JPEDAV (2009) 30:369–371
DOI: 10.1007/s11669-009-9536-8
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Al-C-Fe (Aluminum-Carbon-Iron)

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The early literature on this ternary system was reviewed by [1987Rag], who presented for Fe-rich alloys a liquidus projection, a reaction sequence and four isothermal sections at 1250, 1100, 1000 and 25 °C. Subsequently, [1991Har] computed a liquidus projection and eight isothermal sections at 2000, 1850, 1700, 1300, 1200, 1100, 1000 and 800 °C. This work was updated by [1993Rag]. A second update by [2002Rag] reviewed the experimental results of [1995Pal]. More recently, [2004Oht] carried out a thermodynamic assessment of this system, which was reviewed by [2007Rag]. Most recently, [2008Con] reexamined the thermodynamic analysis and presented a new thermodynamic assessment. The new results of [2008Con] will be reviewed briefly in this update.

Binary Systems

In the Al-C phase diagram, Al_4C_3 is of fixed composition and has the $D7_1$-type of rhombohedral structure. In the Fe-Al phase diagram, the solid solution γ based on face-centered cubic (fcc) Fe is restricted by a loop. The solid solution based on the body-centered cubic (bcc) Fe (α) exists in both the disordered ($A2$) and ordered ($B2$ and $D0_3$) forms. The $A2 \rightarrow B2$ transition is second order down to ~600 °C; below that, a two-phase field of ($A2 + B2$) intervenes indicative of a first-order transition. Apart from the high temperature cubic phase ε ($D8_2$, Cu_5Zn_8-type cubic), there are three intermediate phases in the system with restricted ranges of homogeneity: $FeAl_2$ (triclinic), Fe_2Al_5 (orthorhombic) and $FeAl_3$ or Fe_4Al_{13} (monoclinic). The stable Fe-C phase diagram has a peritectic reaction at 1493 °C, where the γ (fcc) forms from L and δ (bcc). At 1153 °C, a eutectic reaction yields γ + graphite (gr). The stable eutectoid reaction occurs at 740 °C: γ ↔ α (bcc) + gr. Computed phase diagrams of the above binary systems were given by [2008Con].

Computed Ternary Phase Equilibria

The phase equilibria near the γ region in the computed sections of [2004Oht] were not correctly predicted, as pointed by [2007Rag]. [2008Con] reexamined the thermodynamic model parameters in order to rectify this anomaly. They carried out *ab initio* calculations to derive the enthalpy of formation of metastable ordered and disordered fcc phases in the Al-Fe system. The computed phase equilibria from the derived parameters showed good agreement with the experimental data of the γ loop region at the Fe end and of the Fe solubility in Al at the Al-end. These *ab initio* parameters were fed along with experimental data in the

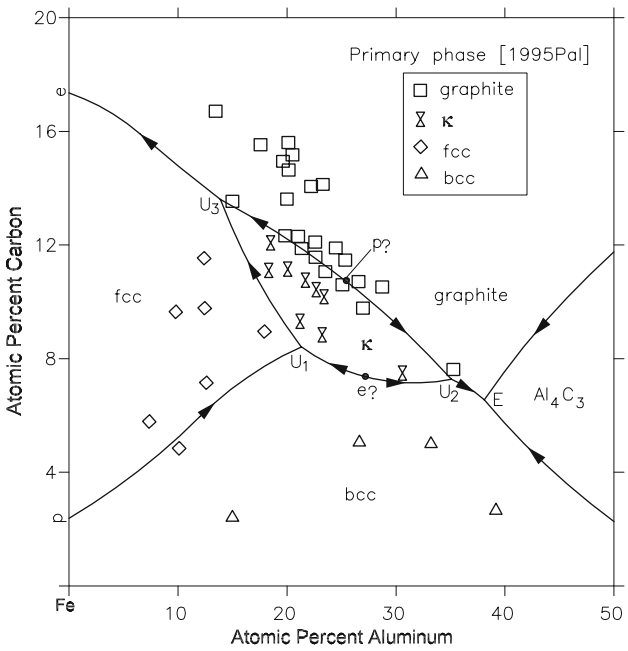

Fig. 1 Al-C-Fe computed liquidus projection [2008Con]

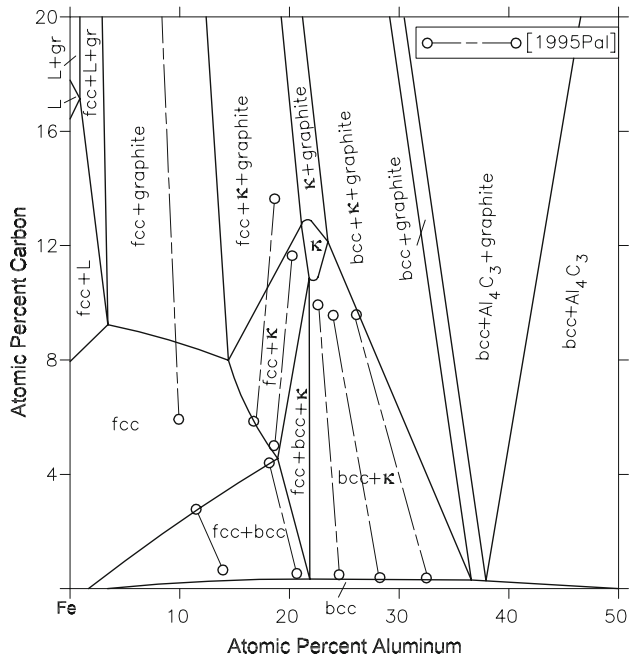

Fig. 2 Al-C-Fe computed isothermal section at 1200 °C [2008Con]

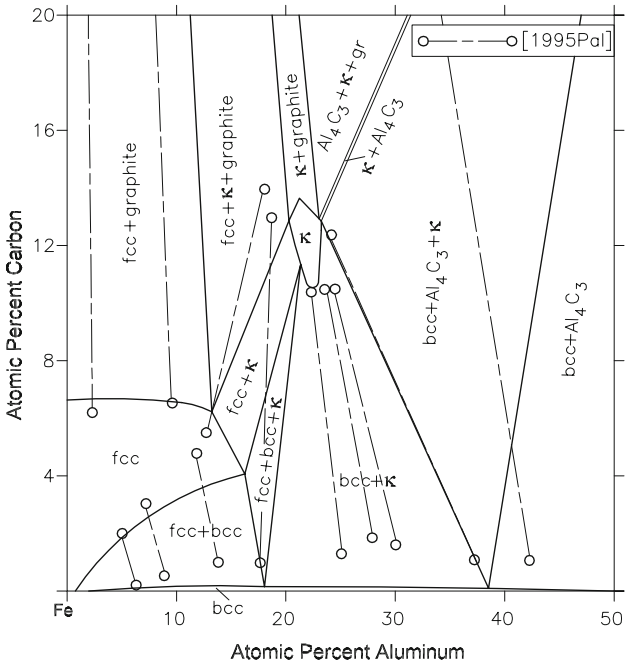

Fig. 3 Al-C-Fe computed isothermal section at 1000 °C [2008Con]

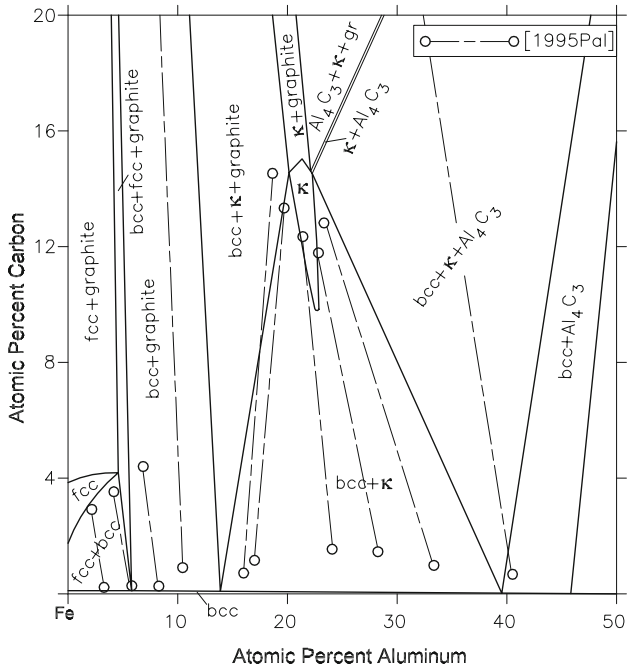

Fig. 4 Al-C-Fe computed isothermal section at 800 °C [2008Con]

Table 1 Al-C-Fe invariant reaction temperatures (°C)

Invariant reaction	[2008Con]	[2004Oht]	[1995Pal]	[1991Har]	[1986Sch]
U_1: L + α ↔ γ + κ	1339	1342	1315	1318	1313
U_2: L + κ ↔ α + gr	1278	1308	1295	1297	1305
U_3: L + κ ↔ γ + gr	1311	1365	1282	1282	1284

optimization. Care was taken to see that the change in the description of the Al-Fe fcc phase had no effect on the phase equilibria of the binary system or its extrapolation to ternary systems such as Al-Fe-Mn and Al-Fe-Ni.

In their thermodynamic modeling, [2008Con] used the substitutional regular solution model for the liquid phase. The ordered and disordered forms of the bcc phase were described with the same Gibbs energy function, with an ordering-energy term. The magnetic contribution to the Gibbs energy was taken into account. The fcc phase was similarly described by taking into account the possible ordering reactions. The $E2_1$-type ternary phase κ (Fe_3AlC_x) was described by combining the $L1_2$-type ordering of Fe and Al, with the interstitial ordering of C within that structure. The main experimental data used in optimization were the liquidus projection and the isothermal sections of [1995Pal].

A liquidus projection, three isothermal sections at 1200, 1000 and 800 °C and three vertical sections at 5C, 10.5C and 22Al (at.%) were computed by [2008Con] and compared with the experimental data of [1995Pal]. Here, the liquidus projection and the three isothermal sections are shown in Fig. 1-4. The agreement is satisfactory. The invariant reaction temperatures computed by [2008Con], however, do not show good agreement with the experimental data of [1986Sch] and [1995Pal] or the computed values of [1991Har], see Table 1.

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