Ca-Fe (Calcium-Iron)

H. Okamoto

The Ca-Fe phase diagram in [Massalski2] was redrawn from [1992Kah]. The Ca-Fe phase diagram near the Fe corner was reported by [1993Gla] partly based on [1960Kre] for the solubility of Ca in liquid Fe, as reviewed by [1994Oka]. This phase diagram is shown in Fig. 1. Formation of a γ loop was concluded in this study.

Solid lines in Fig. 2 show the Ca-Fe phase diagram reported by [1987Sch]. The Ca corner of this phase diagram is enlarged in Fig. 3. The (γFe) phase was not shown in the diagram of [1987Sch]. This can be explained by assuming that the γ loop is so narrow that it is located within the line width of the pure Fe line. This is quantitatively consistent with the diagram of [1993Gla] (Fig. 1). However, the quantitative scale of Fig. 1 is questionable, as discussed below. Figure 4 shows the Fe corner of the Ca-Fe phase diagram calculated by [1994Ang]. The $L_1 + L_2/L_2$ boundary was calculated based on the data of [1964Spo] and [1985Koh]. When Fig. 1 and 4 are compared, it is found

that discrepancy in the solubility of Ca in liquid Fe is about 100 times. It is more reasonable to assume that the scale in Fig. 1 is questionable because the six 9 purity in the horizontal axis is very uncommon.

The (γFe) phase was missing in the diagram of [1987Sch], as described above. However, the van't Hoff relationship demands certain initial angle for the (αFe)/(αFe) + (γFe) boundary away from the 100% Fe line at both highest and lowest temperature limits (1394 and 912 °C). Because the $L_1 + $ (αFe)/(αFe) boundary is located very close to the 100% Fe line, the γ loop must cross this boundary. The temperatures at the crossing should not be much different from the allotropic transformation temperatures of γFe. Two dashed lines have been added in Fig. 2 to reflect this situation. After all, the overall Ca-Fe phase diagram looks like the one proposed by [1992Kah], but the behavior of the (γFe) phase must be clarified (tends to form a γ loop or not).
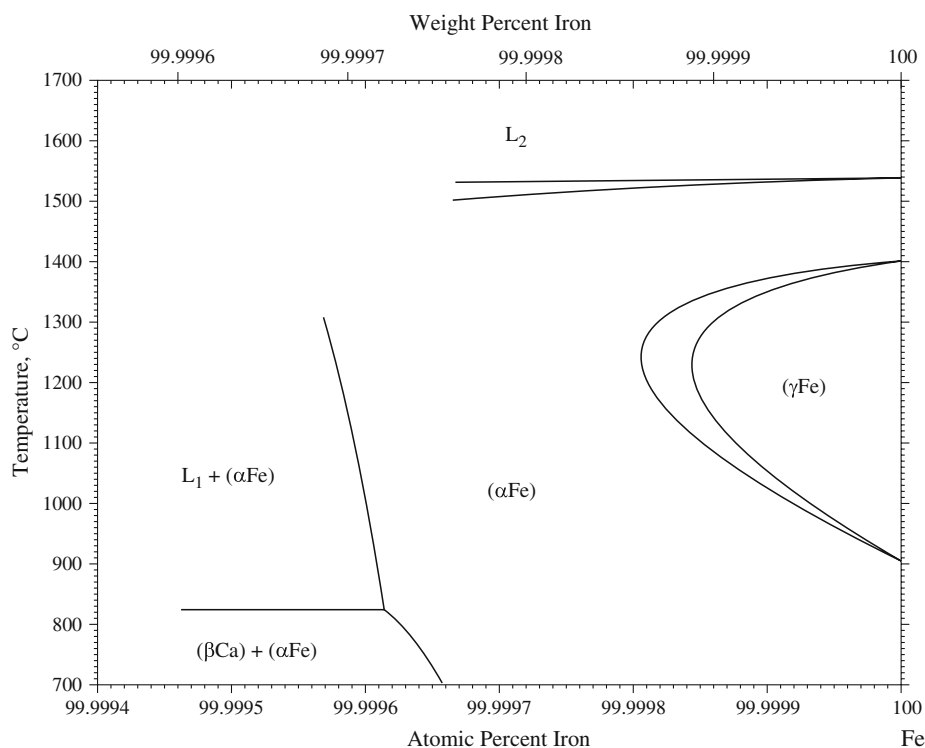
Ca-Fe crystal structure data are given in Table 1.

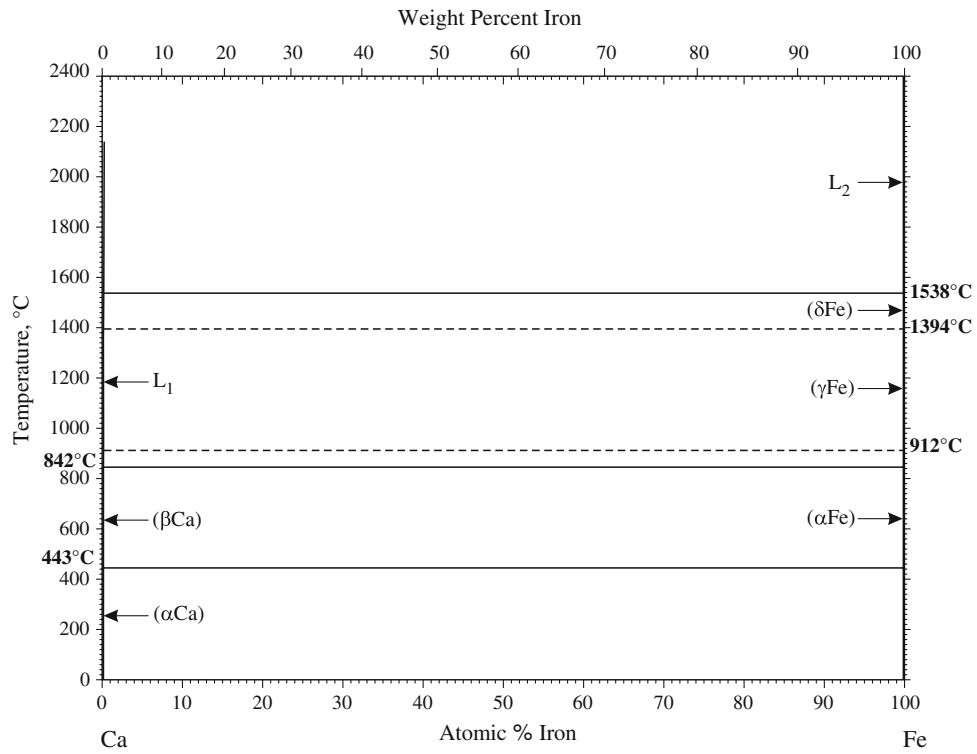**Fig. 1** Fe corner of the Ca-Fe phase diagram [1993Gla] (composition scale may be wrong)
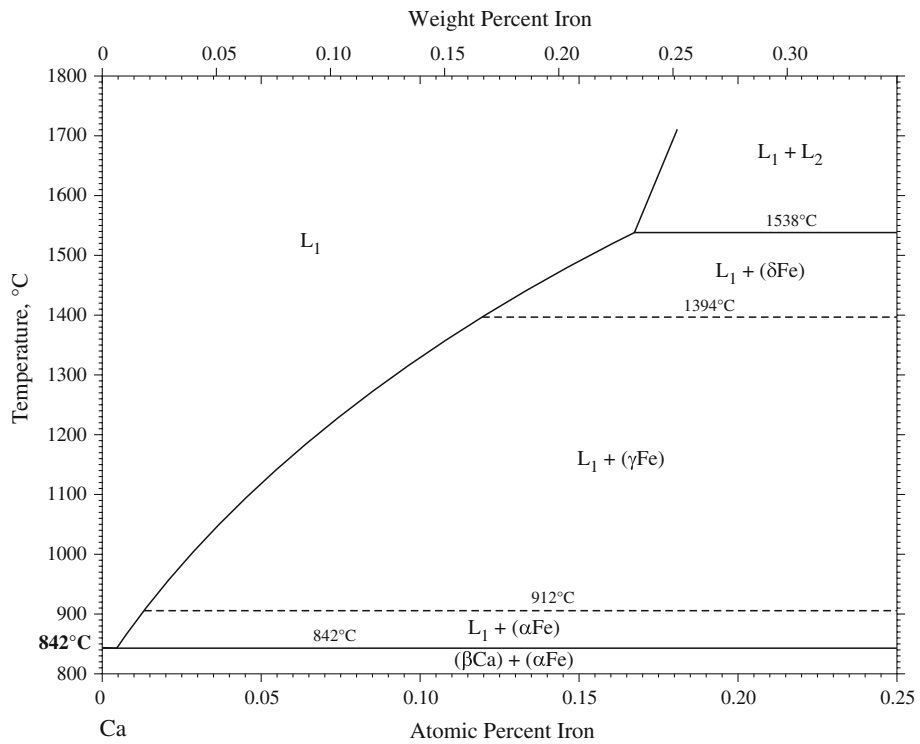
Fig. 2 Ca-Fe phase diagram [1987Sch]

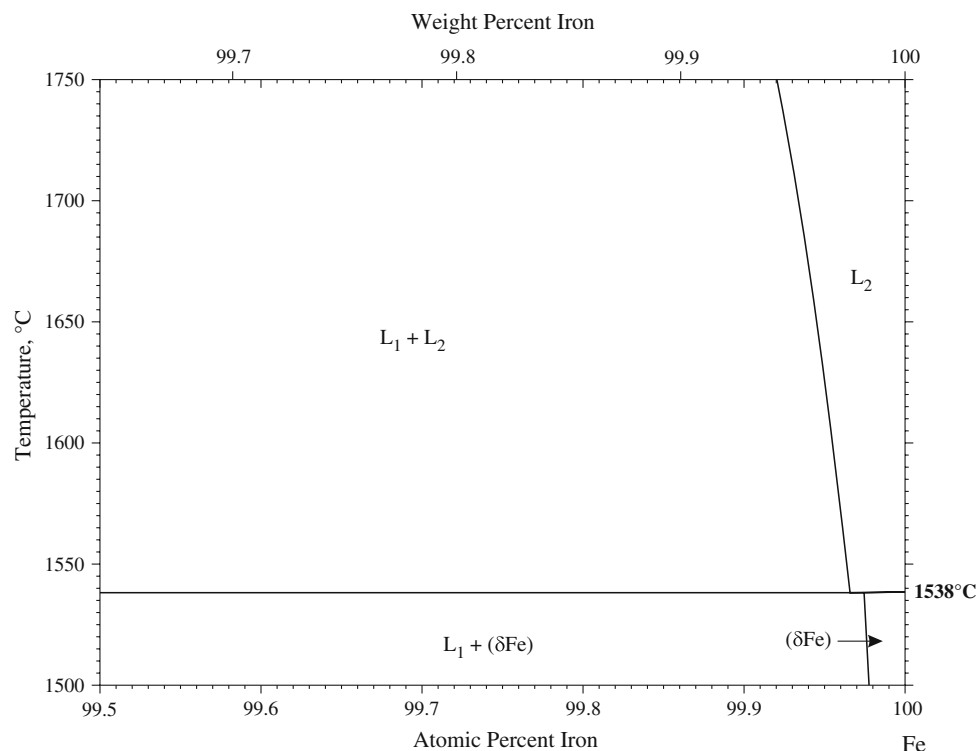**Fig. 3** Ca corner of the Ca-Fe phase diagram shown in Fig. 2

Fig. 4 Fe corner of the Ca-Fe phase diagram calculated by [1994Ang]

Table 1 Ca-Fe crystal structure data

Phase	Composition, at.% Fe	Pearson symbol	Space group	Strukturbericht designation	Prototype
(βCa)	0	$cI2$	$Im\overline{3}m$	$A2$	W
(αCa)	0	$cF4$	$Fm\overline{3}m$	$A1$	Cu
(δFe)	99.97-100	$cI2$	$Im\overline{3}m$	$A2$	W
(γFe)	~100	$cF4$	$Fm\overline{3}m$	$A1$	Cu
(αFe)	~100	$cI2$	$Im\overline{3}m$	$A2$	W

References

1960Kre: N.S. Kreshchanovskii, On the Partition of Calcium in Cast Steel, *Liteinoe Proizvod.*, 1960, (8), p 31; quoted in [1993Gla]

1964Spo: D.L. Sponseller and R.A. Flinn, The Solubility of Calcium in Liquid Iron and Third-Element Interaction Effects, *Trans. Metall. Soc. AIME*, 1964, **230**, p 876-888

1985Koh: M. Köhler, H.J. Engell, and D. Janke, Solubility of Calcium in Fe-Ca-X$_j$ Melts, *Steel Res.*, 1985, **56**(8), p 419-423

1987Sch: E. Schürmann and H. Jacke, Melting Equilibria in the System Fe-C-Ca, *Steel Res.*, 1987, **58**(9), p 399-405, in German

1992Kah: D.J. Kahan and L.J. Swartzedruber, Ca-Fe (Calcium-Iron), *Phase Diagrams of Binary Iron Alloys*, H. Okamoto, Ed., ASM International, Materials Park, OH, 1992, p 84-86

1993Gla: V.N. Gladkii and N.T. Shevelev, New Data on the Fe-Ca Phase Diagram, *Izv. Ross. Akad. Nauk, Metally*, 1993, (6), p 207-209, in Russian, TR: *Russ. Metall.*, 1993, (6), p 113-115

1994Ang: J.C. Anglezio, C. Servant, and I. Ansara, Contribution to the Experimental and Thermodynamic Assessment of the Al-Ca-Fe-Si System—I. Al-Ca-Si, Al-Fe-Si, and Ca-Fe-Si Systems. *Calphad*, 1994, **18**(3), p 273-309

1994Oka: H. Okamoto, Comment on Ca-Fe (Calcium-Iron), *J. Phase Equilib.*, 1994, **15**(5), p 565-566