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Supplemental Literature Review of Binary Phase Diagrams: Cs-In, Cs-K, Cs-Rb, Eu-In, Ho-Mn, K-Rb, Li-Mg, Mg-Nd, Mg-Zn, Mn-Sm, O-Sb, and Si-Sr

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Recent literature on Cs-In, Cs-K, Cs-Rb, Eu-In, Ho-Mn, K-Rb, Li-Mg, Mg-Nd, Mg-Zn, Mn-Sm, O-Sb, and Si-Sr phase diagrams is reviewed in this article in order to update the 1990 compilation *Binary Alloy Phase Diagrams, 2nd edition*, by T.B. Massalski, et al. For some systems reaction tables and crystal structure data have been included, as well. Diagrams have been checked for consistency with rules for phase diagram construction and modified when necessary. In addition, diagrams needing more work have been identified.

Keywords binary phase diagram, crystallography

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 Cs-In, Cs-K, Cs-Rb, Eu-In, Ho-Mn, K-Rb, Li-Mg, Mg-Nd, Mg-Zn, Mn-Sm, O-Sb, and Si-Sr 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.

Systems

Cs-In (Cesium-Indium)

The Cs-In phase diagram in [1990Mas] was redrawn from [1990Pel]. The liquidus boundaries were mostly speculative due to disagreement in available phase boundary data. Figure 1 shows the Cs-In phase diagram calculated by [2010Lee]. The experimental data used in their assessment were essentially the same as those used for assessment by [1990Pel]. The calculated phase boundaries appear to well represent the experimental data.

Cs-In crystal structure data shown in Table 1 have been updated according to [2007Vil].

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Cs-K (Cesium-Potassium)

[1983Bal] assessed the Cs-K system and [1990Mas] accepted the phase diagram. The liquidus and solidus in this phase diagram were very similar to those shown in Fig. 2. The Cs_2K phase was indicated to exist below −88 °C.

Figure 2 shows the Cs-K phase diagram calculated by [2011Ren], which is characterized by the existence of a miscibility gap in the solid phase. [1973Tan] and [1981Som] also predicted independently the existence of such miscibility gap, but with the critical point at a lower temperature of −205 and ∼−130 °C, respectively. The existence of the miscibility gap is in agreement with the concave form of the liquidus and solidus because these features are related through large positive enthalpy of mixing for the (Cs,K) solid phase.

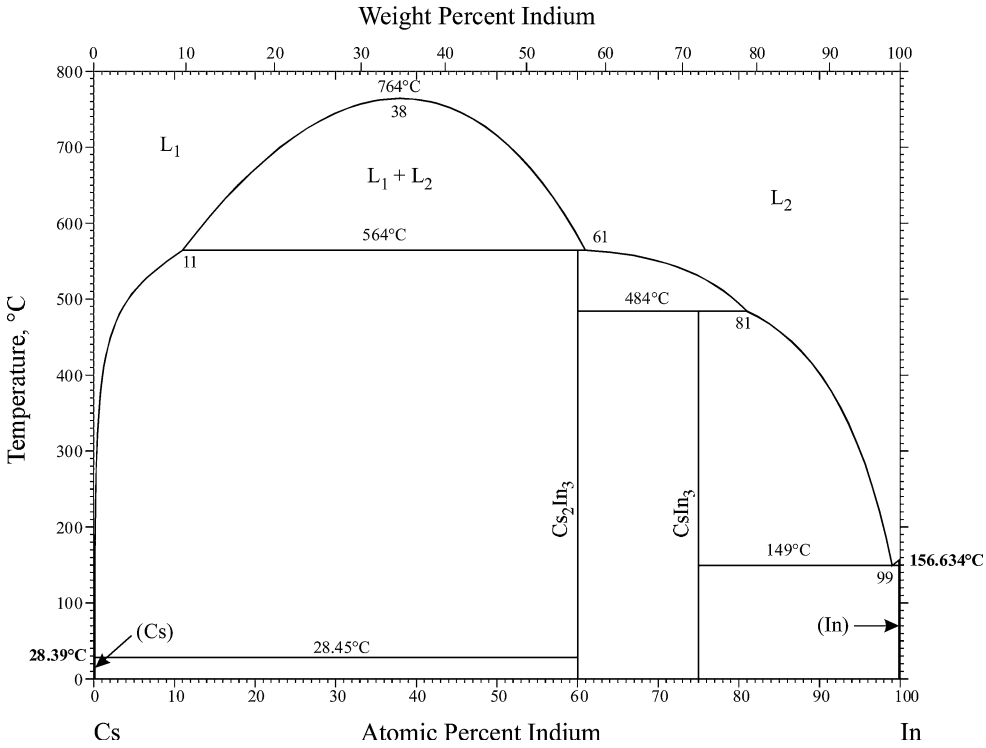

Fig. 1 Cs-In phase diagram [2010Lee]

Table 1 Cs-In crystal structure data

Phase	Composition,at.% In	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Cs)	0	*cI*2	$Im\bar{3}m$	*A*2	W
Cs_2In_3	60	*tI*20	$I\bar{4}m2$	…	…
$CsIn_3$	75	*tI*24	$I\bar{4}m2$	…	Ga_3Rb
(In)	100	*tI*2	*I*4/*mmm*	*A*6	In

[1976Sim] found Cs_6K_7 and Cs_2K in this system. However, the existence of a stable intermediate compound in the center part of the miscibility gap composition range is unlikely [1993Oka], as supported by the absence of such cases in other binary phase diagrams known so far. Because the crystal structures have been determined (Table 2), these two compounds may exist in the metastable state.

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2011Ren: X. Ren, C. Li, Z. Du, and C. Guo, Thermodynamic Assessments of Six Binary Systems of Alkali Metals, *CALPHAD*, 2011, **35**, p 446-454

Cs-Rb (Cesium-Rubidium)

[1983Bal] assessed the Cs-Rb system and [1990Mas] accepted the phase diagram. The liquidus and solidus in this phase diagram were very similar to those shown in Fig. 3. Figure 3 is the Cs-Rb phase diagram calculated by [2011Ren], which is characterized by the existence of a miscibility gap in the solid phase. [1973Tan], [1981Som], and [1983Bal] already predicted the existence of such miscibility gap. The estimated critical temperature was −179, ∼−230, and −251 °C, respectively. The existence of the miscibility gap is in agreement with the concave form of

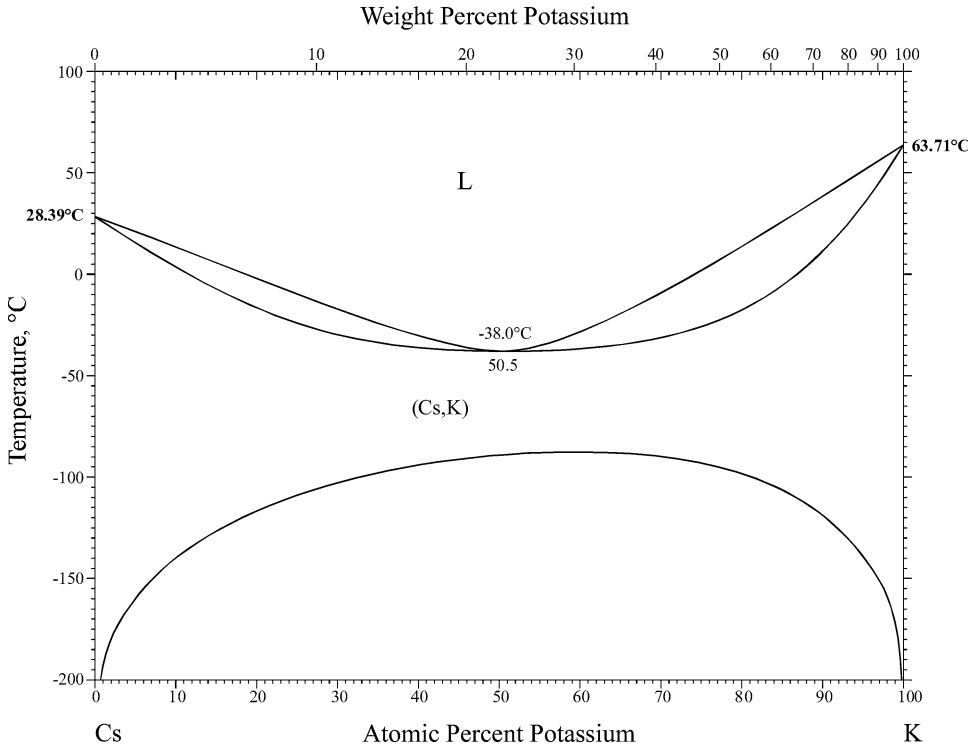

Fig. 2 Cs-K phase diagram

Table 2 Cs-K crystal structure data

Phase	Composition,at.% K	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Cs,K)	0-100	*cI*2	$Im\bar{3}m$	*A*2	W
Cs_6K_7(a)	53.8	*hP*26	$P6_3/mmc$	…	…
CsK_2(a)	66.7	*hP*12	$P6_3/mmc$	*C*14	$MgZn_2$

(a) Metastable?

the liquidus and solidus because these features are related through large positive enthalpy of mixing for the (Cs,Rb) solid phase.

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Eu-In (Europium-Indium)

The Eu-In phase diagram shown in [1990Mas] was redrawn from [1990Oka], who assessed this system based on experimental data published before 1987. There was some uncertainty in the proposed phase boundaries due to disagreement among literature data. According to [1994Oka], the form of the EuIn liquidus of this phase diagram was too asymmetric, exceeding the tolerance limit.

Figure 4 shows the Eu-In phase diagram calculated by [2011Gao]. The result falls within the range of variously reported phase boundary data shown in [1990Oka]. The problem of asymmetry described above has been solved.

Table 3 shows Eu-In crystal structure data updated by referring to [2007Vil].

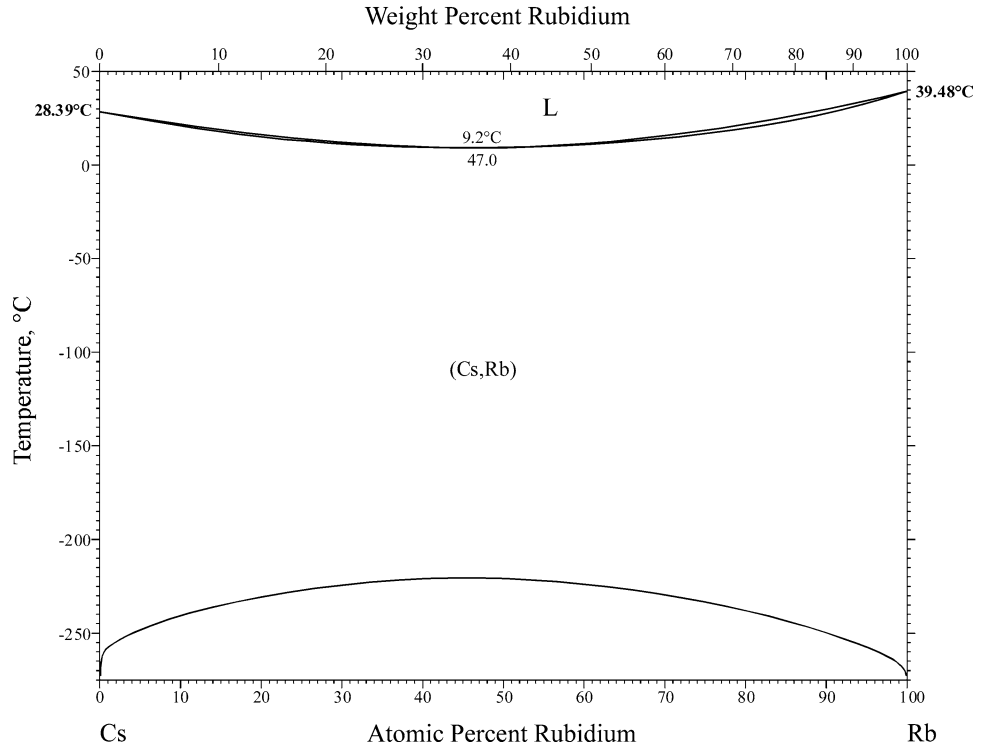

Fig. 3 Cs-Rb phase diagram

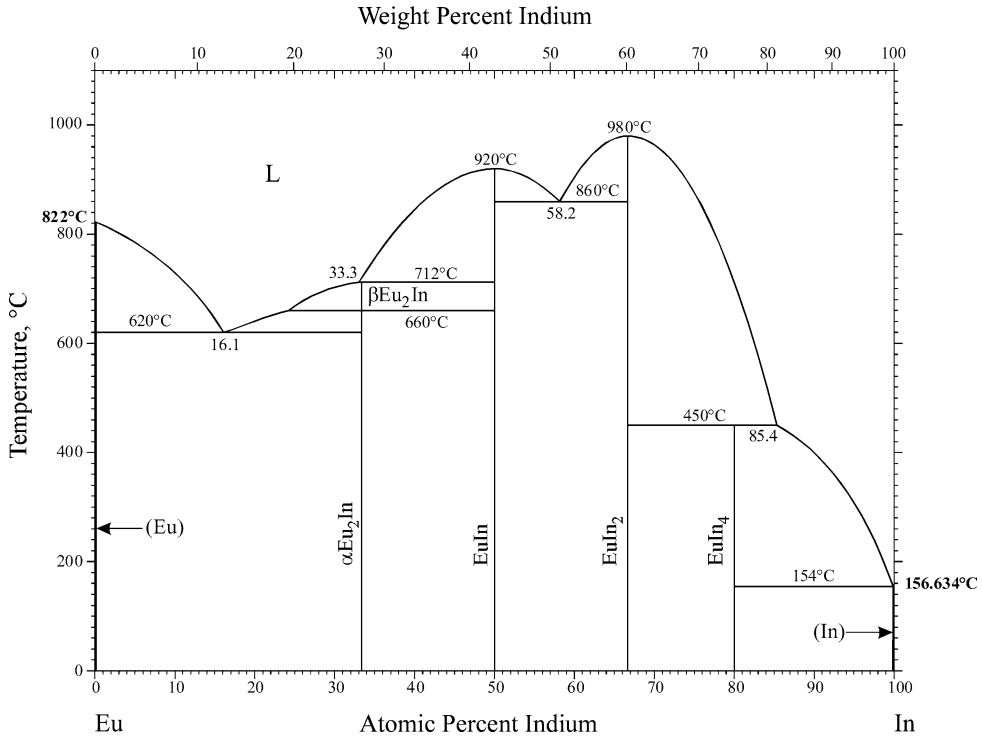

Fig. 4 Eu-In phase diagram

Table 3 Eu-In crystal structure data

Phase	Composition,at.% In	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Eu)	0	*cI*2	$Im\bar{3}m$	*A*2	W
βEu_2In	33.3	…	…	…	…
αEu_2In	33.3	*oP*12	*Pnma*	*C*23	Co_2Si
EuIn	50	*tP*2	*P4/mmm*	…	…
$EuIn_2$	66.7	*hP*6	$P6_3/mmc$	…	$CaIn_2$
$EuIn_4$	80	*mC*20	*C*12/*m*1	…	…
(In)	100	*tI*2	*I*4/*mmm*	*A*6	In

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Ho-Mn (Holmium-Manganese)

The Ho-Mn phase diagram in [1990Mas] was redrawn from [1967Kir]. According to [1994Oka], the liquidus boundaries of compounds in this phase diagram are too flat from the viewpoint of self consistency in thermodynamic properties. In addition, the initial slope of the (δMn) liquidus also seems to be too flat in view of the van't Hoff relationship between the liquidus and the solidus.

Figure 5 shows the Ho-Mn phase diagram calculated by [2009Wan]. The problem of the flat initial slope of the (δMn) liquidus has been solved. The calculated liquidus did not agree with the flat liquids curve shown in [1990Mas].

The rest of the calculated phase diagram was in good agreement with the phase diagram shown in [1990Mas]. However, the temperature dependence of the Gibbs energy for compounds used in the thermodynamic model appears to be too small when the flatness of the liquidus is taken into consideration [1991Oka]. In addition, it is difficult to imagine the liquidus of, e.g., $HoMn_{12}$ extended to the metastable Mn-rich side without causing unlikely strong asymmetry. These inconsistencies, as well as the inconsistency in the (δMn) liquidus described above, suggest that

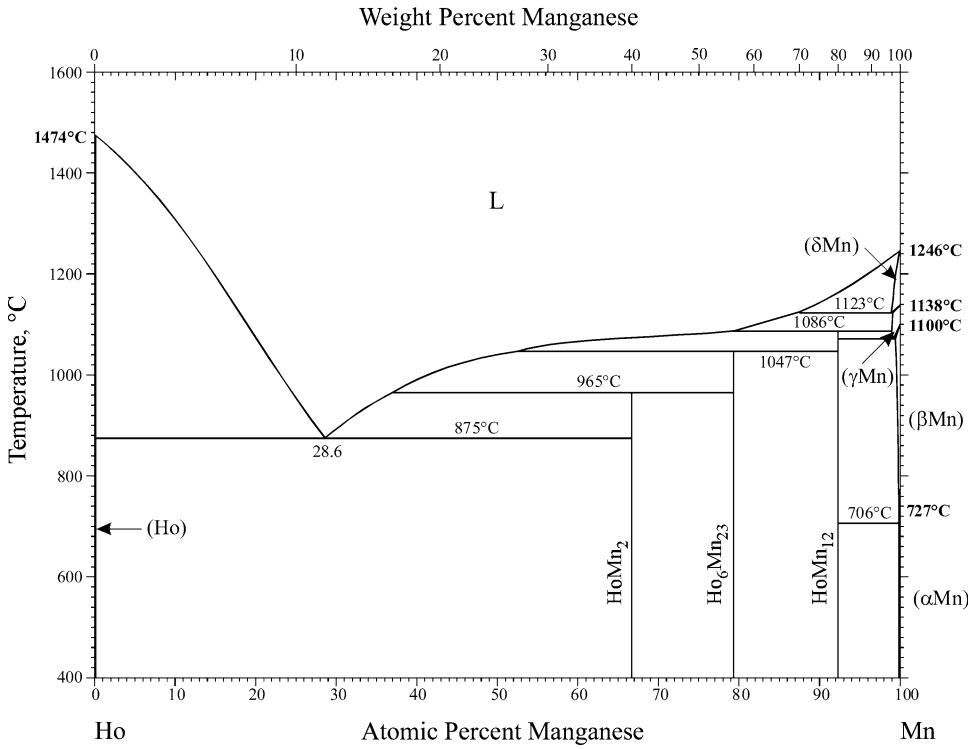

Fig. 5 Ho-Mn phase diagram [2009Wan]

the phase diagram requires reexamination experimentally or reinterpretation of the data points is necessary.

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K-Rb (Potassium-Rubidium)

[1983Bal] assessed the K-Rb system and [1990Mas] accepted the phase diagram. The liquidus and solidus in this phase diagram were very similar to those shown in Fig. 6. Figure 6 is the K-Rb phase diagram calculated by [2011Ren], which is characterized by the existence of a miscibility gap in the solid phase. [1973Tan], [1981Som], and [1983Bal] already predicted the existence of the miscibility gap. The estimated critical temperature was −180, ∼−230, and −215 °C, respectively. The existence of the miscibility gap is in agreement with the concave form of the liquidus and solidus because these features are related through large positive enthalpy of mixing for the (K,Rb) solid phase.

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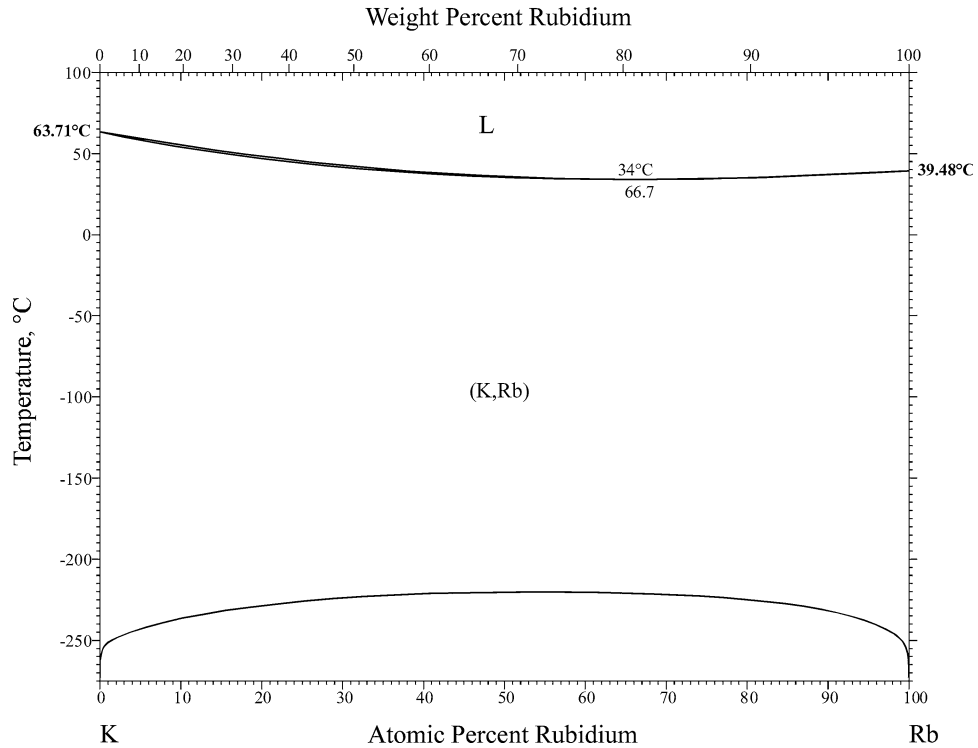

Fig. 6 K-Rb phase diagram

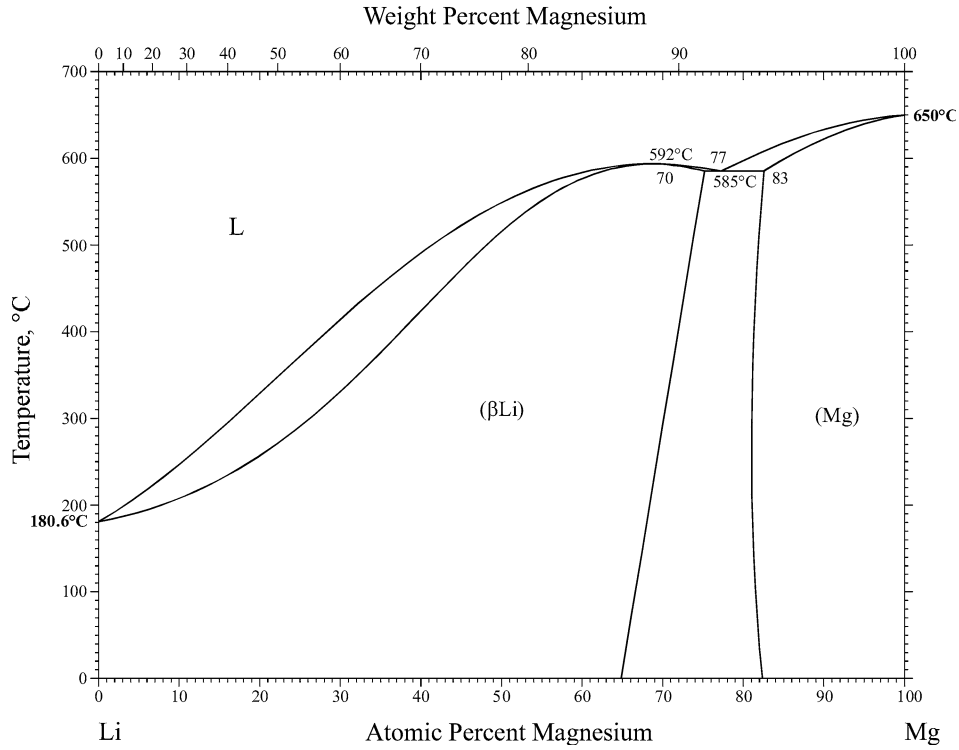

Fig. 7 Li-Mg phase diagram [2011Wan]

Li-Mg (Lithium-Magnesium)

The Li-Mg system was assessed by [1984Nay], who proposed the Li-Mg phase diagram based on experimental data published before 1978. This phase diagram was accepted in [1990Mas]. Thermodynamic modeling based on this phase diagram was attempted by [1984Nay] and [1990Sau].

New phase boundary data not shown in [1984Nay] were published by [1955Row], [1980Sch] and [1981Sch]. Thermodynamic modeling was carried out by [1996Gas] and [2000Bra] by including some of these new data. According to [2011Wan], however, the thermodynamic models used by these authors require refinement because unlikely phase separations would develop in the metastable solid and liquid regions, respectively. Figure 7 shows the Li-Mg phase diagram proposed by [2011Wan], who claimed that the calculated phase diagram agreed well with the experimental phase boundary data reported by [1945Hum], [1955Row], [1975Sab], [1981Sch], and [1996Gas]. Thermodynamic modeling of this system was attempted by [1977Sab] and [2001Kev] also.

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Mg-Nd (Magnesium-Neodymium)

The Mg-Nd phase diagram in [1990Mas] was updated by [1991Oka] based on the experimental work of [1990Del]. [2007Oka] updated the phase diagram again based on the thermodynamic assessment reported by [2005Gor].

Since then, [2006Guo], [2007Men], [2010Niu], and [2011Qi] evaluated this system thermodynamically. In these works, Mg_3Nd and MgNd phases were treated to have finite solubility ranges based on the experimental data reported by [1990Del], whereas [2005Gor] assumed them to be line compounds. From the names of authors, it is evident that [2010Niu] and [2011Qi] superseded [2006Guo] and [2007Men], respectively. [2011Qi] disclosed that the thermodynamic models adopted by [2006Guo] and [2007Men] were inappropriate because a solid phase becomes stable at high temperatures. Thus the Mg-Nd phase diagram calculated by [2011Qi] is chosen for the new updated diagram. Slight modifications have been made in Fig. 8 for transition temperatures of pure Nd for consistency with other Nd-based phase diagrams.

Table 4 shows Mg-Nd crystal structure data.

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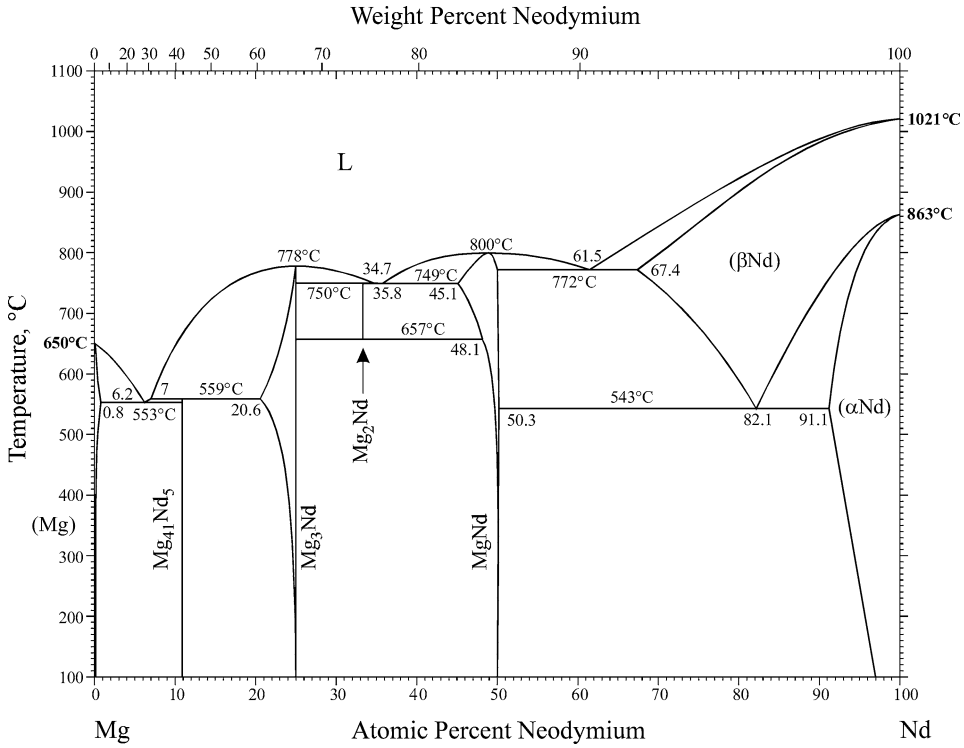

Fig. 8 Mg-Nd phase diagram

Table 4 Mg-Nd crystal structure data

Phase	Composition,at.% Nd	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Mg)	0-0.8	*hP*2	$P6_3/mmc$	*A*3	Mg
$Mg_{41}Nd_5$	10.9	*tI*92	*I*4/*m*	…	Ce_5Mg_{41}
Mg_3Nd	20.6-25	*cF*16	$Fm\bar{3}m$	$D0_3$	BiF_3
Mg_2Nd	33.3	*cF*24	$Fd\bar{3}m$	*C*15	Cu_2Mg
MgNd	45.1-50.3	*cP*2	$Pm\bar{3}m$	*B*2	CsCl
(βNd)	67.4-100	*cI*2	$Im\bar{3}m$	*A*2	W
(αNd)	91.1-100	*hP*4	$P6_3/mmc$	*A*3′	αLa

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Mg-Zn (Magnesium-Zinc)

The Mg-Zn phase diagram in [1990Mas] was adopted from [1988Cla] and updated by [1994Oka] based on the thermodynamic assessment done by [1992Aga].

The Mg-Zn phase diagram shown in Fig. 9 is based on [2012Gho]. This work superseded the earlier version proposed by the same authors' group [2009Was]. The calculated phase boundaries were in excellent agreement with the experimental data reported in [1988Cla]. The phases $Mg_{12}Zn_{13}$ and Mg_2Zn_3 in [2012Gho] have been changed to $Mg_{21}Zn_{25}$ and Mg_4Zn_7, respectively, according to the crystal structure data (Table 5). The former phase was shown as MgZn in [1990Mas] but no phase was found at the equiatomic composition. Its crystal structure has never been reported in spite of its simple formula. Therefore, its existence is doubtful.

Earlier thermodynamic calculations done by [1992Aga], [1998Lia], and [2008Mie] assumed that the $MgZn_2$ phase was a line compound. However, [1994God] observed a measurable width in this phase. This feature has been included in the assessment of [2009Was] and [2012Gho].

Table 5 shows Mg-Zn crystal structure data. The data for $Mg_{21}Zn_{25}$ and Mg_4Zn_7 were taken from [2002Cer] and [1975Yar], respectively.

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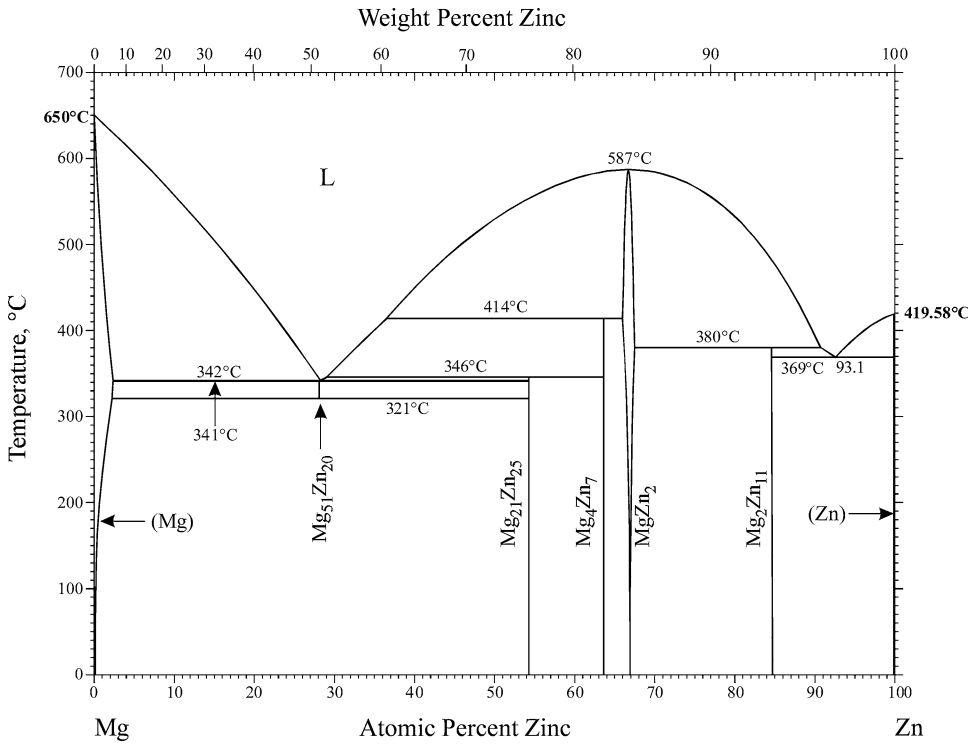

Fig. 9 Mg-Zn phase diagram

Table 5 Mg-Zn crystal structure data

Phase	Composition,at.% Zn	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Mg)	0-2	*hP*2	$P6_3/mmc$	*A*3	Mg
$Mg_{51}Zn_{20}$	28.1	*oI*158	*Immm*	…	…
$Mg_{21}Zn_{25}$	54.3	*hR*276	$R\bar{3}c$	…	…
Mg_4Zn_7	63.6	*mC*110	*C*12/*m*1	…	…
$MgZn_2$	66-67.5	*hP*12	$P6_3/mmc$	*C*14	$MgZn_2$
Mg_2Zn_{11}	84.6	*cP*39	$Pm\bar{3}$	$D8_c$	Mg_2Zn_{11}
(Zn)	100	*hP*2	$P6_3/mmc$	*A*3	Mg

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Mn-Sm (Manganese-Samarium)

The Mn-Sm phase diagram in [1990Mas] was redrawn from [1970Kir]. [1994Oka] pointed out that the (δMn) and (γSm) liquidus boundaries of this phase diagram are too flat in comparison with the slopes expected from the van't Hoff relationship between the liquidus and the solidus.

This problem was solved in the Mn-Sm phase diagrams calculated by [2009Wan] and [2012Kim]. Figure 10 shows the result of [2012Kim], who claimed that the thermodynamic model used by [2009Wan] did not agree well with experimental thermodynamic data. This disagreement probably caused why both (δMn) and (γSm) liquidus calculated by [2009Wan] showed unlikely change in the sign of curvature within a short span of about 20 at.% from either end of the phase diagram. The (αSm) phase has been added

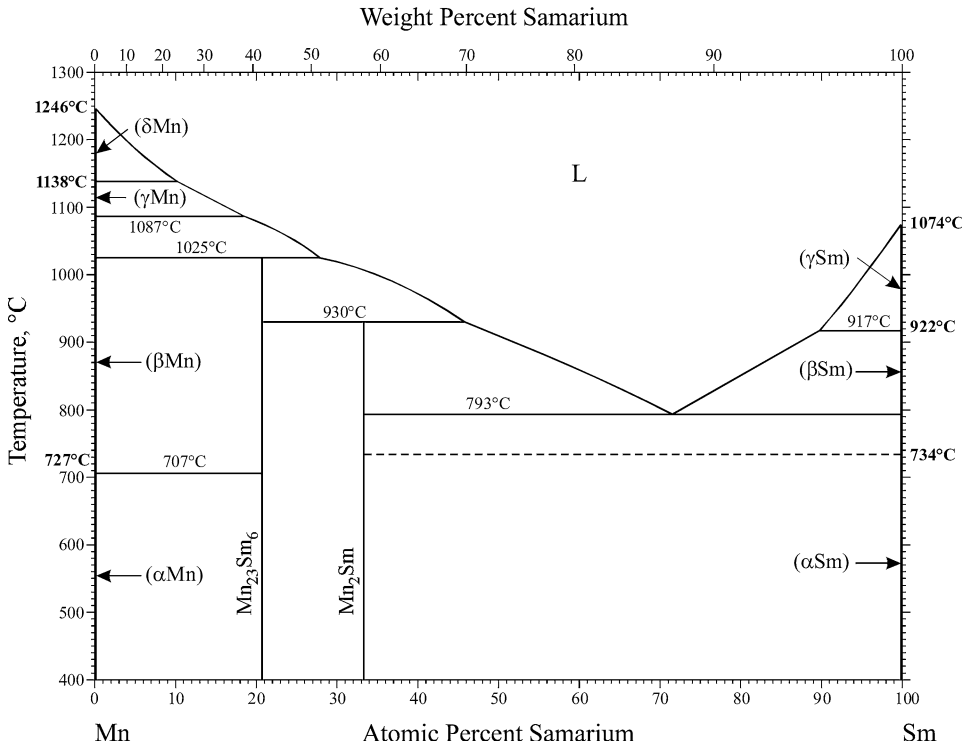

Fig. 10 Mn-Sm phase diagram

Table 6 Mn-Sm crystal structure data

Phase	Composition,at.% Sm	Pearson symbol	Space group	Strukturbericht designation	Prototype
(δMn)	0	*cI*2	$Im\bar{3}m$	*A*2	W
(γMn)	0	*cF*4	$Fm\bar{3}m$	*A*1	Cu
(βMn)	0	*cP*20	$P4_132$	*A*13	βMn
(αMn)	0	*cI*58	$I\bar{4}3m$	*A*12	αMn
$Mn_{23}Sm_6$	20.7	*cF*116	$Fm\bar{3}m$	$D8_a$	$Mn_{23}Th_6$
Mn_2Sm	33.3	*hP*12	$P6_3/mmc$	*C*14	$MgZn_2$
(γSm)	100	*cI*2	$Im\bar{3}m$	*A*2	W
(βSm)	100	*hP*2	$P6_3/mmc$	*A*3	Mg
(αSm)	100	*hR*3	$R\bar{3}m$	…	αSm

in Fig. 10 for consistency with other Sm-based phase diagrams.

Table 6 shows Mn-Sm crystal structure data. [1990Mas] indicated the existence of a Cu_2Mg type modification for the Mn_2Sm phase. However, this modification has never been confirmed.

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O-Sb (Oxygen-Antimony)

The partial Sb-O phase diagram (50-80 at.% O) in [1990Mas] was based primarily on [1957Hen]. Fragmental information from other sources has been added. The existence of SbO was reported by [1957Hen] but its crystal structure was unknown.

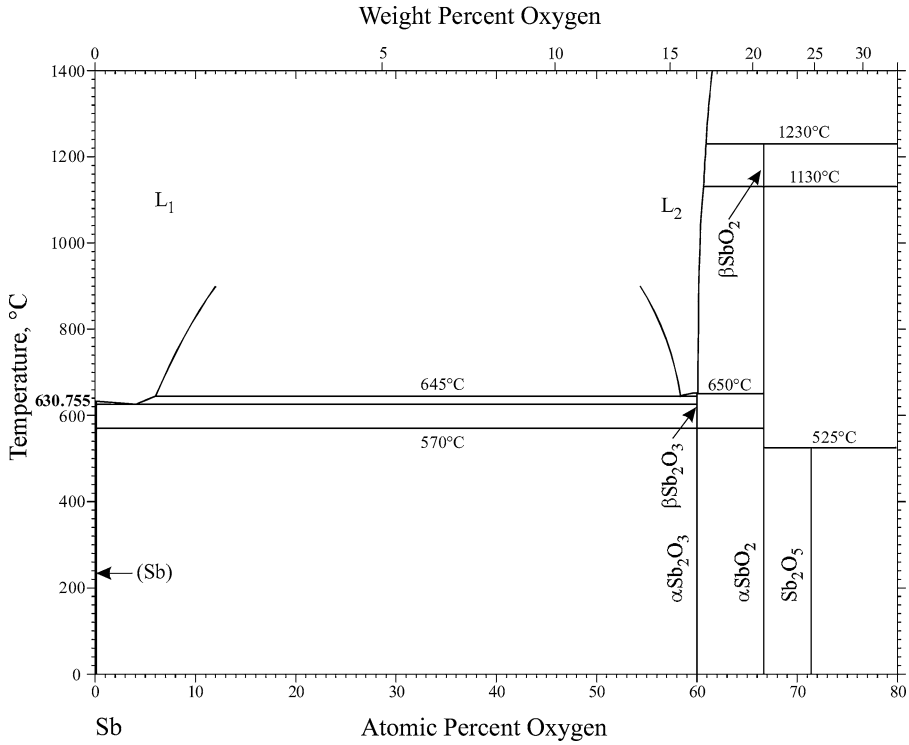

Fig. 11 Sb-O phase diagram

Table 7 Sb-O crystal structure data

Phase	Composition,at.% O	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Sb)	0	*hR*2	$R\bar{3}m$	*A*7	αAs
βSb_2O_3	60	*oP*20	*Pccn*	…	…
αSb_2O_3	60	*cF*80	$Fd\bar{3}m$	…	As_2O_3
βSbO_2	66.7	*mC*24	*C*12/*c*1	…	…
αSbO_2	66.7	*oP*24	$Pna2_1$	…	…
Sb_2O_5	71.4	…	*C*12/*c*1	…	…

[1981Dem] investigated the Sb-O system by means of DTA and x-ray diffraction for the composition range 0-66.7 at.% O. A liquid phase miscibility gap was found instead of a compound SbO. Figure 11 shows the Sb-O phase diagram constructed by combining [1981Dem] (0-50 at.% O) and [1990Mas] (50-80 at.% O). The shape of the miscibility gap has been modified because the one speculated by [1981Dem] was very asymmetric. According to [1981Dem], the temperature of the L → βSb_2O_3 + αSbO_2 eutectic is 585 °C, too significant disagreement with the phase diagram shown in Fig. 11 to disregard. Further clarification is needed in this range because the phase diagram in [1990Mas] was tentative.

Table 7 shows Sb-O crystal structure data according to [2007Vil].

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2007Vil: P. Villars and K. Cenzual, Pearson's Crystal Data CD-ROM, ASM International, Materials Park, OH, 2007

Si-Sr (Silicon-Strontium)

The Si-Sr phase diagram in [1990Mas] was updated by [2006Oka] based on the work of [2004Pal]. The β/α transition of Si_2Sr was not clearly shown. In addition, a question was raised with regard to the strong asymmetry of the βSi_2Sr liquidus.

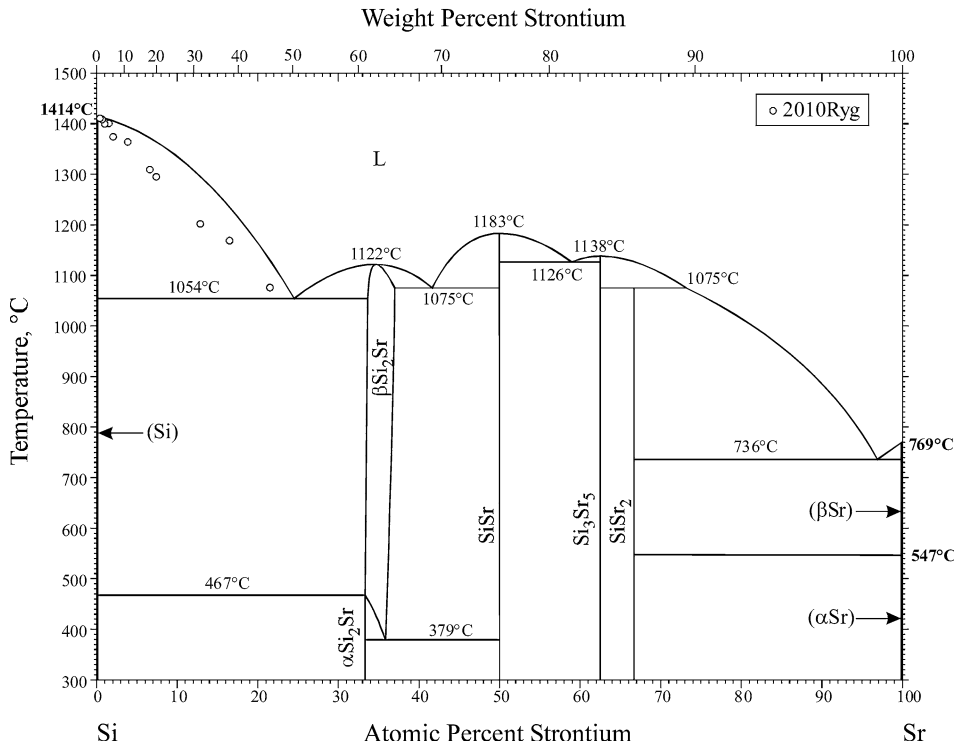

Fig. 12 Si-Sr phase diagram [2011Li]

These shortcomings have been alleviated in the phase diagrams thermodynamically assessed by [2009Gar] and [2011Li]. [2011Li] disclosed that the thermodynamic model used by [2009Gar] may be inappropriate because unlikely inversed miscibility gap would be developed at high temperatures. Figure 12 shows the Si-Sr phase diagram calculated by [2011Li] with an associated model for the liquid phase. [2011Li] calculated also with a substitutional solution model for the liquid phase and obtained a similar result. Both results were in good agreement with the experimental data reported by [2004Pal]. Recently, [2010Ryg] measured the (Si) liquidus. The result is shown in Fig. 12. There are no data points in this range in the work of [2004Pal]. The experimentally determined liquidus temperature is as much as ~100 °C lower than the thermodynamically estimated value by [2009Gar] or [2011Li] at around 10 at.% Sr. This difference is rather large to disregard. If the result of [2010Ryg] is confirmed experimentally, refinement is needed in the thermodynamic modeling.

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