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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 Al-rich alloys, a liquidus projection, a reaction scheme, and four isothermal sections at 1250, 1100, 1000 and 25 °C. A thermodynamic evaluation by [1991Har] presented a tentative reaction scheme for the entire composition range, a computed liquidus projection, and isothermal sections at 2000, 1850, 1700, 1300, 1200, 1100, 1000, and 800 °C. An update by [1993Rag] reviewed the results of [1991Har]. A second update by [2002Rag] reviewed the detailed experimental investigation of this system by [1995Pal]. Recently, [2004Oht] carried out a new thermodynamic analysis covering the whole system. The more recent experimental results of [1995Pal] were used in the optimization. The formation energy of the ternary $\kappa$ phase was estimated from first principle band energy calculations.

## 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 $\gamma$ based on face-centered cubic (fcc) Fe is restricted by a loop. The solid solution based on the body-centered cubic (bcc) Fe ($\alpha$) exists in both the disordered ($A2$) and ordered ($B2$ and $D0_3$) forms. The $\alpha(A2) \rightarrow B2$ transition is second order down to ~ 600 °C; below that a two-phase field of $(\alpha + B2)$ intervenes indicative of a first-order transition. Apart from the high temperature phase $\varepsilon$ , 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 $\gamma$ (fcc) forms from $L$ and $\delta$ (bcc). At 1153 °C, a eutectic reaction yields $\gamma$ + graphite (gr). The stable eutectoid reaction occurs at 740 °C, yielding $\alpha$ (bcc) + gr.

## Computed Ternary Phase Equilibria

The ternary compound $Fe_3AlC$ ($\kappa$) has the perovskite-type of structure and was modeled by [2004Oht] with three sublattices: $(Fe,Al)_3(Fe,Al)_1(C,Va)_1$. Carbon resides in the octahedral void at the body center of the $L1_2$-type lattice. The formation energy of $\kappa$ in the ground state was evaluated using the Full Potential Linearized Augmented Plane Wave (FLAPW) method. The details of this method are given by [2004Oht]. The calculated cohesive energy was modified by considering the interactions between atoms on the same sublattice. The entropy term was estimated using experimental phase boundaries. The calculated homogeneity range of $\kappa$ at 1200 °C is $Fe_{2.8\text{-}2.9}Al_{1.1\text{-}1.2}C_{0.7}$[2004Oht].

In the absence of data on the extension of the $A2 \rightarrow B2$ transition into the ternary region, the word 'bcc' (instead of $\beta$ used by [2004Oht]) is used here to denote the disordered and ordered forms. The solubility of C in bcc computed by [2004Oht] is significantly lower than that found by

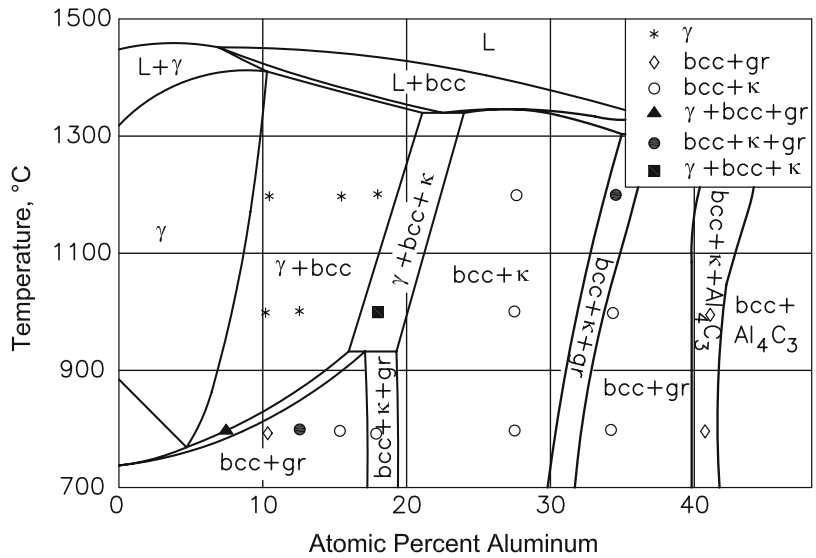


**Fig. 1** Al-C-Fe computed vertical section at 5 at.% C [2004Oht], compared with the experimental data of [1995Pal]

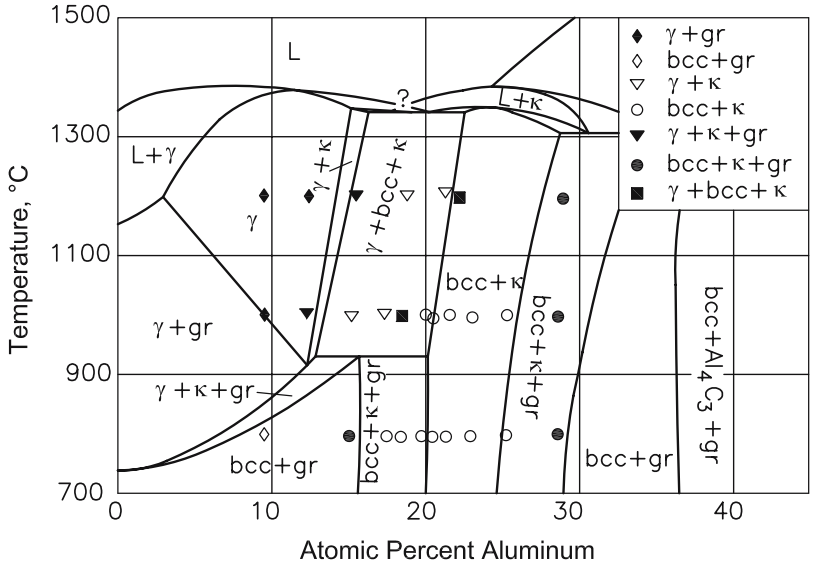


**Fig. 2** Al-C-Fe computed vertical section at 10.5 at.% C [2004Oht], compared with the experimental data of [1995Pal]

[1995Pal]. The computed isothermal sections at 1200, 1000 and 800 °C (not shown here) are in agreement with those experimentally determined by [1995Pal]. In Fig. 1 and 2, the computed vertical sections of [2004Oht] at 5 and 10.5 at.% C are compared with the experimental results of [1995Pal]. The agreement is generally satisfactory, except near the γ region.

## References

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