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# Assessment of the Al corner of the ternary Al–Fe–Si system

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**Abstract.** The present work provides a review of the information available on the Al-rich corner of the Al–Fe–Si system as well as a CALPHAD type assessment making use of the COST 507 database as a starting point. The description of the intermetallic compounds has been modified to account for substitution of Al and Si in the ternary Al-Fe-Si system and to take new experimental information into account.

## Introduction

Cast Al–Si aluminium alloys always contain additional species, either added intentionally or present as impurities, the control of which being more and more important as the use of scrap material increases. As a rule of thumb, manganese is added to Al–Si alloys containing iron in order to avoid precipitation of the so-called  $\beta(\tau_6)$ -AlFeSi phase that forms as elongated plates, thus decreasing the mechanical properties of the cast parts. This rule has been applied since long for improving the quality of cast parts but should be mastered through an appropriate description of phase equilibria in the Al–Fe–Mn–Si system. In order to improve the thermodynamic description of the quaternary, it is necessary to reassess the description of the ternary systems as given in the COST 507 database [1], particularly the Al–Fe–Si system.

## Experimental information and previous assessments

The complete ternary Al–Fe–Si system has been re-evaluated recently [2, 3] but the Al-rich corner still shows some controversies amongst the available experimental information. Most of the features of the Al–Fe–Si system were described in the extensive work of Takeda and Mutuzaki [4], who investigated the complete composition range. Earlier works are mentioned in reviews of the system [5–7]. Using the COST 507 as a starting point, Liu and Chang [8] evaluated the whole composition range in a thermodynamic assessment. Since then, further experimental work [2, 9–13] has become available, which motivates a new assessment of the system. The new experimental data consist basically of formation enthalpy measurements [12, 13] and a reevaluation of the liquidus projection [9–11], which updates and corrects previous evaluations [e.g., 14]

The most recent assessment for the whole composition range has been done by Du et al. [3] for the complete system, but treating the Al-rich ternary phases as stoichiometric compounds and with some discrepancies with experiments in the Al-rich corner, mainly with regard to the extension of the primary solidification range of the  $\beta(\tau_6)$  phase.

## Thermodynamic modelling

To remain compatible with COST database only thermodynamic descriptions of the  $\alpha(\tau_5)$ ,  $\beta(\tau_6)$ ,  $\gamma(\tau_2)$ , and  $\delta(\tau_4)$  phases were altered. Table 1 summarises the sublattice models of these phases used in the present assessment.

Table 1: Modelled ternary phases with references to crystal structure reports.

Phase	Model Structure	ref.
$\alpha(\tau_5)$	$\text{Al}_{0.6612}\text{Fe}_{0.19}\text{Si}_{0.0496}(\text{Al},\text{Si})_{0.0992}$	[15]
$\beta(\tau_6)$	$\text{Al}_{0.598}\text{Fe}_{0.152}\text{Si}_{0.10}(\text{Al},\text{Si})_{0.15}$	[16, 17]
$\gamma(\tau_2)$	$\text{Al}_{0.5}\text{Fe}_{0.2}\text{Si}_{0.1}(\text{Al},\text{Si})_{0.2}$	[18]
$\delta(\tau_4)$	$\text{Al}_{0.4166}\text{Fe}_{0.1667}\text{Si}_{0.25}(\text{Al},\text{Si})_{0.1667}$	[19]

The model for the  $\alpha(\tau_5)$  phase was kept the same as in the COST database, since it already considered composition range as a line compound. For the  $\beta(\tau_6)$  phase, the model from Liu and Chang [8] was employed. The composition ranges for both phases match well the experimental evidence.

Sublattices which would allow mixing between Al and Si were added to the models of  $\gamma(\tau_2)$  and  $\delta(\tau_4)$  phases. The crystal structure of the  $\delta(\tau_4)$  phase is known [19], however X-ray diffraction can not distinguish neighbouring elements Al and Si. Munson [18] give either a monoclinic or cubic structure for  $\gamma(\tau_2)$ , while Pontevichi et al. [9] reports only a powder diffraction file. Coefficients of mixing sublattices for these compounds were therefore not based on crystal structures, but rather chosen to match observed composition ranges.

For all four compounds only linear temperature dependence of the excess parameters of the end-members was considered. The ideal solution model was used for the four line compounds. The models for all other phases were kept the same as in the COST 507 database, apart for the liquid phase, to which was added a ternary interaction parameter.

The PARROT module of the Thermocalc [20] software was used for the optimization of the model parameters. Firstly, the data from Pontevichi et al. [9] at 1000 K were fitted using only temperature-independent constants as excess parameters of the end-members. Then, enthalpies of formation at 298 K [12, 13, 21] were used to recalculate the linear temperature dependence.

A further optimization step was the introduction of data at 570°C and 600°C [22]. Then, a ternary interaction parameter for the liquid was introduced, to take into account the invariant equilibria involving the liquid phase [2, 11], which corrects and improves previous results [5]. Krendelsberger et al. [2] provided the temperatures for the invariant reactions, while the compositions were taken from Pontevichi et al. [11]. Finally, data for the isopleth with 13.5 wt. % Si [10] were also fitted. Since this is a section of technological importance, a slightly higher weight in the optimization was assigned to these last results.

After the optimization, the model parameters were rounded following the recommendations of Lukas et al. [23]. The final set of parameters is as follows:

$$G_{\text{Al:Fe:Si:Al}}^{\alpha(\tau_5)} - 0.7604G_{\text{Al}}^{\text{fcc}} - 0.19G_{\text{Fe}}^{\text{bcc}} - 0.0496G_{\text{Si}}^{\text{dia}} = -28100 + 9.1T \quad (1)$$

$$G_{\text{Al:Fe:Si:Si}}^{\alpha(\tau_5)} - 0.6612G_{\text{Al}}^{\text{fcc}} - 0.19G_{\text{Fe}}^{\text{bcc}} - 0.1488G_{\text{Si}}^{\text{dia}} = -25310 + 5T \quad (2)$$

$$G_{\text{Al:Fe:Si:Al}}^{\beta(\tau_6)} - 0.748G_{\text{Al}}^{\text{fcc}} - 0.152G_{\text{Fe}}^{\text{bcc}} - 0.10G_{\text{Si}}^{\text{dia}} = -26900 + 12T \quad (3)$$

$$G_{\text{Al:Fe:Si:Si}}^{\beta(\tau_6)} - 0.598G_{\text{Al}}^{\text{fcc}} - 0.152G_{\text{Fe}}^{\text{bcc}} - 0.25G_{\text{Si}}^{\text{dia}} = -19800 + 3T \quad (4)$$

$$G_{\text{Al:Fe:Si:Al}}^{\gamma(\tau_2)} - 0.7G_{\text{Al}}^{\text{fcc}} - 0.2G_{\text{Fe}}^{\text{bcc}} - 0.1G_{\text{Si}}^{\text{dia}} = -27300 + 6.8T \quad (5)$$

$$G_{\text{Al:Fe:Si:Si}}^{\gamma(\tau_2)} - 0.5G_{\text{Al}}^{\text{fcc}} - 0.2G_{\text{Fe}}^{\text{bcc}} - 0.3G_{\text{Si}}^{\text{dia}} = -28700 + 8T \quad (6)$$

$$G_{\text{Al:Fe:Si:Al}}^{\delta(\tau_4)} - 0.5833G_{\text{Al}}^{\text{fcc}} - 0.1667G_{\text{Fe}}^{\text{bcc}} - 0.25G_{\text{Si}}^{\text{dia}} = -18100 \quad (7)$$

$$G_{\text{Al:Fe:Si:Si}}^{\delta(\tau_4)} - 0.4166G_{\text{Al}}^{\text{fcc}} - 0.1667G_{\text{Fe}}^{\text{bcc}} - 0.4167G_{\text{Si}}^{\text{dia}} = -24700 + 7T \quad (8)$$

$$L_{Al,Fe,Si}^{Liq} = -110000 + 100T \quad (9)$$

## Results and discussion

A calculated isothermal section at 590°C is shown in Fig 1(a), together with experimental data from Stefániay et al. [22]. It is seen that we have a good agreement with the experimental points, even though they show a large scattering. On the other hand, the fitted tie-triangle (filled squares in Fig. 1(a)) is broader in the calculated diagram. This fact is not contradicted by the experiments, precisely because of their scattering.

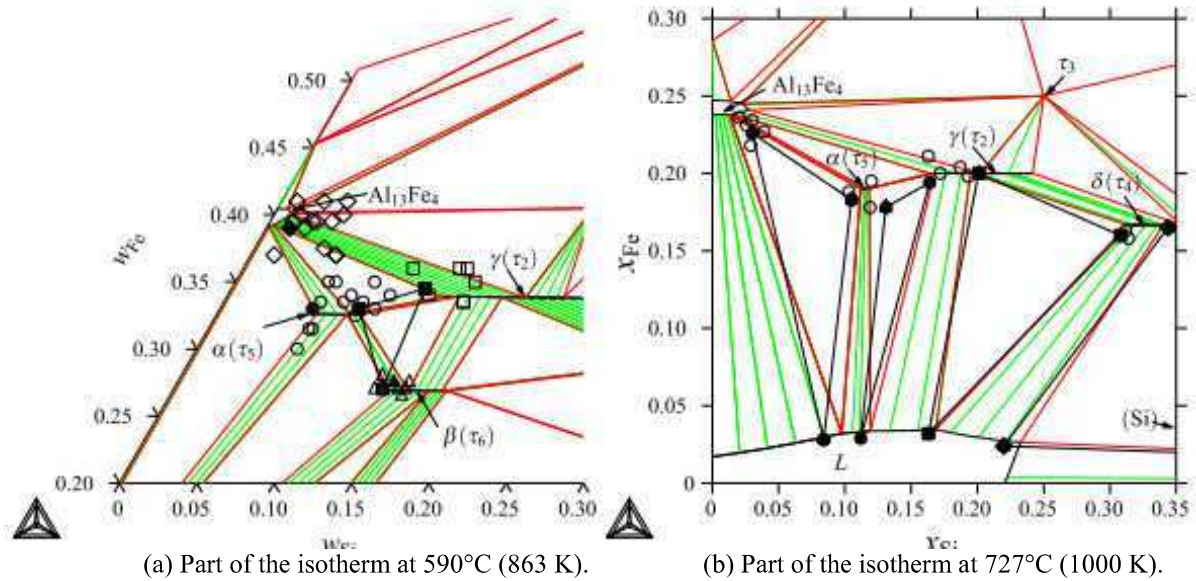


Fig. 1: Isotherms at (a) 590°C (863 K) and (b) 727°C (1000 K). The data from Stefániay et al. [22] at 570°C and 600°C was used in the fit at 590°C, while the measurements of Pontevichi et al. [9] was used in the optimization at 727°C. (Filled symbols denote data used in the optimization.)

Fig. 1(b) shows an isothermal section at 727°C (1000 K), compared with data from Pontevichi et al. [9]. The calculation shows a slightly higher Fe content in the  $\alpha(\tau_5)$  phase, which cannot be varied without changing the model of the phase, since it does not allow substitution of Fe. The agreement for the other tie-triangles is quite acceptable.

Table 2 compares the calculated and the experimental values [2, 11] of the invariant equilibria in the Al-rich corner of the ternary system. It is seen that the agreement is excellent. On the other hand, the calculated compositions for the invariant reactions, as seen from Fig. 2 is good for all reactions, except for P<sub>1</sub> and U<sub>4</sub>, both involving the  $\alpha(\tau_5)$  and the  $Al_{13}Fe_4$  phases. The data of Takeda and Mutuzaki [4], Munson [18], and Zakharov et al. [24] (see Fig. 2) for these phases show a good agreement with our calculations, even though they disagree strongly with respect to the range of  $\beta(\tau_6)$  primary solidification. On the other hand, a higher weight has been assigned to the data from Pontevichi et al. [11], which justifies the above mentioned disagreement. The filled triangle in Fig 2 is an averaged composition for the P<sub>1</sub> reaction, used only for the sake of the optimization. It is not given by Pontevichi et al. [11], but its temperature was determined by Krendelsberger et al. [2].

The isopleth section corresponding to 13.5 wt. % Si is shown in Fig 3(a). There is an excellent agreement between the calculated liquidus line and the experimental values. As a further check, the isopleth with 5 wt. % Fe is shown in Fig. 3(b), with experimental data from Takeda and Mutuzaki [4], and Zakharov et al. [24] (not used in the optimization), showing again an overall good agreement.

Table 2: Calculated (present work) and measured [2, 11] invariant reaction temperatures in the Al-rich corner of the Al–Fe–Si system.

Invariant Equilibrium	Temperature (°C)		
	Ref. 2	Ref. 11	Calculated
P <sub>1</sub> $L + Al_{13}Fe_4 + \gamma(\tau_2) \leftrightarrow \alpha(\tau_5)$	766		757
P <sub>2</sub> $L + \gamma(\tau_2) + \delta(\tau_4) \leftrightarrow \beta(\tau_6)$	665	667	669.7
U <sub>3</sub> $L + \gamma(\tau_2) \leftrightarrow \alpha(\tau_5) + \beta(\tau_6)$	648	661	647.5
U <sub>4</sub> $L + Al_{13}Fe_4 \leftrightarrow (Al) + \alpha(\tau_5)$	636	630	634
U <sub>5</sub> $L + \alpha(\tau_5) \leftrightarrow (Al) + \beta(\tau_6)$	609	613	614.4
U <sub>6</sub> $L + \delta(\tau_4) \leftrightarrow \beta(\tau_6) + (Si)$	596	596	597
E <sub>7</sub> $L \leftrightarrow (Al) + (Si) + \beta(\tau_6)$	577	576	576

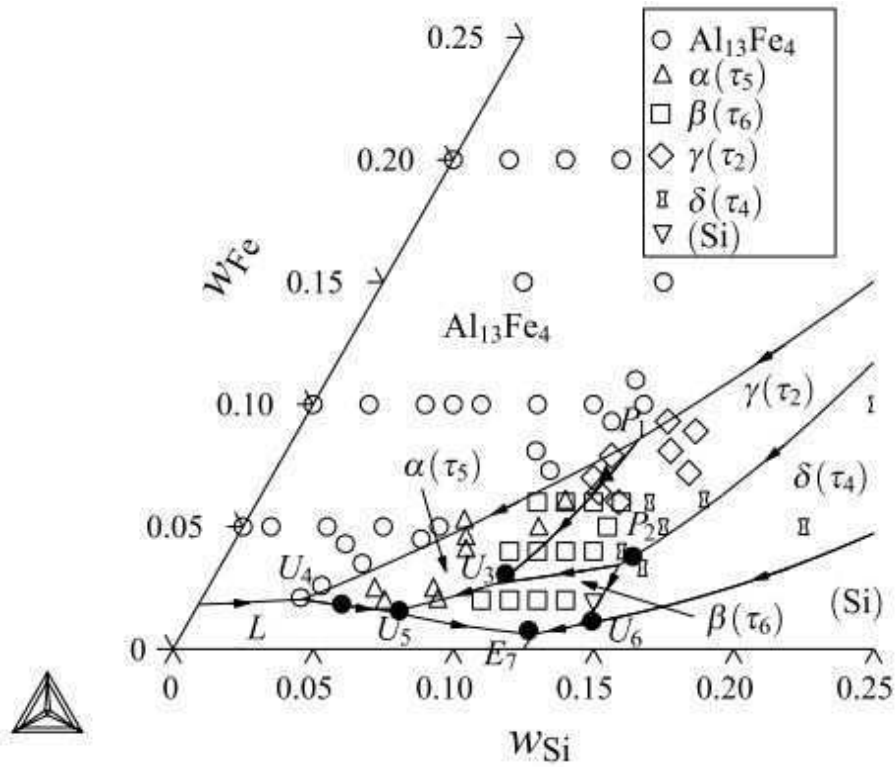


Fig. 2: Projection of the liquid troughs close to the Al-rich corner. The invariant points used in the fit (●) are from Pontevichi et al. [11] (compositions) and Krendelsberger et al. [2] (temperatures, not shown in the figure). The remaining data come from Takeda and Mutuzaki [4], Munson [18], and Zakharov et al. [24]. For the invariant reaction temperatures, see Table 2. The filled triangle is an averaged point for the P<sub>1</sub> reaction, used only for the sake of the optimization.

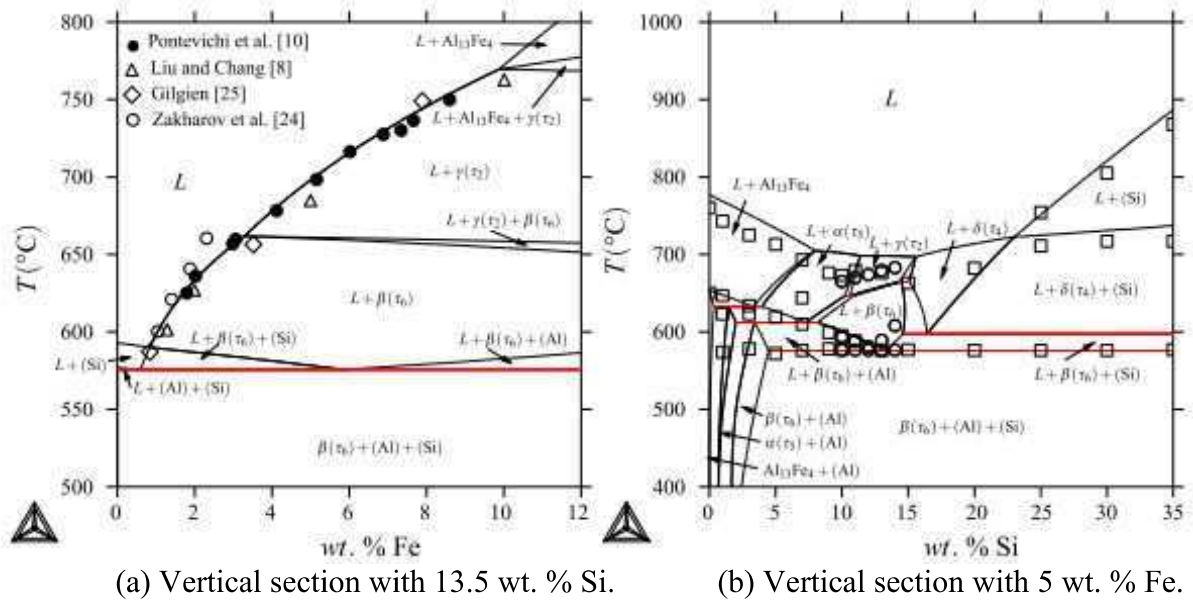


Fig. 3: (a) Isopleth with 13.5 wt. % Si. The data used in the fit are those from Pontevischi et al. [10]. (b) Isopleth with 5 wt. % Fe, with data from Takeda and Mutuzaki [4] (5 wt. % Fe,  $\square$ ) and Zakharov et al. [24] ( $\approx$ 6 wt. % Fe,  $\circ$ ). None of the data in Fig. 3(b) were used in the optimization.

## Conclusion

The Al-rich corner of the Al–Fe–Si ternary system was reassessed in order to take new experimental evidence into account. The starting point for the thermodynamic optimization was the COST 507 database, allowing for substitution of Al and Si in the  $\beta(\tau_6)$ ,  $\gamma(\tau_2)$  and  $\delta(\tau_4)$  phases. That transformed the models of these phases into line compounds. The results show a good agreement with the available literature.

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