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Predicting the Q-Phase in Al-Cu-Mg-Si Alloys

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The objective of this work was to predict whether or not $Al_5Cu_2Mg_8Si_6$, the Q-phase, can be dissolved by solutionizing depending on the composition of Al-Cu-Mg-Si alloys. The procedure was to predict a series of isopleths at 505 °C using ThermoCalc software with a newly constructed database. Then zero-phase-fraction lines for the Q-phase on the isopleths were projected onto various planes to form isothermal, polyisopleth projections that show the effect of Si, Mg, and Cu on Q-phase stability.

Keywords aluminum alloys, equilibrium diagram, isopleths, isothermal equilibration, multicomponent, phase diagram, thermodynamic modeling

1. Introduction

Alloys in the Al-Cu-Mg-Si system serve as important structural materials in the automotive and aerospace industry. The compound $Al_5Cu_2Mg_8Si_6$, is known as the Q-phase and forms during solidification in many of these alloys. The Q-phase has a hexagonal structure[1] and can be detrimental to mechanical properties.[2,3]

In this work the ability to remove Q during solutionizing is predicted for a range of Al-Cu-Mg-Si alloys using thermodynamic software and a database constructed from several sub-databases in the literature and a model for the Q-phase. The prediction is displayed as calculated isothermal polyisopleth projections. Such projections provide a two-dimensional representation of phase stability that is obtained from a three-dimensional, isothermal phase diagram.

2. Procedure

There are four ternary sub-systems in the Al-Cu-Mg-Si quaternary. Databases for three of the sub-systems, Al-Cu-Mg, Al-Mg-Si and Cu-Mg-Si, were obtained from the COST Action 507 program developed in Europe.[4] The fourth was from an earlier work[5] in which a more accurate thermodynamic description of the liquid phase was obtained from experimental data on Al-rich alloys in the Al-Cu-Si sub-system and was then combined with other thermodynamic assessments of that sub-system.[4,6] The databases for the ternary sub-systems were extrapolated into quaternary space by the Muggianu model[7] in the ThermoCalc software.[8]

Since $Al_5Cu_2Mg_8Si_6$ is a true quaternary phase (i.e. a phase that only exists in a four component alloy), the ternary databases contain no information about it. In the current work a model for the Q-phase was added that treats Q as a line compound with a Gibbs energy expressed as:

$$G_{Al_5Cu_2Mg_8Si_6} = \frac{5}{21}{}^0G_{Al} + \frac{2}{21}{}^0G_{Cu} + \frac{8}{21}{}^0G_{Mg} + \frac{6}{21}{}^0G_{Si} + A + BT \quad \text{(Eq 1)}$$

in which ${}^0G_{Al}$, ${}^0G_{Cu}$, ${}^0G_{Mg}$ and ${}^0G_{Si}$ are standard Gibbs energies of pure Al, Cu, Mg and Si as functions of temperature, T, while A and B are parameters that were evaluated in this work from previous experimental data on the Al-Cu-Mg-Si quaternary system.[9-13] According to that body of work there are three invariant reactions (listed in Table 1) that occur in the Al-rich corner, which involve the Q-phase. The A and B parameters were adjusted to minimize the difference between the measured and calculated invariant reaction temperatures. These adjustments only influence phase boundaries associated with the Q-phase.

Finally ThermoCalc software was used with the evaluated database to predict a series of isopleths. One series of

Table 1 Calculated invariant reaction temperatures and compositions compared with experimental invariant reaction temperatures

	Temperature, °C		Mole fraction concentrations of the invariant liquid phase			
Reaction on cooling	Experiment	Calculation	Al	Cu	Mg	Si
L + Mg_2Si → (Al) + (Si) + Q	521(10) 541.6 (11)	532	Bal	0.073	0.046	0.096
L + Mg_2Si → (Al) + θ-Al_2Cu + Q	513 (9) 510 (10) 512 (11)	520	Bal	0.15	0.05	0.028
L → (Al) + θ-Al_2Cu + (Si) + Q	505 (10) 510 (9) 509 (10, 11)	514	Bal	0.13	0.027	0.067

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isopleths were at constant Si, another series at constant Mg, and a third series at constant Cu. All were at the typical solutionizing temperature of 505 °C (778 K). The zero-phase-fraction (ZPF) lines[14-16] for the Q-phase on each series of isopleth were then projected onto an X-Y plane, in which X and Y are the solute elements that were not held constant. For example the constant Si isopleths were projected on the Cu-Mg plane. The result is what can be termed an "isothermal, polyisopleth projection." The predictions were then compared with experimental evidence. Each ZPF line on an isopleths surrounds the area where the Q-phase occurs under equilibrium conditions. When viewed together, the projected lines define contours of the three dimensional ZPF surface much like constant temperature lines define contours of a liquidus surface on the polythermal projection of a ternary system.

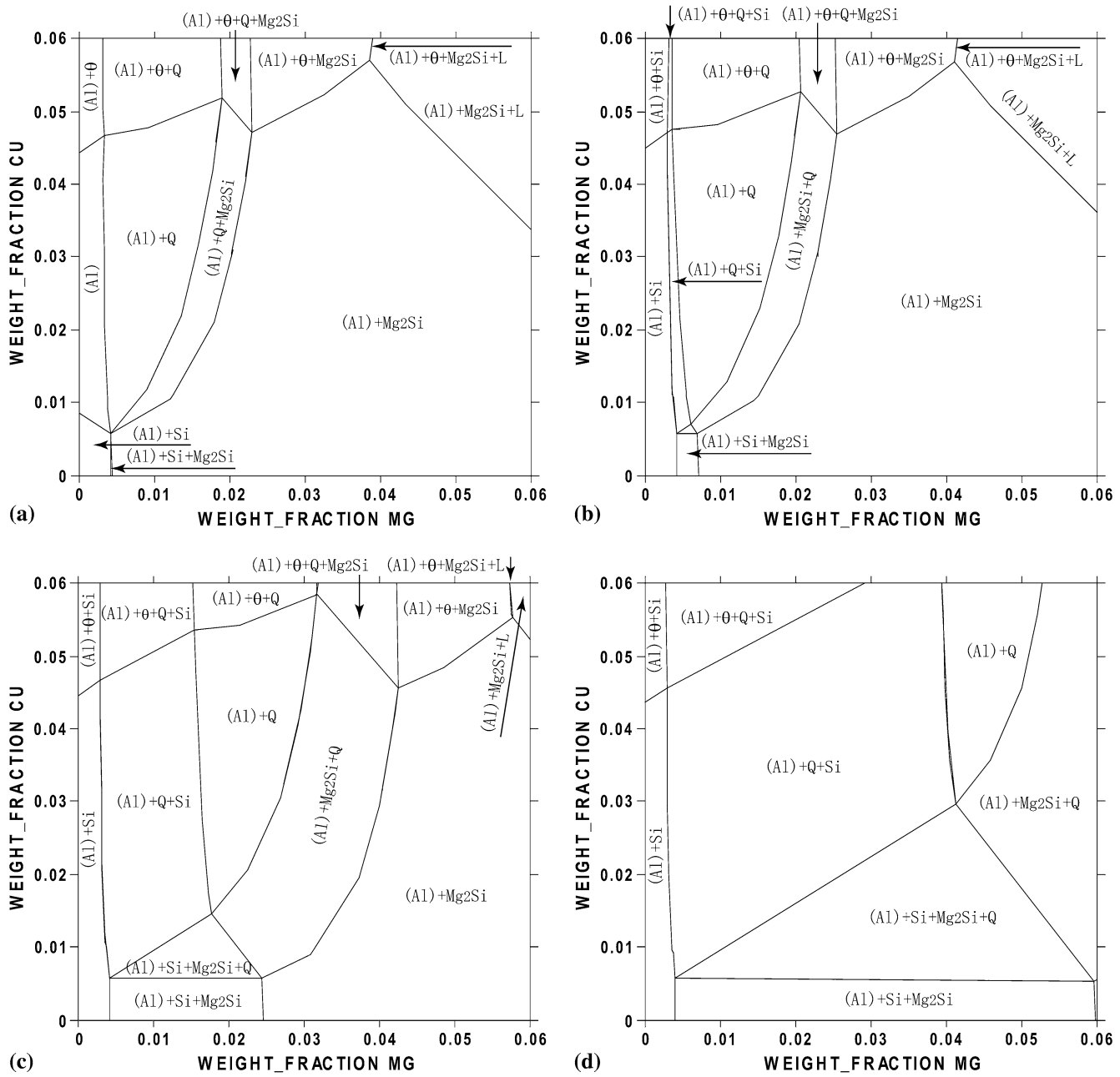

Fig. 1 ThermoCalc predictions of four isopleths sections of the Al-Cu-Mg-Si phase diagram at $T = 505$ °C (778 K) for different Si concentrations. (a) W(Si) = 0.008; the θ-phase is Al_2Cu and the Q-phase is $Al_5Cu_2Mg_8Si_6$. (b) W(Si) = 0.010; the θ-phase is Al_2Cu and the Q-phase is $Al_5Cu_2Mg_8Si_6$. (c) W(Si) = 0.020; the θ-phase is Al_2Cu and the Q-phase is $Al_5Cu_2Mg_8Si_6$. (d) W(Si) = 0.040; the θ-phase is Al_2Cu and the Q-phase is $Al_5Cu_2Mg_8Si_6$

3. Results

When the values for A and B are set equal to 784.6 kJ/mol and 0.574 kJ/mol/K, the three invariant reaction temperatures given in Table 1 are calculated. It can be seen that the predicted temperatures are within ±10 °C of measured values. Predicted compositions of the invariant liquids are given in Table 1 as well, but no experimental values were found in the literature for comparison.

Figure 1 gives four predicted isopleths, each with Mg versus Cu axes and each with a different value of weight fraction Si between 0.0085 and 0.0400. From the labels on the multiphase regions one can determine which of the phase boundary lines are ZPF lines for the Q-phase. Similar diagrams were obtained for constant weight fractions of Mg and Cu.

It is known from the topology of phase diagrams that two-dimensional sections of isothermal phase diagrams should appear as a collection of intersecting ZPF lines.[14-16] Accordingly all intersections should appear as four line junctions except in peculiar cases when three or more lines intersect at the same point or, as in the apparent three line junctions in Fig. 1, when two ZPF lines are so close together that they appear as one line. The lines are labeled as multiphase regions, which they are, but the width of the region is less than a line width.

Figure 2(a) and (b) gives two isothermal isopleths of the Al-Cu-Mg-Si system. The isopleths contain ZPF lines for the Q-phase at 505 °C. The Q+ on the figure indicates the side of the ZPF line where the Q-phase occurs while Q− indicates the side of the line where the Q-phase is absent. Also on Fig. 2(a) and (b) are experimental data[13] taken after annealing a series of alloys at 500 °C. The data indicate whether or not the Q-phase was found at various compositions. Figure 3 gives three isothermal polyisopleth projections. Each was obtained by combining a series of isopleths. The result is three views of the phase diagram volume where the Q-phase is stable at equilibrium as predicted by the current database.

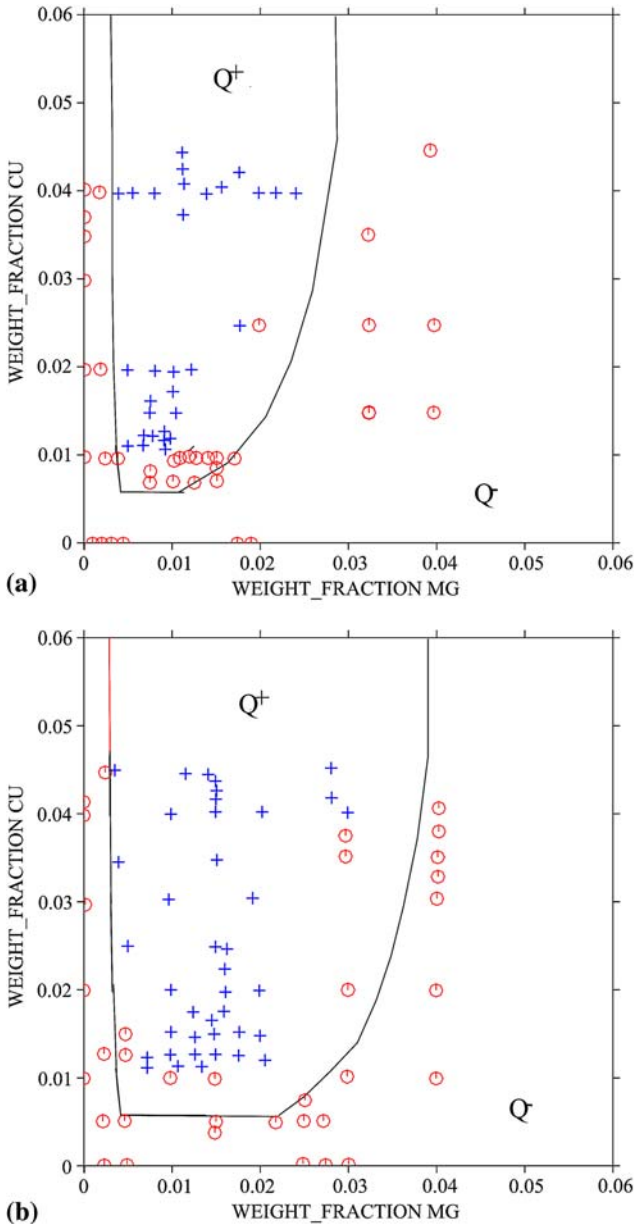

Fig. 2 ThermoCalc predictions of the zero-phase-fraction Q lines for the Al-Cu-Mg-Si system at T = 505 °C (778 K) and (a) W(Si) = 0.012. (b) W(Si) = 0.018 with experimental data from Ref 13. (a, b) The + symbols indicate that Q was present while the ○ symbols indicate that no Q was present

4. Discussion

The predictions in Fig. 1 give a detailed view of the phases that form in quaternary Al-Cu-Mg-Si alloys. However this is more information than is needed if the objective is to reduce or eliminate the formation of the Q-phase during solutionizing at 505 °C. In fact the additional information plus the need to compare multiple figures interferes with having a global view of how alloy additions affect Q-phase stability.

In Fig. 2 comparison of experimental data with the predicted ZPF line for the Q-phase one finds that the predicted line and the data agree to within less than one atomic percent. In general the predicted diagram over estimates the stability by making the stability region larger than is seen experimentally.

Figure 3 gives three isothermal, polyisopleth projections. The projections provide a compact view of Q-phase formation on a single figure. From these one can predict how each of the elements affects Q-phase stability. For example Fig. 3(a) shows that in alloys with Cu concentrations less than 0.7% or Mg less than about 0.2% one can avoid the Q-phase regardless of other concentrations in Al-Cu-Mg-Si alloys. The right side of the Q-phase region is limited by the formation of Mg_2Si. In this regard, Fig. 3(a) shows that increasing the amount of Si requires adding more Mg in order that Mg_2Si form instead of the Q-phase.

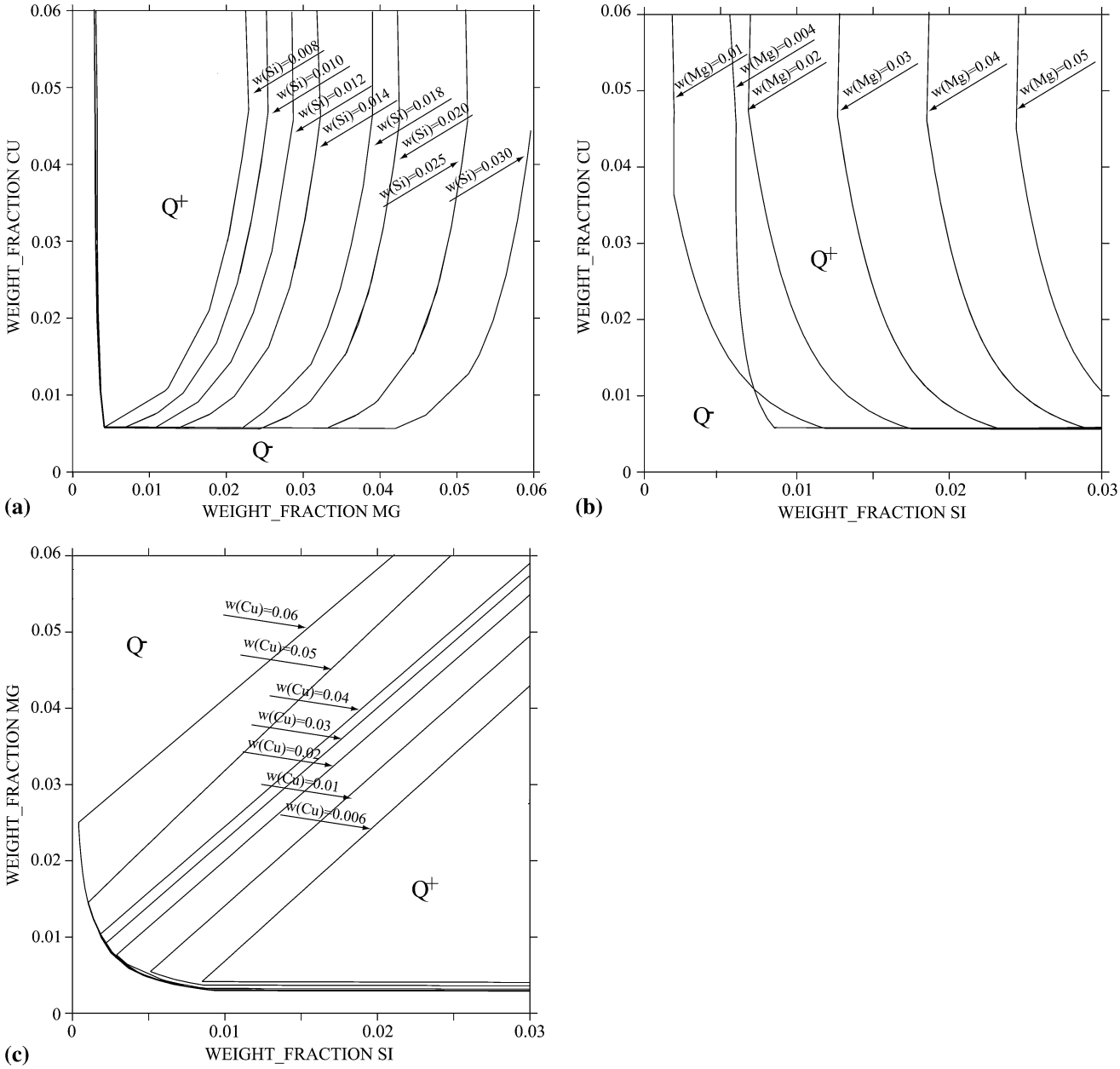

Fig. 3 (a)-(c) Polyisopleth projections illustrating the effect of Si, Mg and Cu on Q-phase formation

Figure 3(b) contains some of the same information as Fig. 3(a) as it should since it is just another view of the same volume. For example it shows that the Q-phase does not form in alloys containing less than 0.7% Cu and that adding Mg can limit the amount of Q-phase because Mg_2Si will form instead. Figure 3(b) shows that two of the ZPF lines cross. This occurs when there are contour lines from both the top and bottom of a volume on the figure. Figure 3(c) shows again that Q-phase does not form for low Mg concentrations. In addition it shows how Cu has a small effect on the minimum Mg concentration, but for a broad range of Si and Mg concentrations, adding Cu will increase the amount of Q-phase at 505 °C.

5. Conclusions

A database for Al-Cu-Mg-Si alloys developed for this program was used to predict isothermal polyisopleth projections that indicate Q-phase stability. Agreement between predictions and previous experimental work showed that boundaries predicted for Q-phase formation at 505 °C over estimate the stability range, but by no more than 1%. The polyisopleth projections predict that the Q-phase can be solutionized in alloys containing either less than 0.7% Cu or 0.2% Mg. Also they show that adding Mg can reduce the amount of Q-phase by forming Mg_2Si

instead, while adding Cu had the affect of increasing the amount of Q-phase whenever it was present in an alloy. These diagrams show that an advantage of the isothermal polyisopleth projections is that they eliminate unneeded phase boundaries, while providing a global view of three-dimensional predictions on a two-dimensional figure.

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