

# THERMODYNAMIC CALCULATION OF SOLIDIFICATION MICROSTRUCTURE

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## SUMMARY

Software and a general algorithm have been developed to permit the thermodynamic calculation of the amounts and compositions of the microstructural constituents formed during the cooling of an alloy from above the liquidus temperature to below the temperature of final disappearance of the liquid for the cases of equilibrium cooling and Scheil-Gulliver cooling conditions.

## I. INTRODUCTION

Following solidification of an alloy from the liquid state, as in casting processes, it is important to know the compositions and amounts of the microstructural constituents (primary constituents, binary and ternary eutectic constituents, etc.). At any overall alloy composition and temperature, during either equilibrium cooling or Scheil-Gulliver cooling, thermodynamic database computing systems<sup>[1-3]</sup> can calculate the amounts and compositions of all phases by Gibbs energy minimization, with the required data being retrieved from databases of model parameters for the thermodynamic properties. Similarly, phase diagram sections can be calculated and plotted. However, this information does not readily permit the direct calculation of the compositions and amounts of the microstructural constituents, particularly in the case of ternary and higher-order systems.

The present article describes an algorithm that permits such calculations under either equilibrium or Scheil-Gulliver cooling conditions. The algorithm has been programmed and incorporated into the FactSage<sup>[1]</sup> software system.

## II. BINARY ALLOYS

As a simple example, consider the Al-Li equilibrium phase diagram in Fig. 1 and consider first the case of equilibrium cooling. When an alloy of overall composition  $X_{Li} = 0.4$  (where  $X_{Li}$  is the Li mole fraction) is cooled at equilibrium from the liquid state, the composition of the liquid follows the crystallization path shown on the figure. Solidification starts at the liquidus temperature, 954 K, with precipitation of a primary AlLi solid. When the temperature has decreased to 874 K the following eutectic reaction occurs isothermally:



with the formation of a eutectic constituent. When solidification is complete at 874 K (i.e. after the final disappearance of the liquid) the microstructure consists of grains of a homogeneous primary AlLi constituent with composition at point **b** and grains of a eutectic constituent of overall composition at point **e** consisting of FCC and AlLi phases with compositions at points **a** and **b** respectively. In this simple example the relative amounts of the two constituents as well as the relative amounts of the two phases in the eutectic constituent could be calculated by simple applications of the Lever Rule with no need for special software. However, this initial example serves as an introduction to the operation of the new solidification software.

With the new algorithm, one enters the overall alloy composition ( $X_{Li} = 0.40$ ). Then, starting at the calculated liquidus temperature, the software repeatedly calculates the equilibrium conditions as the temperature,  $T$ , is decreased in steps of  $\Delta T$ . Typically,  $\Delta T = 1$  K or 5 K. Whenever the calculated equilibrium phases after a step are different than they were before the step, the program recognizes that one or more phase transformations have occurred and iterates back to calculate the transition temperature(s) with high precision. By comparing the amounts of the various phases present before and after the transition, the program can determine which phases are the reactants and which are the products of the precipitation reaction which is occurring.

For the present example, the output is shown in Table I. A summary of the precipitation reactions occurring during the entire course of the solidification from the liquidus to the final disappearance of the liquid is given along with the final amount and composition of each constituent at the moment of final disappearance of the liquid at 873.55 K and the amounts and

compositions of the FCC and AlLi phases in the two-phase eutectic constituent. (In this example, the basis of the calculation is 1.0 g-atom of the pure elemental components.)

A detailed output of the amounts and compositions of the constituents after each incremental cooling step can also be listed, but is not shown in Table I.

Upon cooling and annealing below 874 K, further precipitation reactions within the grains may occur. This will be treated in Section IV.

Equilibrium cooling conditions are generally approached only when the cooling rate is extremely slow. In practice, conditions often approach more closely to those of Scheil-Gulliver cooling<sup>[4]</sup> in which solids, once precipitated, cease to react with the liquid or with each other, there is no diffusion in the solids, the liquid phase remains homogeneous, and the liquid and surfaces of the solid phases are in equilibrium.

To calculate the course of Scheil-Gulliver cooling at a fixed overall composition the following simulation strategy is adopted. At a given overall composition the liquidus temperature is first calculated. Then, starting at the liquidus, the temperature is decreased by increments  $\Delta T$  and the compositions and amounts of precipitated solids at equilibrium with the liquid are calculated. These solids are then “removed” from further equilibrium calculations, but their compositions and amounts are retained in memory. The remaining liquid is then cooled by successive increments  $\Delta T$  and the process is repeated until all the liquid has solidified. Generally, a value of  $\Delta T = 5\text{K}$  is sufficient to give a good approximation to Scheil-Gulliver cooling conditions, but occasionally a smaller value may be required.

Consider the same example of an Al-Li alloy with composition  $X_{Li} = 0.4$ . Under Scheil-Gulliver conditions the crystallization path followed by the liquid is shown in Fig. 2 (which, in this particular example, is the same as the equilibrium path in Fig. 1). Between 954 K and 874 K a primary AlLi constituent precipitates just as in the case of equilibrium cooling, but now the solid grains are in equilibrium with the liquid only at their surface. The amount and composition of solid deposited during each incremental step  $\Delta T$  are stored in memory, and the program keeps track of the accumulated amount and composition of the (now inhomogeneous) primary AlLi constituent. The solidification terminates at 874 K with the eutectic Reaction [1].

The output is shown in Table I where calculated temperatures have been rounded off to  $\pm 0.01\text{K}$ . (The calculated temperatures shown on Fig. 1 have been rounded off to the nearest degree.) In this particular example the reaction steps are the same as in the case of equilibrium

cooling, but the final compositions and/or amounts of the constituents are different. It may be noted that, in the case of Scheil-Gulliver cooling, neither the average composition of the primary constituent nor the relative amounts of the constituents can be simply read from the equilibrium diagram. That is, the Lever Rule does not apply.

At each cooling step, a detailed output can also be requested of the amounts and compositions of the constituents precipitated during that step, or cumulatively up to that point. This is not shown in Table I.

As a second example, consider an Al-Li alloy of composition  $X_{Li} = 0.1$ . Calculated crystallization paths of the liquid are shown for equilibrium and Scheil-Gulliver cooling in Figs. 1 and 2 respectively, and the output of the solidification software is shown in Table II. Solidification of the FCC primary phase commences at the liquidus temperature of 918 K. In the case of equilibrium cooling, the composition of the solid phase, which remains homogeneous, follows the solidus until solidification is complete at 904.40 K with a single homogeneous solid primary phase of composition  $X_{Li} = 0.1$ . In the case of Scheil-Gulliver cooling, the liquid phase remains present down to the eutectic temperature because, after each incremental cooling step, the solid which precipitates and is subsequently “removed” from the calculations always has a lower Li content than the liquid phase.

*Hence, in general during Scheil-Gulliver cooling, for an alloy of any composition in a system of any number of components, the final disappearance of the liquid always occurs at a minimum on the liquidus surface.*

In the preceding examples, it is assumed that all the FCC and AlLi phases produced during the eutectic Reaction [1] go to form the eutectic constituent (that is, none precipitates onto the surfaces of the already precipitated primary grains), as is consistent with the mechanism of eutectic formation.

As a third example for a binary system, consider an Al-Li alloy of composition  $X_{Li} = 0.65$ . Crystallization paths of the liquid for the cases of equilibrium and Scheil-Gulliver cooling are shown in Figs. 1 and 2 respectively and the output of the solidification software is shown in Table III.

In the case of equilibrium cooling in Fig. 1, solidification begins on the liquidus at 901 K. The primary AlLi solution precipitates between 901 K and 793 K. At 793 K the peritectic reaction



occurs isothermally until all the AlLi phase has been consumed. Cooling then continues between 793 K and 604 K with precipitation of Al<sub>2</sub>Li<sub>3</sub>. At 604 K the peritectic reaction



occurs isothermally until all the liquid has been consumed. Solidification is complete at 604 K.

It is assumed that full equilibrium conditions apply. Hence, the peritectic Reaction [2] proceeds to completion until all the AlLi primary constituent has been consumed. Therefore, the amount of “constituent 1” remaining when solidification is complete is zero, as shown in Table III. Of course, in practice peritectic reactions rarely proceed to completion due to kinetic constraints.

Similarly, it is assumed that the peritectic Reaction [3] proceeds to completion isothermally at 604 K until all the liquid has been consumed although, in practice, some liquid will most likely persist down to lower temperatures.

Note the distinction in Table III between “constituent 2” which is the Al<sub>2</sub>Li<sub>3</sub> constituent formed during the peritectic Reaction [2] at 793.01 K and “constituent 2A” which is the Al<sub>2</sub>Li<sub>3</sub> constituent formed during the subsequent precipitation between 793.01 K and 604.35 K.

During the peritectic Reaction [3] at 604.35 K the liquid is assumed to react with the Al<sub>2</sub>Li<sub>3</sub> of constituents 2 and 2A in proportion to their relative amounts. Specifically, just before Reaction [3] begins, the amounts of Al<sub>2</sub>Li<sub>3</sub> in constituents 2 and 2A are calculated to be 10.44 g and 2.198 g respectively. The amounts consumed in Reaction [3] are thus assumed to be in the ratio 10.44/2.198.

*In general, if a phase  $\alpha$  is a reactant of a peritectic reaction, then during the reaction the  $\alpha$  phases in all previously precipitated constituents are assumed to be consumed in proportion to their relative amounts.* In practice, of course, this is not necessarily true, but the actual proportions could only be calculated by taking kinetic factors into account.

The situation for Scheil-Gulliver cooling of the alloy at  $X_{Li} = 0.65$  requires fewer assumptions than in the case of equilibrium cooling since, *under Scheil-Gulliver conditions, peritectic reactions cannot occur.* Since Reaction [2] does not take place, the primary AlLi constituent

remains unchanged at all temperatures below 793.01 K. Between 793.01 K and 604.35 K  $\text{Al}_2\text{Li}_3$  precipitates. At 604.35 K the peritectic Reaction [3] does not occur, and all the  $\text{Al}_2\text{Li}_3$  that precipitated remains unchanged at all temperatures below 604.35 K. Between 604.35 K and 452.05 K, precipitation of  $\text{Al}_4\text{Li}_9$  occurs. At the eutectic temperature of 452.05 K the eutectic reaction



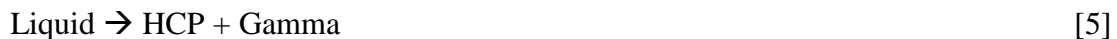
occurs isothermally and solidification is complete at this temperature.

### III. TERNARY ALLOYS

To illustrate solidification calculations in a ternary system, the Mg-Al-Zn system is chosen as example. The calculated projection of the liquidus surface is shown in Fig. 3. There are 12 primary phase fields as shown, and many of the solid phases are solutions with extended binary or ternary ranges of stoichiometry. There are 10 ternary invariant points as labeled. Two of these (at 624.15 K (351 °C) and 618.15 K (345 °C)) are eutectic points; the others are peritectic.

Enlargements of the Mg-rich corner of Fig. 3 are shown in Figs. 4 and 5. Two alloy compositions, A(80 Mg, 15 Al, 5 Zn) and B(59 Mg, 27 Al, 14 Zn) (in mol %), are shown along with the calculated crystallization paths of the liquid during equilibrium cooling in Fig. 4, and Scheil-Gulliver cooling in Fig. 5. Outputs from the solidification software are shown in Tables IV and V. In these examples, a basis of a total mass of 100 g-atoms was chosen.

For alloy A in Fig. 4, equilibrium solidification commences at the liquidus temperature, 768.87 K (495.72 °C), and proceeds with precipitation of a primary HCP phase to 681.95 K (408.80 °C). Thereafter the liquid crystallization path follows the univariant line down to 644.39 K (371.24 °C) with precipitation of a binary (HCP + Gamma) eutectic constituent:

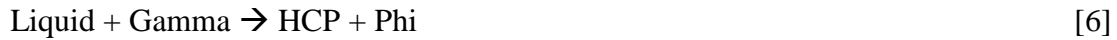


During this stage, the composition of the already precipitated primary HCP constituent (constituent 1) will change since it always remains at equilibrium. It is assumed that the total number of g-atoms of constituent 1 remains constant at all temperatures below 681.95 K (408.80

°C) despite these possible changes of composition. While this is not strictly true, the actual change in the total amount of constituent 1 could only be calculated by taking kinetic factors into account.

*In general, unless one or more of the phases in a constituent are consumed in subsequent peritectic reactions, it is assumed that the total number of g-atoms of a constituent remains constant once precipitation of that constituent is complete.*

At 644.39 K (371.24 °C) the following peritectic reaction occurs isothermally:



Full equilibrium is assumed such that Reaction [6] proceeds to completion isothermally with complete consumption of the liquid. “Constituent 3” is the mixture of (HCP + Phi) formed isothermally during Reaction [6].

In the case of Scheil-Gulliver cooling of alloy A, as shown in Fig. 5 and Table IV, the liquid crystallization path during precipitation of the primary HCP phase is nearly, but not exactly, the same as in the case of equilibrium cooling. The primary precipitation is complete at 683.3 K (410.15 °C) (*cf.* 681.95 K (408.80 °C) for equilibrium cooling). In the Scheil-Gulliver case, the peritectic reactions at 644.39 K (371.24 °C) and 620.93 K (347.78 °C) are prohibited. Therefore, solidification continues down to the ternary eutectic temperature of 618.07 K (344.92 °C) (a minimum on the liquidus surface) where the ternary eutectic constituent (HCP + Tau + Mg<sub>12</sub>Zn<sub>13</sub>) precipitates isothermally.

In the case of equilibrium cooling of alloy B as shown in Fig. 4 and Table V, precipitation of the primary constituent proceeds between the liquidus temperature, 720.26 K (447.11 °C), and 697.6 K (424.45 °C). Thereafter, the reaction steps as shown in Table V are, in order: precipitation of a binary (Gamma + Tau) eutectic constituent; an isothermal ternary peritectic reaction at 665.32 K (392.17 °C) which proceeds until the Tau phase is completely consumed; precipitation of a binary (Gamma + Phi) eutectic constituent; and an isothermal ternary peritectic reaction at 644.39 K (371.24 °C) which proceeds until the liquid phase is completely consumed. As described above, it is assumed that the Gamma phase which is consumed during this isothermal reaction is taken partially from the Gamma phase of constituent 2 and partially from

the Gamma phase of constituent 4 in proportion to their relative amounts. Again it can be appreciated that, in the case of full equilibrium cooling involving peritectic reactions, the actual final microstructure is very dependent upon kinetic factors and several assumptions must be made. Nevertheless, the calculations provide a useful limiting scenario.

In the case of Scheil-Gulliver cooling of alloy B, as shown on Fig. 5 and Table V, the peritectic reactions at 665.32 K (392.17 °C) and 644.39 K (371.24 °C) are prohibited. Hence, solidification continues down to the ternary eutectic temperature of 618.07 K (344.92 °C).

In general, since peritectic reactions do not occur during Scheil-Gulliver cooling, fewer assumptions are needed. Therefore, the final calculated microstructure is expected to approximate the actual observed microstructure more closely than in the case of equilibrium cooling.

A final example is shown in Fig. 6 and Table VI for an alloy of composition C (15% Mg, 5% Al, 80% Zn) (in mol %). In the case of equilibrium cooling, precipitation of a primary Laves constituent is followed between 647.15 K (374.00 °C) and 638.51 K (365.36 °C) by the binary peritectic reaction:



This is followed by an isothermal ternary peritectic reaction at 638.51 K (365.36 °C) which is the temperature of final disappearance of the liquid.

In the case of Scheil-Gulliver cooling of alloy C, the peritectic Reaction [7] is prohibited. Hence, upon reaching the univariant line at 647.29 K (374.14 °C) the crystallization path crosses the  $\text{Mg}_2\text{Zn}_{11}$  liquidus surface with precipitation of  $\text{Mg}_2\text{Zn}_{11}$  down to 626.34 K (353.19 °C). Thereafter, precipitation of a binary (HCP Zn +  $\text{Mg}_2\text{Zn}_{11}$ ) eutectic constituent occurs down to 623.78 K (350.63 °C) where the ternary eutectic constituent (FCC + HCP Zn +  $\text{Mg}_2\text{Zn}_{11}$ ) precipitates isothermally.

#### IV. PRECIPITATION DURING SUBSEQUENT ANNEALING

Often, in alloy processing, an alloy is solidified relatively rapidly under approximately Scheil-Gulliver conditions to below the temperature of final disappearance of the liquid and is subsequently annealed at a temperature below the solidus. During annealing, precipitation can



occur within the grains. This process can be simulated with the current solidification software.

As an example, consider the Mg-Al-Zn alloy with composition B in Table V. Suppose that this alloy has been solidified under Scheil-Gulliver conditions down to 523.15 K (250 °C). Upon arriving at 523.15 K (250 °C) the primary Tau constituent (constituent 1) has a total mass of 614.75 g and a composition 31.765 w/o Mg, 29.481 w/o Al, 38.754 w/o Zn. At 523.15 K (250 °C) the phase is supersaturated and, upon annealing at this temperature, precipitation will occur within the phase. To calculate the amount and composition of the precipitates after complete annealing, one ‘clicks’ on the name of the phase in the tabular output in Table V. The components of the phase (614.75 X 0.31765 g Mg, etc.) are then automatically transferred as input to the FactSage equilibrium calculation module. One then enters the annealing temperature (250 °C) and the conditions after equilibration are calculated. In this case, the calculations show that 54.53 g of Gamma phase are formed, with 560.22 g of residual Tau phase. The total mass remains constant. That is, it is assumed that no reaction with other phases occurs during annealing. This is a reasonable approximation in most cases.

The calculation assumes full annealing. In reality, annealing will often be terminated before the equilibrium amount of precipitates has formed. Nevertheless, the calculation indicates which phases will precipitate and shows the maximum amount of precipitates which can be formed. Similar calculations can, of course, be carried out for all the other phases in the various constituents in Table V.

## **V. OTHER FEATURES OF THE SOLIDIFICATION SOFTWARE**

There are several features of the solidification software which have not been illustrated but which may be briefly listed.

The calculations are not limited to systems of three components.

Since the FactSage databases contain data for the molar volumes and expansivities of many phases, the molar volumes of the various constituents can be calculated and displayed in the output.

The enthalpy changes associated with the formation of each of the constituents are also calculated and can be displayed in the output.

In the examples selected here, it has been assumed that during Scheil-Gulliver cooling all solid phases, once precipitated, no longer remain in equilibrium with the liquid. This is the usual

assumption in the case of Scheil-Gulliver cooling. However, the software is flexible and permits one to specify that certain specified solid phases remain in equilibrium with the liquid.

## VI. DISCUSSION – SCHEIL-GULLIVER CONSTITUENT DIAGRAMS

The solidification software permits the course of Scheil-Gulliver cooling to be simulated, but only at one overall alloy composition at a time. By analogy with equilibrium phase diagrams which apply to equilibrium cooling, it would be very useful to calculate and plot “Scheil-Gulliver constituent diagrams” which would permit one to better visualize the course of Scheil-Gulliver solidification as temperature and composition are varied. Software for calculating and plotting such diagrams is now available in the FactSage system and is the subject of another publication<sup>[5]</sup>. As an example, the calculated Scheil-Gulliver constituent diagram for the Al-Li system is shown in Fig. 7. The labeled fields show the microstructural constituents which precipitate progressively as temperature is decreased at any composition. For example, if an alloy of overall composition  $X_{Li} = 0.65$  (*cf.* Table 3) is cooled under Scheil-Gulliver conditions to a temperature below 725.15 K (452 °C) it will consist of the following constituents: AlLi primary, Al<sub>2</sub>Li<sub>3</sub>, Al<sub>4</sub>Li<sub>9</sub> and an (Al<sub>4</sub>Li<sub>9</sub> + BCC) eutectic.

As a second example, a partial Scheil-Gulliver constituent diagram for the Al-Mg-Zn system along an isopleth where  $X_{Zn} = 0.05$  is shown in Fig. 8. The composition of alloy A (see Fig. 4 and Table 4) is shown on the diagram. The sequence of reactions occurring as this alloy is cooled can be seen to correspond to those calculated in Table IV.

## VII. CONCLUSIONS

Following solidification of an alloy from the liquid state, as in casting processes, it is important to know the compositions and amounts of the microstructural constituents. During either equilibrium or Scheil-Gulliver cooling, thermodynamic database computing systems<sup>[1-3]</sup> can calculate the amounts and compositions of all phases by decreasing the temperature by small increments and performing calculations after each step. However, this information does not readily permit the direct calculation of the compositions and amounts of the microstructural constituents, particularly in the case of ternary and higher-order systems.

With the new algorithm and software, whenever a phase transition is observed to occur, the

nature of the transition reaction is deduced by noting which phases are present before and after the transition. In this way the cumulative amounts and compositions of all microstructural constituents (primary constituents, binary, ternary and higher-order eutectic constituents, etc.) are calculated from the liquidus down to the temperature of final disappearance of the liquid.

As well, the amount of precipitation occurring in all constituents during subsequent full annealing at lower temperatures can be calculated.

In the case of equilibrium cooling, several assumptions must be made, due mainly to the occurrence of peritectic reactions which, in practice, seldom proceed to completion. Nevertheless, the results for the limiting case of complete peritectic reactions provide a useful limiting scenario.

In the case of Scheil-Gulliver cooling, far fewer assumptions are required since peritectic reactions are prohibited in this case.

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**Table II. Output of solidification software for 1.0 g-atom of an Al-Li alloy of composition  $X_{Li} = 0.10$ .**

<b>EQUILIBRIUM COOLING</b>	<b>SCHEIL-GULLIVER COOLING</b>
SUMMARY OF REACTIONS	
Cooling 1000 to 918.29 K Liquid cooling	
Constituent 1 918.29 to 904.40 K Liquid -> FCC	
COMPOSITION OF PHASES IN CONSTITUENTS AT 904.40 K (temperature of final disappearance of Liquid)	
<b><u>Constituent 1</u></b>	
Phase FCC	
	MOLE FRACTION    MASS FRACTION
Al	9.0000E-01    9.7221E-01
Li	1.0000E-01    2.7789E-02
	TOTAL AMT/g.atom    TOTAL
AMT/gram	1.0000E+00    2.4977E+01
SUMMARY OF REACTIONS	
Cooling 1000 to 918.29 K Liquid cooling	
Constituent 1 918.29 to 873.55 K Liquid -> FCC	
Constituent 2 873.55 K (isothermal) Liquid -> FCC + ALi	
COMPOSITION OF PHASES IN CONSTITUENTS AT 873.55 K (temperature of final disappearance of Liquid)	
<b><u>Constituent 1</u></b>	
Phase FCC	
	MOLE FRACTION    MASS FRACTION
Al	9.0868E-01    9.7480E-01
Li	9.1320E-02    2.5201E-02
	TOTAL AMT/g.atom    TOTAL
AMT/gram	9.3839E-01    2.3602E+01
<b><u>Constituent 2</u></b>	
Phase FCC	
	MOLE FRACTION    MASS FRACTION
Al	8.5939E-01    9.5961E-01
Li	1.4061E-01    4.0390E-02
	TOTAL AMT/g.atom    TOTAL
AMT/gram	4.3019E-02    1.0395E+00
Phase ALi	
	MOLE FRACTION    MASS FRACTION
Al	5.5580E-01    8.2947E-01
Li	4.4420E-01    1.7053E-01
	TOTAL AMT/g.atom    TOTAL
AMT/gram	1.8588E-02    3.3607E-01

**Table III. Output of solidification software for 1.0 g-atom of an Al-Li alloy of composition  $X_{Li} = 0.65$ .**

<b>EQUILIBRIUM COOLING</b>	<b>SCHEIL-GULLIVER COOLING</b>
<b>SUMMARY OF REACTIONS</b>	
Cooling 1000 to 901.42 K    Liquid cooling	
Constituent 1 901.42 to 793.01 K    Liquid -> AlLi	
Constituent 2 793.01 K (isothermal) Liquid + AlLi -> Al <sub>2</sub> Li <sub>3</sub>	
Constituent 2A 793.01 to 604.35 K Liquid -> Al <sub>2</sub> Li <sub>3</sub>	
Constituent 3 604.35 K (isothermal) Liquid + Al <sub>2</sub> Li <sub>3</sub> -> Al <sub>4</sub> Li <sub>9</sub>	
<b>COMPOSITION OF PHASES IN CONSTITUENTS AT 604.35 K (temperature of final disappearance of Liquid)</b>	
<b><u>Constituent 1</u></b> Phase AlLi	
	MOLE FRACTION    MASS FRACTION
Al	3.8832E-01    7.1164E-01
Li	6.1168E-01    2.8836E-01
	TOTAL AMT/g.atom    TOTAL
AMT/gram	0.0000E+00    0.0000E+00
<b><u>Constituent 2</u></b> Phase Al <sub>2</sub> Li <sub>3</sub>	
	MOLE FRACTION    MASS FRACTION
Al	4.0000E-01    7.2157E-01
Li	6.0000E-01    2.7843E-01
	TOTAL AMT/g.atom    TOTAL
AMT/gram	3.7846E-01    5.6606E+00
<b><u>Constituent 2A</u></b> Phase Al <sub>2</sub> Li <sub>3</sub>	
	MOLE FRACTION    MASS FRACTION
Al	4.0000E-01    7.2157E-01
Li	6.0000E-01    2.7843E-01
	TOTAL AMT/g.atom    TOTAL
AMT/gram	7.9877E-02    1.1947E+00
<b><u>Constituent 3</u></b> Phase Al <sub>4</sub> Li <sub>9</sub>	
	MOLE FRACTION    MASS FRACTION
Al	3.0769E-01    6.3339E-01
Li	6.9231E-01    3.6661E-01
	TOTAL AMT/g.atom    TOTAL AMT/gram
AMT/gram	5.1138E-02    6.7028E-01
<b><u>Constituent 4</u></b> Phase BCC	
	MOLE FRACTION    MASS FRACTION

	MOLE FRACTION	MASS FRACTION	Al	7.1617E-03	2.7275E-02
Al	3.0769E-01	6.3339E-01	Li	9.9284E-01	9.7272E-01
Li	6.9231E-01	3.6661E-01		TOTAL AMT/g.atom	TOTAL AMT/gram
	TOTAL AMT/g.atom	TOTAL		1.7776E-01	1.2593E+00
AMT/gram	5.4167E-01	7.0998E+00	Phase Al4Li9		
				MOLE FRACTION	MASS FRACTION
			Al	3.0769E-01	6.3339E-01
			Li	6.9231E-01	3.6661E-01
				TOTAL AMT/g.atom	TOTAL AMT/gram
				1.7107E-03	2.2423E-02







	Al	1.3724E-01	8.6536E-02
	Mg	4.2165E-01	2.3950E-01
		TOTAL AMT/g.atom TOTAL	
	AMT/gram		
		1.7657E-01	7.5554E+00
	Phase Mg <sub>12</sub> Zn <sub>13</sub>		
		MOLE FRACTION	MASS FRACTION
	Zn	4.6034E-01	6.9390E-01
	Al	5.9665E-02	3.7116E-02
	Mg	4.8000E-01	2.6898E-01
		TOTAL AMT/g.atom TOTAL	
	AMT/gram		
		1.6407E+00	7.1163E+01





		1.3896E+00	3.5359E+01
	Phase Tau		
		MOLE FRACTION	MASS FRACTION
	Zn	4.4042E-01	6.7334E-01
	Al	1.3784E-01	8.6969E-02
	Mg	4.2174E-01	2.3969E-01
		TOTAL AMT/g.atom	TOTAL
	AMT/gram		
		1.1513E+00	4.9234E+01
	<b>Constituent 6</b>		
	Phase HCP		
		MOLE FRACTION	MASS FRACTION
	Zn	2.6012E-02	6.6832E-02
	Al	2.7314E-02	2.8962E-02
	Mg	9.4667E-01	9.0421E-01
		TOTAL AMT/g.atom	TOTAL
	AMT/gram		
		2.5019E+00	6.3666E+01
	Phase Tau		
		MOLE FRACTION	MASS FRACTION
	Zn	4.4111E-01	6.7397E-01
	Al	1.3724E-01	8.6536E-02
	Mg	4.2165E-01	2.3950E-01
		TOTAL AMT/g.atom	TOTAL
	AMT/gram		
		2.4807E-01	1.0615E+01
	Phase Mg <sub>12</sub> Zn <sub>13</sub>		
		MOLE FRACTION	MASS FRACTION
	Zn	4.6034E-01	6.9390E-01
	Al	5.9665E-02	3.7116E-02
	Mg	4.8000E-01	2.6898E-01
		TOTAL AMT/g.atom	TOTAL
	AMT/gram		
		2.3051E+00	9.9981E+01



Phase Mg2Zn11			Mg	2.3835E-03	8.9860E-04
	MOLE FRACTION	MASS FRACTION	TOTAL AMT/g.atom TOTAL		
Zn	8.0841E-01	9.1742E-01	AMT/gram		
Al	3.7743E-02	1.7677E-02		6.1642E-02	3.9739E+00
Mg	1.5385E-01	6.4904E-02	Phase Mg2Zn11		
TOTAL AMT/g.atom TOTAL				MOLE FRACTION	MASS FRACTION
AMT/gram			Zn	8.1811E-01	9.2246E-01
	2.0275E-01	1.1681E+01	Al	2.8043E-02	1.3049E-02
			Mg	1.5385E-01	6.4487E-02
			TOTAL AMT/g.atom TOTAL		
			AMT/gram		
				4.1368E-02	2.3987E+00
			<b>Constituent 4</b>		
			Phase FCC		
				MOLE FRACTION	MASS FRACTION
			Zn	6.4960E-01	8.1797E-01
			Al	3.4929E-01	1.8151E-01
			Mg	1.1089E-03	5.1909E-04
			TOTAL AMT/g.atom TOTAL		
			AMT/gram		
				8.2854E-02	4.3020E+00
			Phase HCP_Zn		
				MOLE FRACTION	MASS FRACTION
			Zn	9.7560E-01	9.8988E-01
			Al	2.2039E-02	9.2282E-03
			Mg	2.3577E-03	8.8931E-04
			TOTAL AMT/g.atom TOTAL		
			AMT/gram		
				2.0879E-01	1.3454E+01
			Phase Mg2Zn11		
				MOLE FRACTION	MASS FRACTION
			Zn	8.1719E-01	9.2199E-01
			Al	2.8962E-02	1.3485E-02
			Mg	1.5385E-01	6.4527E-02
			TOTAL AMT/g.atom TOTAL		
			AMT/gram		
				1.5469E-01	8.9640E+00

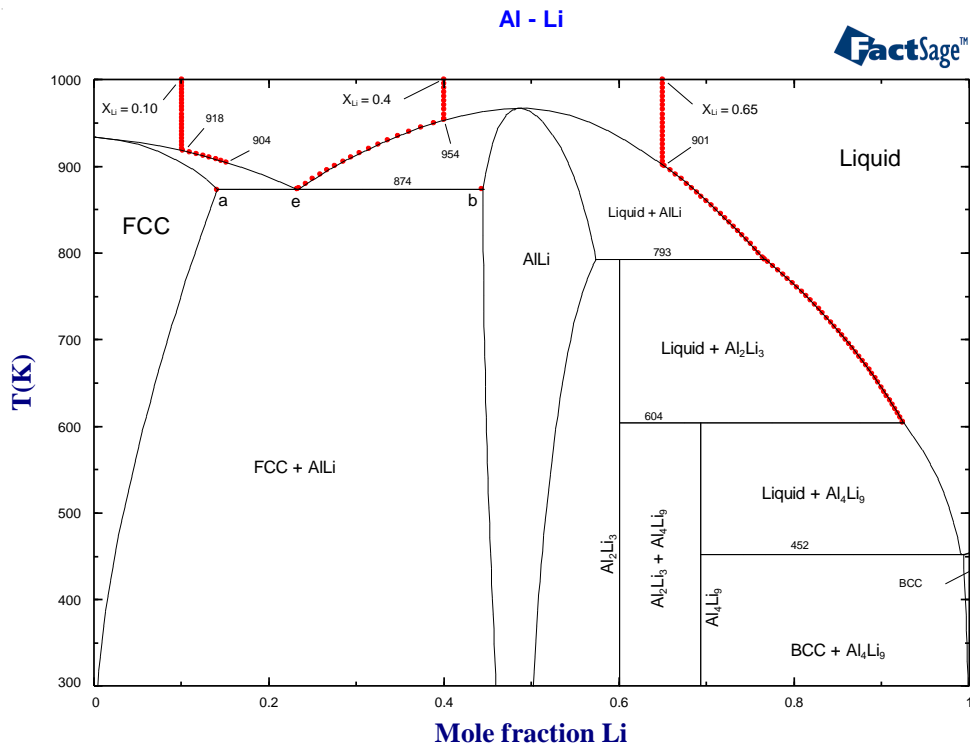


Fig. 1 Al-Li phase diagram showing liquid crystallization paths for equilibrium cooling at three alloy compositions.

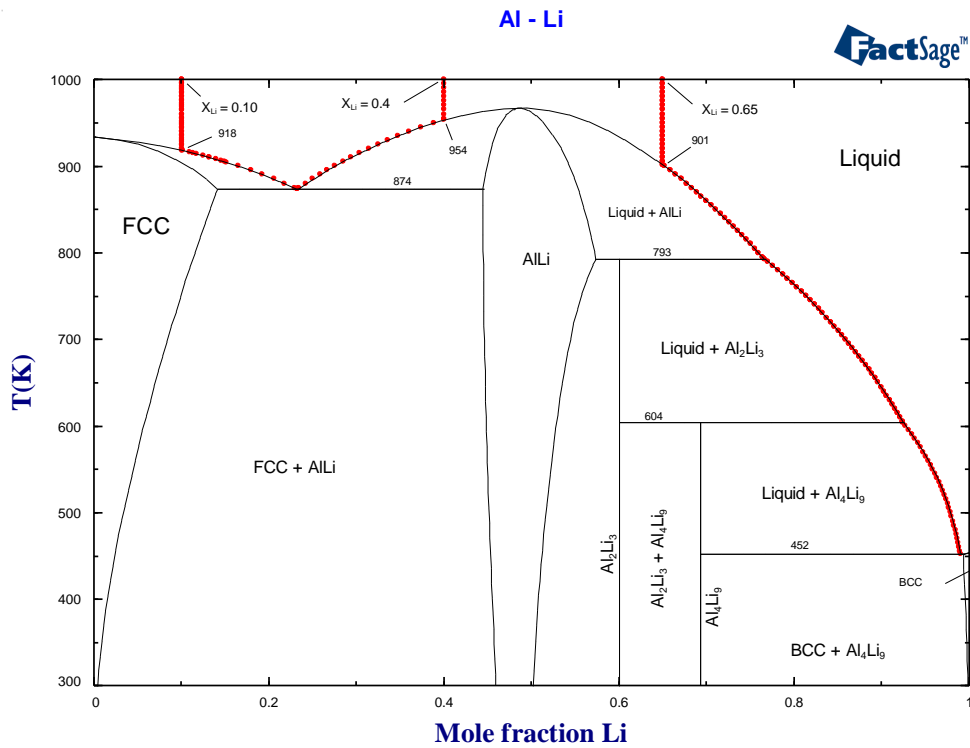


Fig. 2 Al-Li phase diagram showing liquid crystallization paths for Scheil-Gulliver cooling at three alloy compositions.



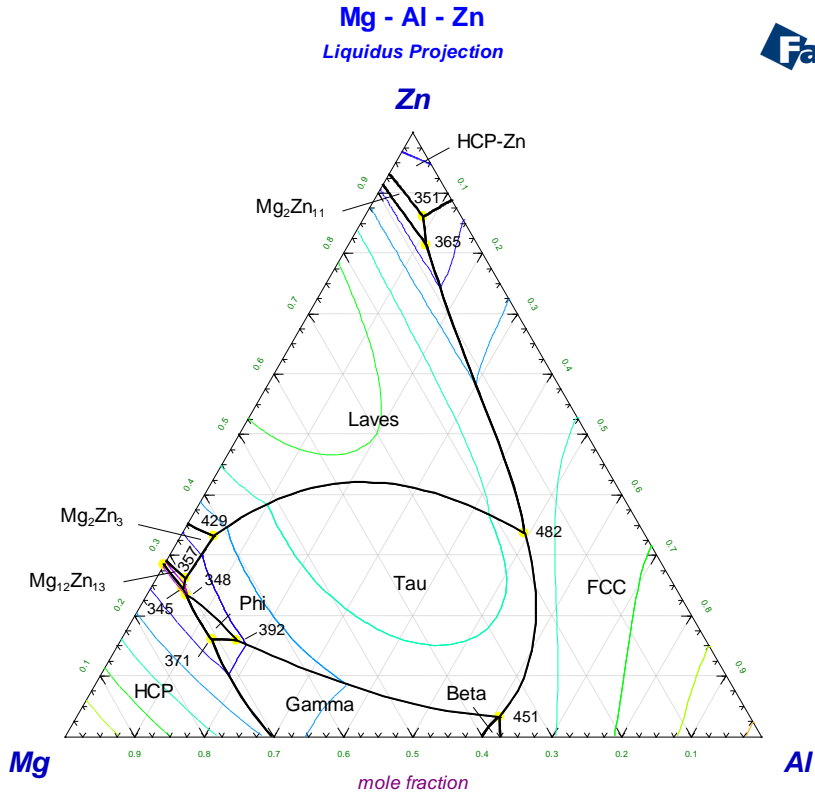


Fig. 3 Liquidus surface of the Mg-Al-Zn system. (Temperatures in °C).

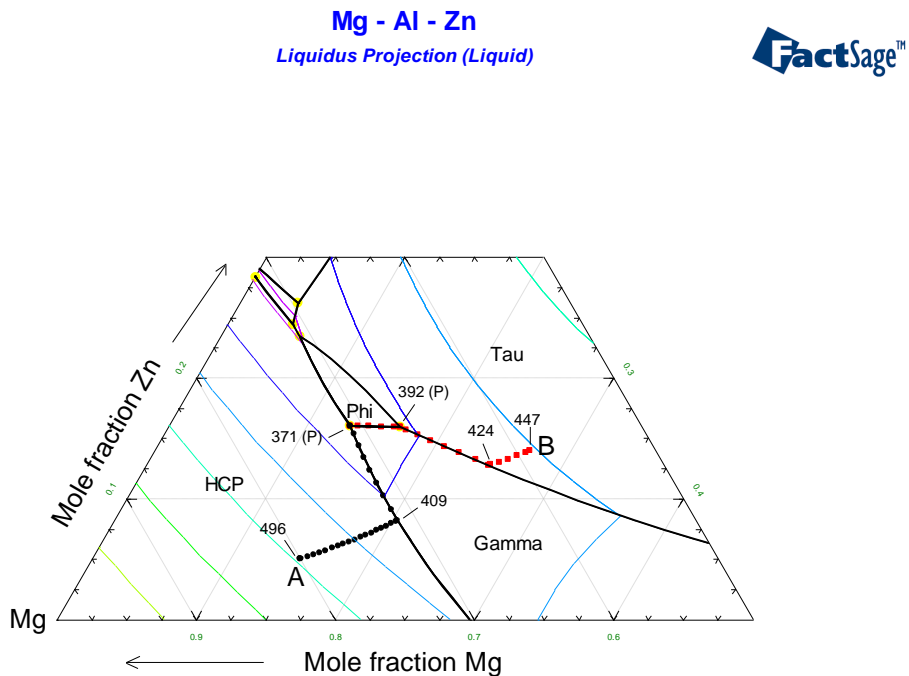


Fig. 4 Enlargement of the Mg-rich corner of Fig. 3 showing liquid crystallization paths for equilibrium cooling of alloy compositions A and B. (Temperatures in °C; E and P indicate eutectic or peritectic invariant points).

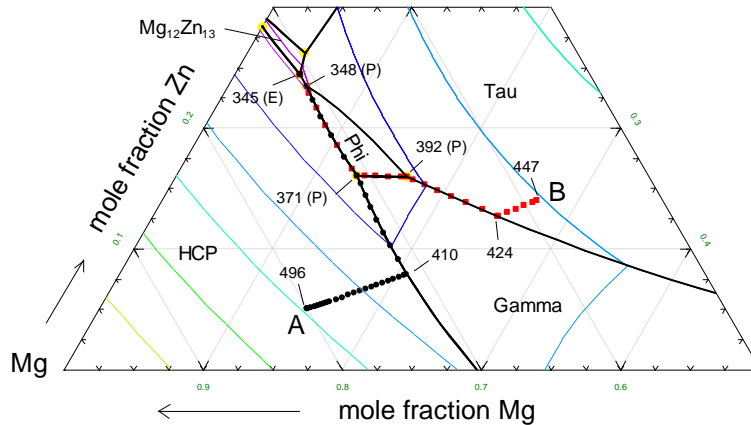


Fig. 5 Enlargement of the Mg-rich corner of Fig. 3 showing liquid crystallization paths for Scheil-Gulliver cooling of alloy compositions A and B. (Temperatures in °C; E and P indicate eutectic or peritectic invariant points).

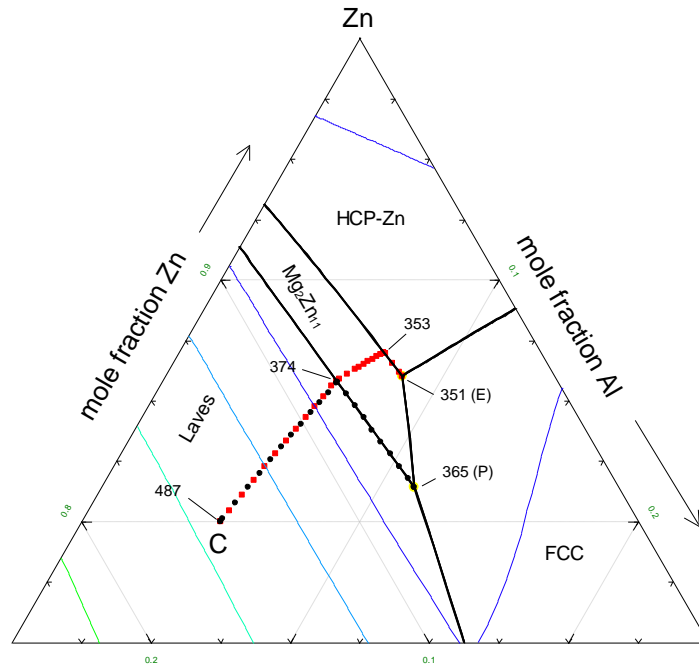


Fig. 6 Enlargement of the Mg-rich corner of Fig. 3 showing liquid crystallization paths for alloy composition C for equilibrium cooling (black circles) and Scheil-Gulliver cooling (red diamonds). (Temperatures in °C; E and P indicate eutectic or peritectic invariant points).

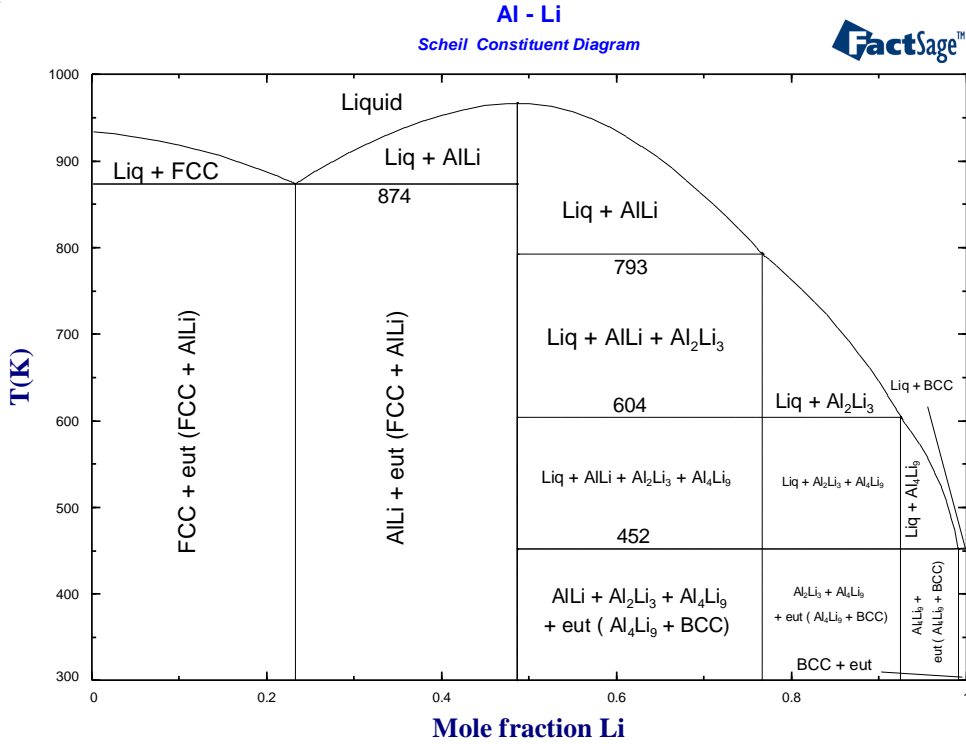


Fig. 7 Calculated Scheil-Gulliver constituent diagram of the Al-Li system<sup>[5]</sup>.

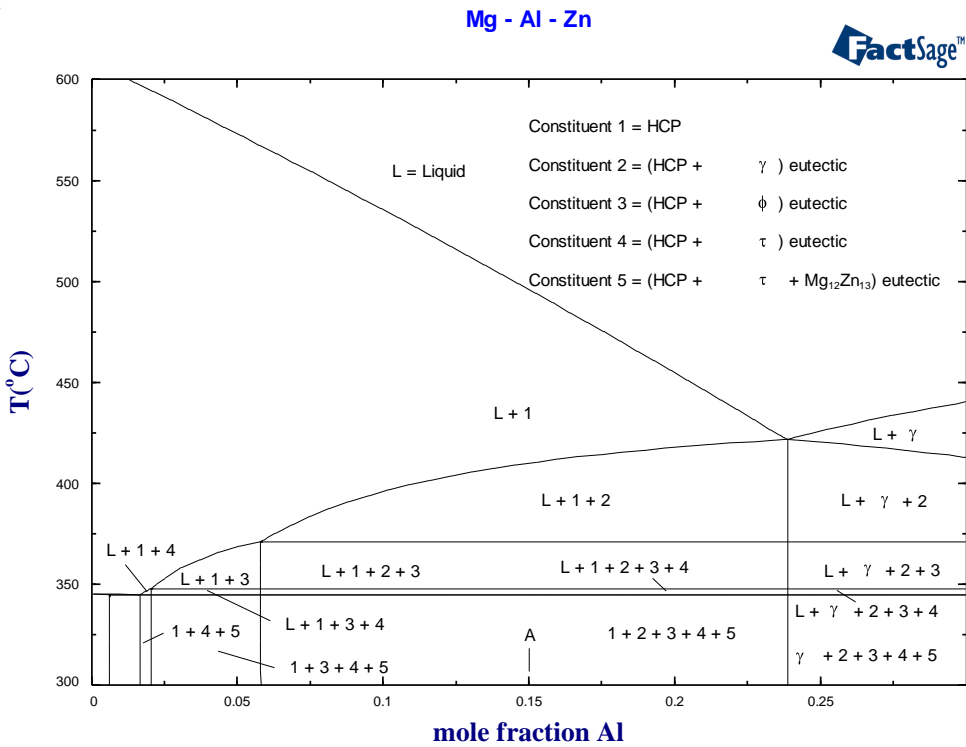


Fig. 8 Calculated Scheil-Gulliver constituent diagram of the Mg-Al-Zn system<sup>[5]</sup> at constant mole fraction  $X_{Zn} = 0.05$ .