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Al-Fe-Si (Aluminum-Iron-Silicon)

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The first review of this system by [1988Ray] presented a liquidus surface, liquidus and solidus projections near the Al corner, a full isothermal section at 1000 °C and partial sections near the Al corner at 560, 550, and 450 °C. An update by [1994Rag] presented isothermal sections at 700 and 450 °C in the order-disorder region of Fe-rich alloys and an isothermal section at 600 °C near the Al corner. The computed results of the thermodynamic assessment of [1999Liu] were summarized by [2002Rag]. [2005Gho] presented an updated review of this system. A better understanding of the nature and occurrence of the ternary compounds in this system, a re-determination of the solidification characteristics and several isothermal sections are now available from the studies of [2004Bos], [2004Pon1], [2004Pon2], [2007Kre] and [2008Du].

Binary Systems

The Al-Fe phase diagram [Massalski2] depicts several intermediate phases. Apart from the high temperature phase Fe_4Al_5 (ε), there are three phases stable down to room temperature: $FeAl_2$ (triclinic), Fe_2Al_5 (70-73 at.% Al; orthorhombic), and $FeAl_3$ (or Fe_4Al_{13}) (74.5-76.6 at.% Al; monoclinic). The Al-Si phase diagram is a simple eutectic system with the eutectic reaction at 577 °C and 12.2 at.% Si. In the Fe−Si system [Massalski2], the Fe−based face−centered cubic phase γ is enclosed by a loop. The intermediate phases are: α_2 (*B*2, CsCl-type cubic), α_1 ($D0_3$, BiF_3-type cubic), Fe_2Si (stable between 1212 and 1040 °C; hexagonal), Fe_5Si_3 ($D8_8$, Mn_5Si_3-type hexagonal), FeSi (*B*20-type cubic), $\beta FeSi_2$ (tetragonal) and $\alpha FeSi_2$ (orthorhombic).

Table 1 Al-Fe-Si crystal structure and lattice parameter data [2004Bos, 2007Kre]

Phase	Composition, at.%	Pearson symbol	Space group	Lattice parameter, nm
$Al_2Fe_3Si_3$ (τ_1 or τ_9)	44.5-21.5 Al ~37 Fe 18.5-41.5 Si	*aP*16	*P*1	a = 0.4651; b = 0.6326; c = 0.7499; α = 101.4°; β = 105.9°; γ = 101.2°
Al_3FeSi (τ_2 or γ)	64.8-54.4 Al ~20 Fe 15.2-25.6 Si	*mC*?	…	a = 1.78; b = 1.025; c = 0.890; β = 132°
Al_2FeSi (τ_3)	55.5-53.5 Al ~24 Fe 20.5-22.5 Si	*oC*128	*Cmma*	a = 0.7995; b = 1.5162; c = 1.5221
Al_3FeSi_2 (τ_4 or δ)	53.5-46 Al ~16 Fe 30.5-38 Si	*tI*24	*I*4/*mcm*	a = 0.6061; c = 0.9525
$Al_{7.4}Fe_2Si$ (τ_5 or α)	71.25-68.75 Al ~18.75 Fe 10-12.5 Si	*hP*~244	$P6_3/mmc$	a = 1.2404; c = 2.6234
$Al_{4.5}FeSi$ (τ_6 or β)	67-65 Al ~16 Fe 17-19 Si	*mC*52	*C*2/*c*	a = 2.0813; b = 0.6175; c = 0.6161; β = 90.42°
$Al_3Fe_2Si_3$ (τ_7)	48.2-39.7 Al ~24 Fe 27.8-36.3 Si	*mP*64	$P2_1/n$	a = 0.7179; b = 0.8354; c = 1.4455; β = 93.80°
$Al_2Fe_3Si_4$ (τ_8)	28.1-24.6 Al ~32.4 Fe 39.5-43 Si	*oC*48	*Cmcm*	a = 0.3669; b = 1.2385; c = 1.0147
$Al_9Fe_4Si_3$ (τ_{10})	58.5-57.5 Al ~24.5 Fe 17-18 Si	hex.	…	a = 1.5518; c = 0.7297
Al_5Fe_2Si (τ_{11})	66-64.5 Al ~24.5 Fe 9.5-11 Si	*hP*28	$P6_3/mmc$	a = 0.7509; c = 0.7594

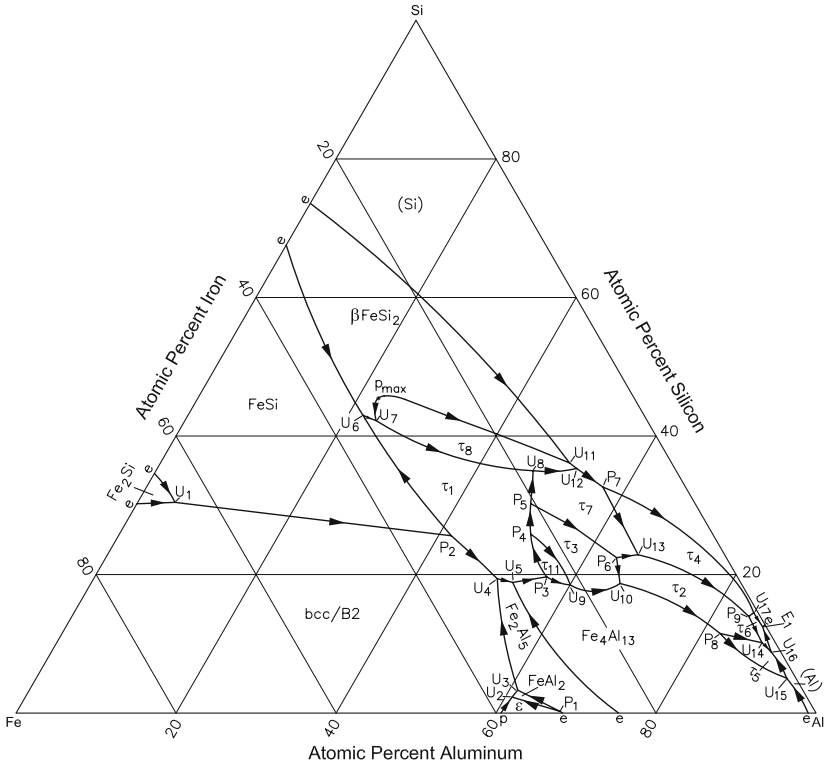

Fig. 1 Al-Fe-Si liquidus projection [2007Kre]

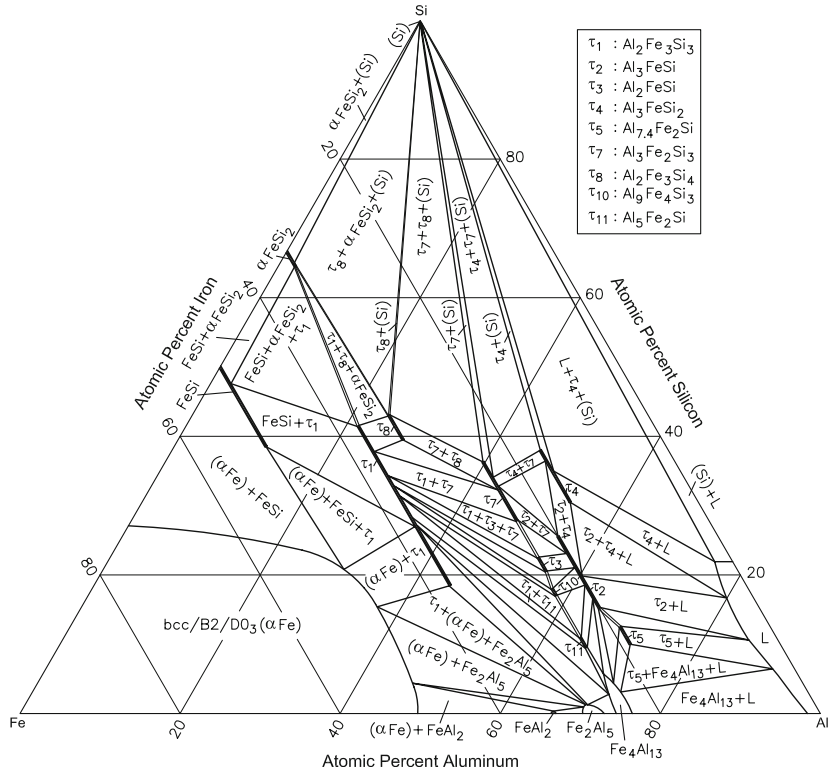

Fig. 2 Al-Fe-Si isothermal section at 727 °C [2004Bos]

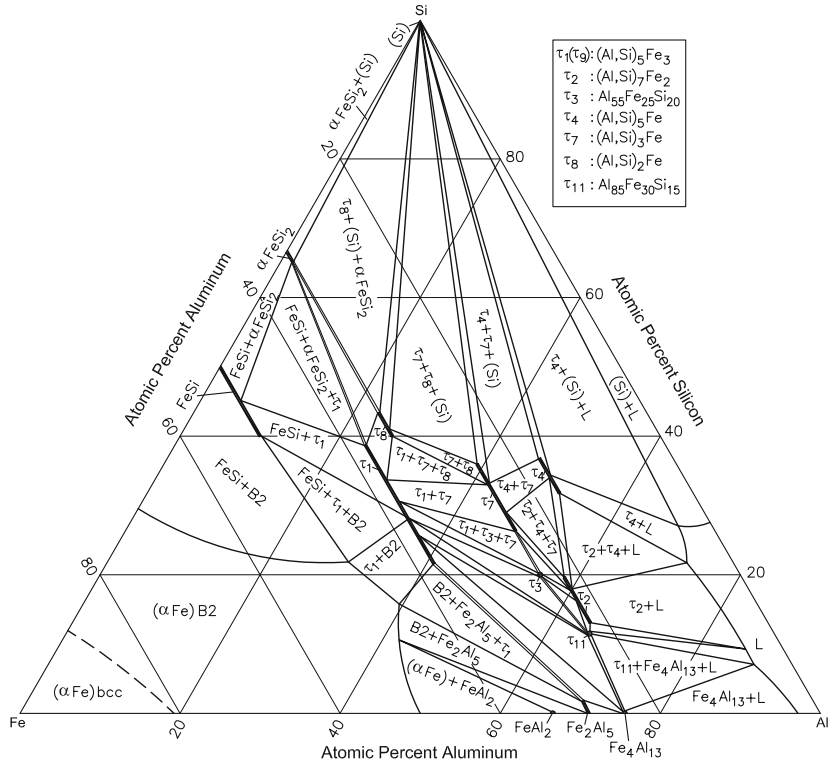

Fig. 3 Al-Fe-Si computed isothermal section at 800 °C [2008Du]

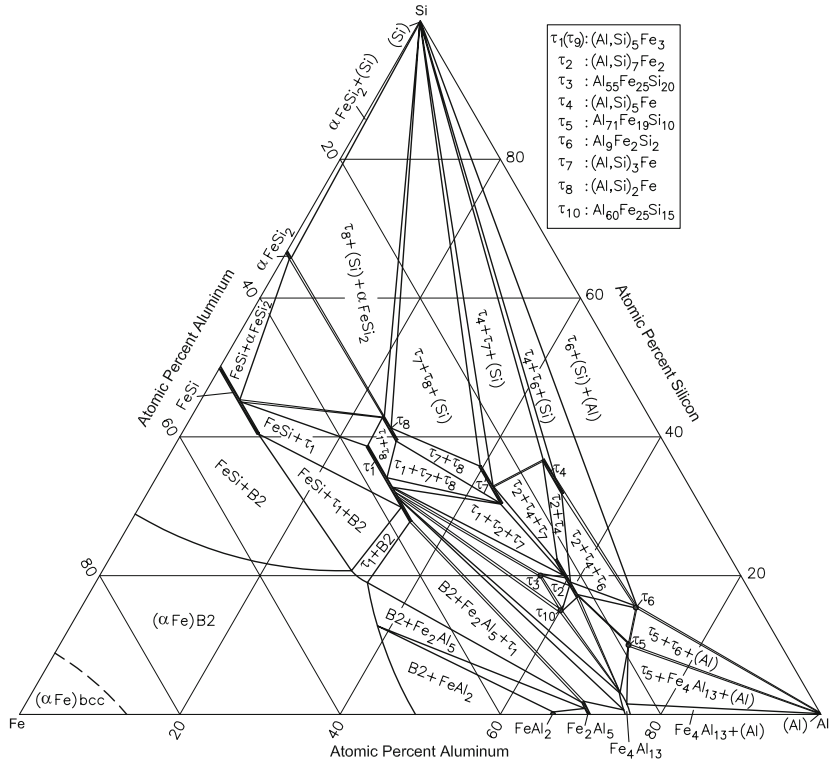

Fig. 4 Al-Fe-Si computed isothermal section at 550 °C [2008Du]

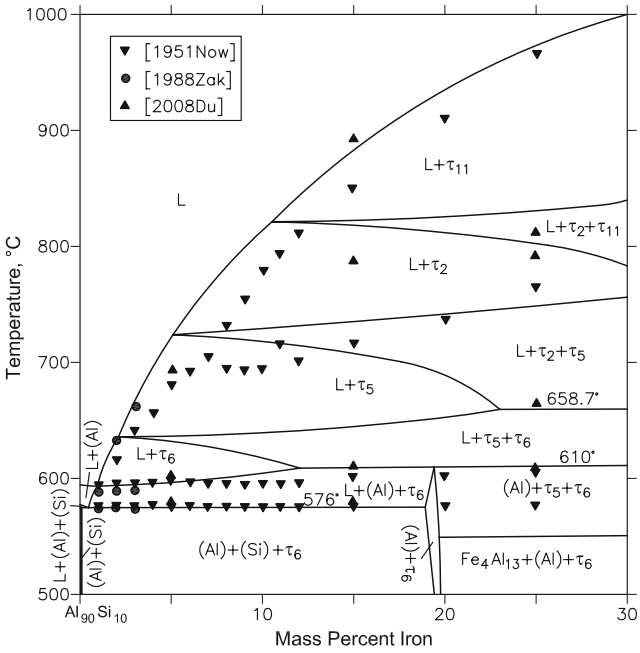

Fig. 5 Al-Fe-Si computed vertical section at 10 mass% Si [2008Du]

Ternary Phases

A number of reports discuss the occurrence and structure of the ternary phases in this system [1988Ray, 2002Rag, 2004Bos, 2005Gho, 2008Du]. The discussion indicates the existence of metastable and unconfirmed phases, with several differing notations used by authors to denote the ternary phases. The notations for the established stable phases adopted by [2004Bos], [2005Gho], [2007Kre] and [2008Du] are in agreement and will be used here. There are ten stable ternary phases in this system: τ_1 (or τ_9) ($Al_2Fe_3Si_3$), τ_2 (γ) (Al_3FeSi), τ_3 (Al_2FeSi), τ_4 (δ) (Al_3FeSi_2), τ_5 (α) ($Al_{7.4}Fe_2Si$), τ_6 (β) ($Al_{4.5}FeSi$), τ_7 ($Al_3Fe_2Si_3$), τ_8 ($Al_2Fe_3Si_4$), τ_{10} ($Al_9Fe_4Si_3$) and τ_{11} (Al_5Fe_2Si). In the above, the nominal formulae are given in brackets. The structure type for τ_4 (Al_3FeSi_2) is $GaPd_5$. τ_{11} (Al_5Fe_2Si) is Co_2Al_5-type hexagonal. The structural details and the homogeneity ranges are listed in Table 1. The Fe content of the ternary phases remains approximately constant, with a small variation of 1 at.% in most cases. The mean value of the Fe content is listed in Table 1. Al and Si substitute for each other at approximately constant Fe content.

Ternary Phase Equilibria

With starting metals of 99.99% Al, 99.98% Fe, and 99.99% Si, [2007Kre] arc-melted under Ar atm more than 80 alloys. For isothermal studies, the alloys were annealed at 800, 700, and 550 °C for 2, 2 and 4 weeks respectively. The phase equilibria were studied with x-ray powder diffraction, scanning electron microscope equipped with energy dispersive analyzer, and differential thermal analysis at a heating rate of 5 °C per min. The liquidus surface constructed by them is shown in Fig. 1. Their results agree with the liquidus projection near the Al corner reported by [2004Pon1]. The ternary phases τ_1(τ_9), τ_2, τ_3, τ_4, τ_5, τ_6, τ_7 and τ_{11} form through ternary peritectic reactions P_2 (1052 °C), P_6 (934 > T > 900 °C), P_4 (940 °C), P_7 (875°C), P_8 (766 °C), P_9 (665 °C), P_5 (934 °C), and P_3 (997 °C) respectively. The phase τ_8 forms at a peritectic maximum (p_{max}) at 1010 °C. The binary phase $FeAl_2$ nucleates in the ternary region through the reaction P_1 (1153 °C [2008Du]). The phase τ_{10} does not take part in the liquid equilibria. [2007Kre] also presented a schematic isothermal section at 550 °C and a reaction sequence for the solidification reactions.

[2004Bos] annealed more than 60 alloys at 727 °C for 200-350 h, followed by air cooling. The phase structure was examined with optical and electron microscopy, electron probe microanalysis, and x-ray powder diffraction. Differential thermal analysis was carried out at a heating/cooling rate of 5-60 °C per min. The isothermal section constructed by [2004Bos, 2004Pon2] at 727 °C is redrawn in Fig. 2. All ternary phases (except τ_6) are present at this temperature. In plotting the ternary phases, the small variation in Fe content is ignored in Fig. 2. Correspondingly, they lie parallel to the Al-Si side. Among the binary phases, FeSi dissolves up to ~12 at.% Al and $FeAl_3$ dissolves up to ~5 at.% Si.

Recently, a new thermodynamic assessment of this system was carried out by [2008Du]. The liquid and the disordered bcc phases were modeled as substitutional solutions. The ordered bcc phase (*B2*) was modeled with two sublattices with (Al, Fe, Si, Va) residing in both sublattices. The binary phases with third component solubility $FeAl_2$, Fe_2Al_5, Fe_4Al_{13}, FeSi and $\alpha FeSi_2$ were modeled with Al and Si substituting for each other in the second sublattice. The ternary phases τ_1(τ_9), τ_2, τ_4, τ_7, and τ_8 were modeled as $Fe_y(Al,Si)_z$, with y and z values corresponding to the formulae. The compounds τ_3, τ_5, τ_6, τ_{10} and τ_{11} were taken to be stoichiometric compounds. The experimental data used as input for optimization were primarily the isothermal section at 727 °C by [2004Bos], the invariant reactions and the isothermal section at 550 °C from [2007Kre, 2008Du] and the enthalpy increment of τ_5 [2008Du]. Satisfactory agreement was found between the computed isothermal sections at 800, 727 and 550 °C and the experimental results. Here, the computed isothermal sections at 800 and 550 °C are shown in Fig. 3 and 4. The τ_{11} phase is present at 800 °C (Fig. 3) and at 727 °C (Fig. 2), but not at 550 °C (Fig. 4). The τ_{10} phase is present at 727 °C, and at 550 °C. It forms through the solid-state reaction: $\tau_{10} \leftrightarrow \tau_1 + \tau_3 + \tau_{11}$, at 807 °C [2007Kre] or at 753 °C [2008Du]. [2007Kre] pointed out that the τ_{10}-τ_{11} relationship needs more investigation

A liquidus projection, a reaction sequence and two vertical sections were also computed by [2008Du]. The vertical section at 10 mass% Si is redrawn in Fig. 5. The comparison with the experimental results of [1951Now], [1988Zak] and [2008Du] shows satisfactory agreement. The other vertical section at 15 mass% of Fe (not shown here) was compared by [2008Du] with the early results of [1933Nis] and [1940Tak].

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