodynamic Assessment of the Li-Sn (Lithium-Tin) System, J. Alloys Compd., 2005, 393, p 105-108

2006Du: Z. Du, Z. Jiang, and C. Guo, Thermodynamic Optimizing of the Li-Sn System, Z. Metallkd., 2006, 97, p 10-16

2014Li: D. Li, S. Furtauer, H. Flandorfer, and D.M. Cupid, Thermodynamic Assessment and Experimental Investigation of the Li-Sn System, CALPHAD, 2014, 47, p 181-195

2014Wan: J. Wang, J. Han, I.H. Jung, D. Bairos, and P. Chartrand, Thermodynamic Optimization on the Binary Li-Sn System and Ternary Mg-Sn-Li System, CALPHAD, 2014, 47, p 100-113

Mn-S (Manganese-Sulfur)

The Mn-S phase diagram assessed by [1990Fra] was updated by [2011Oka] according to [2010Kan]. The S-rich side of MnS of this phase diagram was speculative due to lack of experimental data.

Figure 12 shows the complete Mn-S phase diagram assessed by [2015Dil]. The gas phase is suppressed, as in the phase diagram of [2010Kan]. Although the results of [2010Kan] and [2015Dil] are topologically the same, critical point temperatures differ up to about 500 °C. Experimental data are still not available to select a preferable phase diagram.

References

1990Fra: H.F. Franzen, Mn-S (Manganese-Sulfur), T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., *Binary Alloy Phase Diagrams*, *2nd ed*., ASM International, Materials Park, OH, 1990, p 2593, 2597

2010Kan: Y.B. Kang, Critical Evaluations and Thermodynamic Optimizations of the Mn-S and the Fe-Mn-S Systems, CALPHAD, 2010, 34, p 232-244

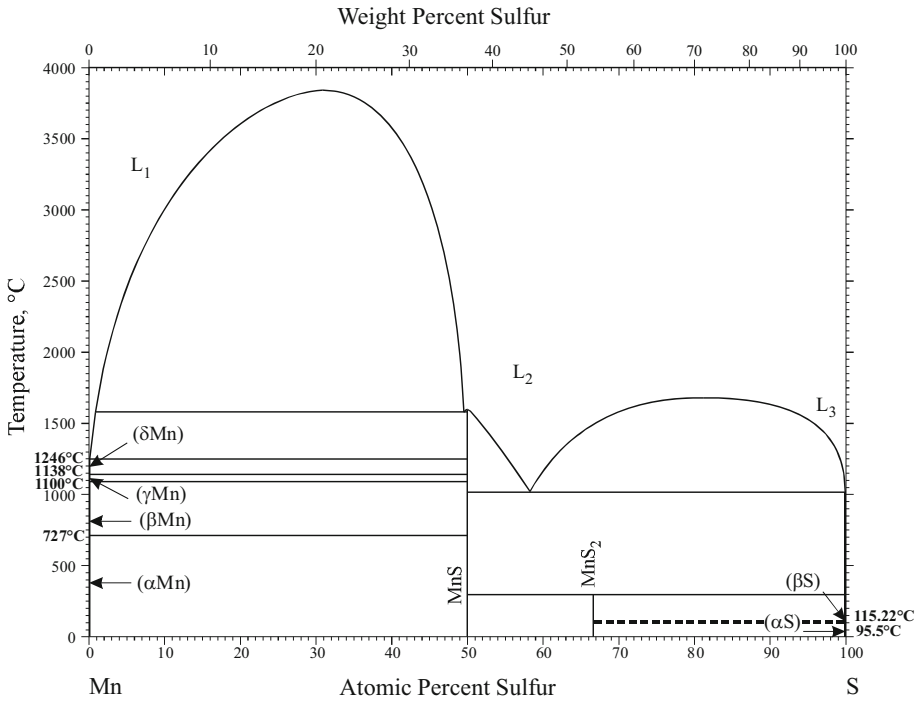

Fig. 12 Mn-S phase diagram [2015Dil] (>227 °C)

2011Oka: H. Okamoto, Mn-S (Manganese-Sulfur), J. Phase Equilib. Diffus., 2011, 32(1), p 78
2015Dil: D. Dilner, H. Mao, and M. Selleby, Thermodynamic Assessment of the Mn-S and Fe-Mn-S Systems, CALPHAD, 2010, 48, p 95-105

Nb-Re (Niobium-Rhenium)

The Nb-Re phase diagram in [1990Mas], redrawn from [1965Ell], was a preliminary version of the diagram reported by [1961Gie].

Figure 13 shows the Nb-Re phase diagram calculated by [2013Liu]. The phase boundary data reported by [1961Gie] were used as the primary basis of the thermodynamic model. Accordingly, the Nb-Re phase diagram in [1990Mas] has been improved in Fig. 13.

This system has been studied repeatedly by [1956Gre], [1959Kna], [1961Eng], [1961Lev], [1961Sav], [1969Sav], [1976Pan], [2008Jou], and [2009Jou], as well as [1961Gie]. These reports generally agreed that a narrow σ phase and a broad χ phase exist in this system, but reported phase boundaries showed significant disagreement. Further experimental studies may be needed for confirmation of the Nb-Re phase diagram shown in Fig. 13.

References

1956Gre: P. Greenfield and P.A. Beck, Intermediate Phases in Binary Systems of Certain Transition Elements, Trans. AIME, 1956, 206, p 265-275
1959Kna: A.G. Knapton, The Niobium-Rhenium System, J. Less-Common Met., 1959, 1, p 480-486
1961Eng: J.J. English, Columbium-Rhenium System, Binary and Ternary Phase Diagrams of Cb, Mo, Ta, and W, DMIC Rep. 152, 1961, p 20
1961Gie: B.C. Giessen, R. Nordheim, and N.J. Grant, The Constitution Diagram Niobium (Columbium)-Rhenium, Trans. Metall. Soc. AIME, 1961, 221, p 1009-1013
1961Lev: P. Levesque, W.R. Bekebrede, and H.A. Brown, The Constitution of Rhenium-Columbium Alloys, Trans. Am. Soc. Met., 1961, 53, p 215-226
1961Sav: J.M. Savitzki, M.A. Tylkina, and K.B. Povarova, Phase Diagram of the Niobium-Rhenium System, Planseeber. Pulvermetall., 1961, 8, p 188-191 in German
1965Ell: R.P. Elliott, Cb-Re, Columbium-Rhenium, Constitution of Binary Alloys, First Supplement, McGraw-Hill, New York, 1965, p 268-269

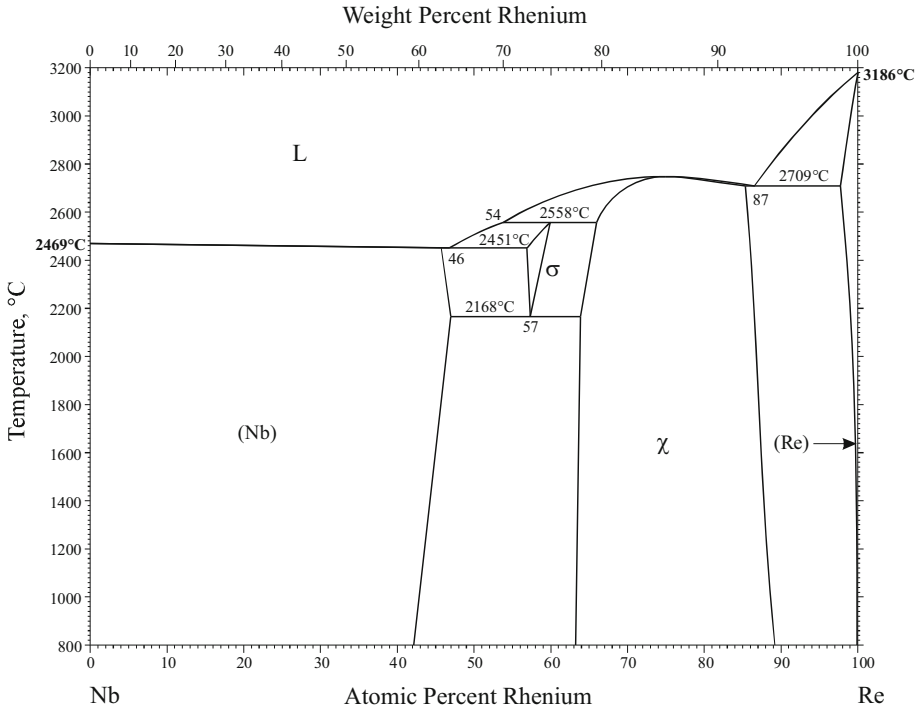

Fig. 13 Nb-Re phase diagram [2013Liu]

1969Sav: E.M. Savitskii, M.A. Tylkina, and O.K. Khamidov, Investigation of the Solid Solubility of Transition Metals in Rhenium and Some Properties of Their Alloys, Russ. Metall., 1969, (4), p 130-135

1976Pan: L.A. Panteleimonov, I.G. Sokolova, and T.O. Mkhitar'yan, A Study of the Properties of Alloys in the Rhenium-Tantalum and Rhenium-Niobium Systems, Moscow Univ. Chem. Bull., 1976, 31(1), p 94-95

1990Mas: T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, ed., Nb-Re (Niobium-Rhenium), *Binary Alloy Phase Diagrams*, *2nd ed*., ASM International, Materials Park, OH, 1990, p 2756-2757

2008Jou: J.M. Joubert, Crystal Chemistry and Calphad Modeling of the σ Phase, Prog. Mater. Sci., 2008, 53(3), p 528-583

2009Jou: J.M. Joubert and M. Phejar, Crystal Chemistry and Calphad Modeling of the χ Phase, Prog. Mater. Sci., 2009, 54(7), p 945-980

2013Liu: X.L. Liu, C.Z. Hargather, and Z.K. Liu, First-Principles Aided Thermodynamic Modeling of the Nb-Re System, CALPHAD, 2013, 41, p 119-127