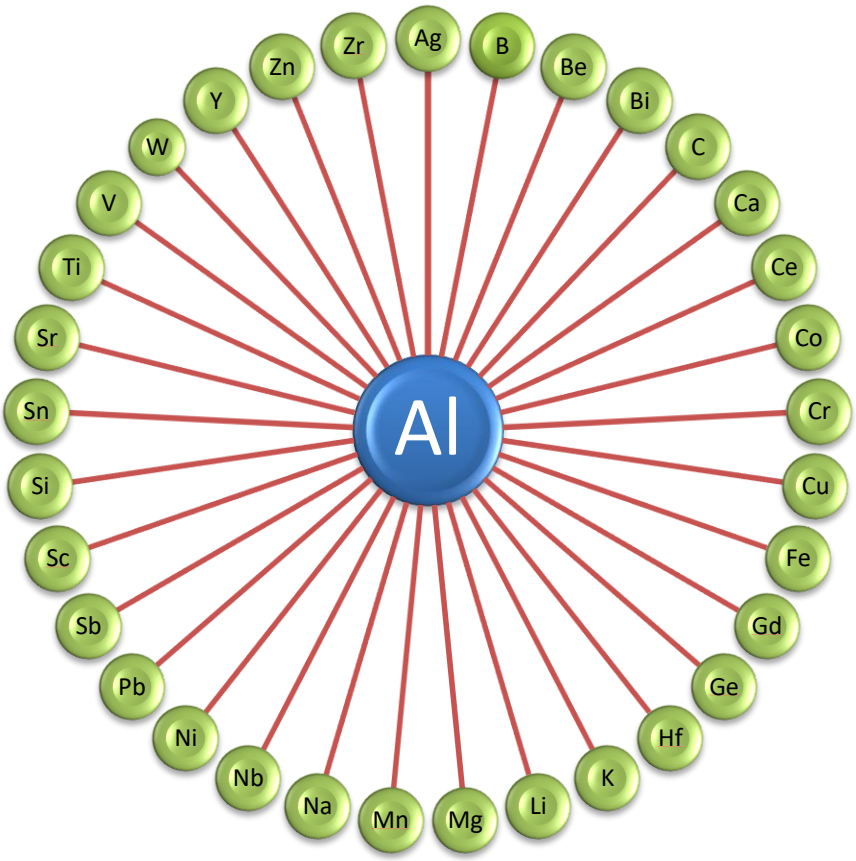
# 1. PanAluminum

Thermodynamic database for multi-component Aluminum-rich casting and wrought alloys

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# 1.1 Components

Total of 34 components are included in the database as listed here:

Major alloying elements: **Al**, Cu, Fe, Mg, Mn, Si and Zn

Minor alloying elements: Ag, B, Be, Bi, C, Ca, Ce, Co, Cr, Gd, Ge, Hf, K, Li, Na, Nb, Ni, Pb, Sb, Sc, Sn, Sr, Ti, V, W, Y, and Zr

# 1.2 Suggested Composition Range

The suggested composition range for each element is listed in Table 1.1. It should be noted that this given composition range is rather conservative. It is derived from the chemistries of the multicomponent commercial alloys that have been used to validate the current database. In the subsystems, many of these elements can be applied to a much wider composition range. In fact, some subsystems are valid in the entire composition range as given in section 1.5.

Table 1.1: Suggested composition range

| Element | Composition Range (wt.%) |
|---|---|
| Al | 80 ~ 100 |
| Cu | 0 ~ 5.5 |
| Fe | 0 ~ 2.0 |
| Mg | 0 ~ 7.6 |
| Mn | 0 ~ 1.2 |
| Si | 0 ~ 17.5 |
| Zn | 0 ~ 8.1 |
| others | 0 ~ 1.0 |

For many binary and ternary systems, there is no composition limit and they are covered in the full range from 0-100% as detailed in the Tables below. The components are classified as "Minor" even though their coverage in binary systems is similar to most "Major" components. However, they are covered less extensively in ternary systems as detailed in section 1.5.

## 1.3 What's new in PanAl2020

Major improvements made in PanAl2020 include enhanced assessment of the Al-Fe-Ni, Al-Mg-Sc, Al-Sc-Si, and Al-Si-Sr ternary systems. Other improvements include extended in depth descriptions concerning mutual interactions of components in multicomponent alloys.

## 1.4 Phases

Total of 851 phases are included in the current database. The names and thermodynamic models of some phases are given in Table 1.2. Information on all phases will be displayed in the TDB viewer of Pandat or can be found at www.computherm.com.

Table 1.2: Phase name and related information

| Name | Lattice Size | Constituent |
|---|---|---|
| Ag5Zn8 | (2)(2)(3)(6) | (Ag,Zn)(Ag)(Ag,Zn)(Ag,Zn) |
| AgMg3 | (0.23)(0.77) | (Ag,Cu)(Al,Mg) |
| AgMg4 | (0.2)(0.8) | (Ag,Cu)(Al,Mg) |
| Al18Mg3V2 | (18)(3)(2) | (Al)(Mg)(V) |
| Al2Fe | (2)(1) | (Al)(Cr,Fe,Mn) |
| Al2LiMg | (0.53)(0.33)(0.14) | (Al)(Li)(Mg) |
| Al2W | (2)(1) | (Al)(W) |
| Al5Fe2 | (5)(2) | (Al)(Cr,Fe,Mn) |
| Al5Fe4 | (1) | (Al,Fe,Mn) |
| Al8FeMg3Si6 | (8)(3)(1)(6) | (Al)(Mg)(Fe)(Si) |
| Al8FeMnSi2 | (16)(2)(2)(3) | (Al)(Fe)(Mn)(Si) |

| | | |
|---|---|---|
| AlCu_Theta | (0.667)(0.333) | (Al)(Ag,Al,Cu) |
| AlMg_Gamma | (10)(24)(24) | (Ca,Mg)(Al,Cu,Li,Mg,Zn)(Al,Cu,Mg,Zn) |
| Alpha_AlFeSi | (0.66)(0.19)(0.05)(0.1) | (Al)(Fe)(Si)(Al,Si) |
| Cu3Mg2Si | (3)(2)(1) | (Cu)(Mg)(Si) |
| Delta_AlFeSi | (5)(1) | (Al,Si)(Fe) |
| Fcc | (1)(1) | (Ag,Al,Be,Bi,Ca,Ce,Co,Cr,Cu,Fe,Gd,Ge,Hf,K,Li,Mg,Mn,Na,Nb,Ni,Pb,Sb,Sc,Si,Sn,Sr,Ti,V,W,Y,Zn,Zr)(B,C,Va) |
| Gamma_AlFeSi | (0.635)(0.205)(0.16) | (Al)(Fe)(Si) |
| Li2MgSi | (0.5)(0.25)(0.25) | (Li)(Mg)(Si) |
| LiMg2Si | (0.5)(0.25)(0.25) | (Mg)(Si)(Li,Va) |
| Mu | (7)(2)(4) | (Co,Fe,Mn,Nb,W)(Nb,W)(Co,Fe,Nb,W) |
| NbSn2 | (1)(2) | (Nb)(Sn) |
| Q_Al5Cu2Mg8Si6 | (0.2381)(0.0952)(0.381)(0.2857) | (Al)(Cu)(Mg)(Si) |
| T10_AlFeSi | (0.6)(0.25)(0.15) | (Al)(Fe)(Si) |
| T11_AlFeSi | (0.6538)(0.2308)(0.1154) | (Al)(Fe)(Si) |

## 1.5 Key Elements and Subsystems

The modeling status for the constituent binaries and ternaries are given in Table 1.3 and Table 1.4. The color represents the following meaning:

: Full description

: Full description for major phases

: Extrapolation

Table 1.3: Modeling status of constituent binary systems

| | Al | B | Be | Bi | C | Ca | Ce | Co | Cr | Cu | Fe | Gd | Ge | Hf | K | Li | Mg | Mn | Na | Nb | Ni | Pb | Sb | Sc | Si | Sn | Sr | Ti | V | W | Y | Zn | Zr |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ag | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Al | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| B | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Be | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Bi | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ca | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ce | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Co | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Cr | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Cu | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Fe | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Gd | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ge | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Hf | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| K | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Li | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Mg | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Mn | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Na | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Nb | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ni | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Pb | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Sb | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Sc | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Si | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Sn | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Sr | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ti | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| W | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Y | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Zn | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table 1.4: Modeling status of constituent ternary systems

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Ag-Al-Cu | Ag-Al-Ge | Ag-Al-Mg | Ag-Al-Si | Ag-Al-Zn | Ag-Cu-Mg | Al-Be-Si | Al-Ca-Mg |
| Al-Ce-Cu | Al-Ce-Mg | Al-Co-Cu | Al-Co-Fe | Al-Co-Mn | Al-Co-Si | Al-Cr-Fe | Al-Cr-Ni |
| Al-Cr-Si | Al-Cu-Fe | Al-Cu-Li | Al-Cu-Mg | Al-Cu-Mn | Al-Cu-Sb | Al-Cu-Si | Al-Cu-Zn |
| Al-Fe-Mg | Al-Fe-Mn | Al-Fe-Ni | Al-Fe-Si | Al-Fe-Zn | Al-Gd-Ni | Al-Ge-Si | Al-Li-Mg |
| Al-Li-Si | Al-Li-Zn | Al-Mg-Mn | Al-Mg-Na | Al-Mg-Sb | Al-Mg-Si | Al-Mg-V | Al-Mg-Zn |
| Al-Mn-Si | Al-Si-Sn | Al-Si-Sr | Al-Si-Ti | Al-Si-Zn | Al-Si-Zr | Cu-Mg-Si | Cu-Mg-Zn |
| Fe-Mn-Si | Li-Mg-Si | Mg-Li-Si | Mg-Si-Zn | | | | |

# 1.6 Database Validation

The PanAl database is validated by a large amount of phase equilibrium data. Two examples are shown here. Figure 1.1 shows the calculated isotherm of Al-Cu-Mg-Si at 500°C with Si content of 1.8wt%. The experimental data of D.P. Smith [1962Smi] are plotted on it for comparison. Figure 1.2 shows the calculated isopleth of Al-Fe-Mg-Si at 4wt.%Mg and 0.5wt.%Fe with experimental data from Phillips [1961Phi].

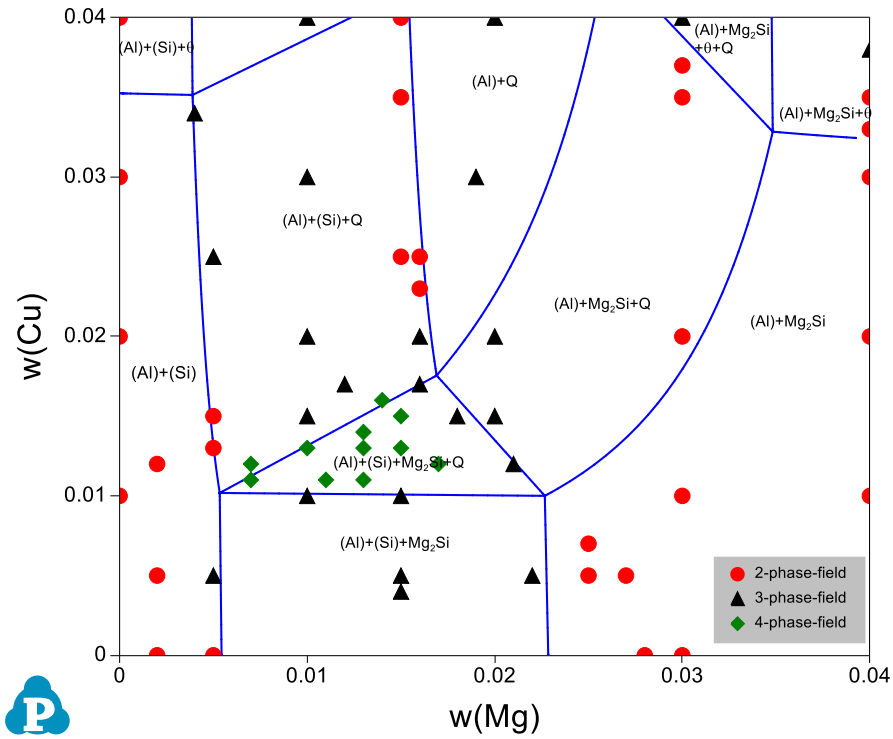


Figure 1.1: Comparison of a calculated isothermal section of Al-Cu-Mg-Si at 1.8wt%Si and at T=500°C with the experimental data [1962Smi]

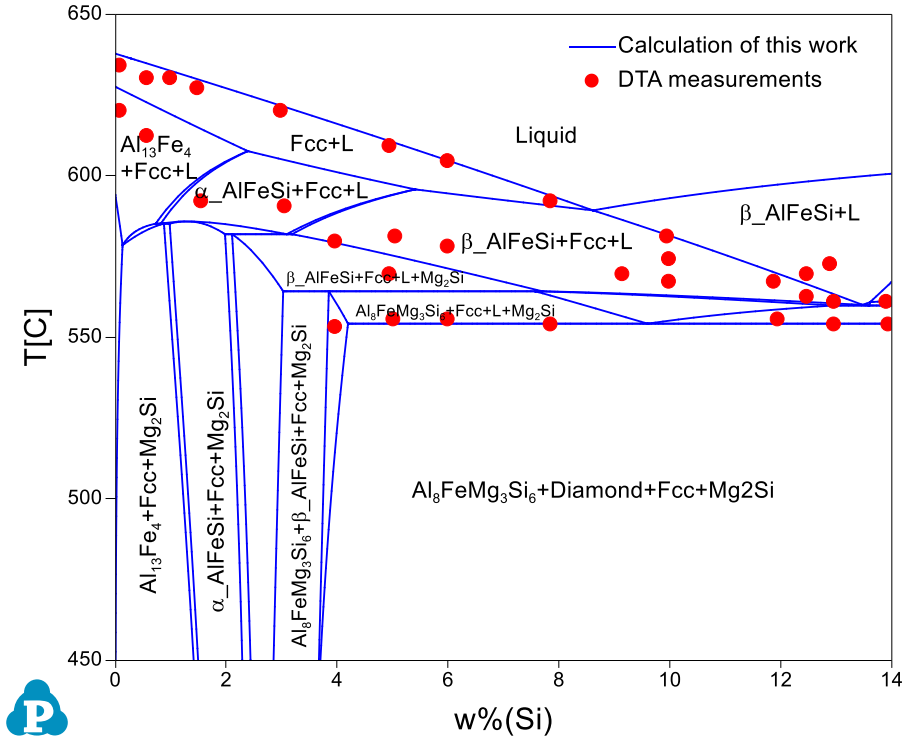


Figure 1.2: Comparison of a calculated isopleth of Al-Fe-Mg-Si at 4wt.%Mg and 0.5wt.%Fe with the experimental data [1961Phi]

In addition to the validation of phase equilibria, the current database has also been subjected to extensive validation by the solidification data of commercial aluminum alloys. The predicted liquidus and solidus temperatures of cast and wrought are shown in Figure 1.3 ~ Figure 1.6 with experimental data, respectively.

**Cast aluminum alloys:** 201, 206, 208, 242, 295, 296, 308, 319, 356, 357, 359, 360, 380, 383, 384, 390, 771, 850

**Wrought aluminum alloys:** 2014, 2017, 2024, 2036, 2124, 2218, 2219, 2319, 3003, 3004, 3105, 4032, 5052, 5056, 5083, 5086, 5154, 5182, 5356, 5454, 5456, 5457, 6005, 6009, 6010, 6061, 6063, 6066, 6070, 6101, 6151, 6201, 6205, 6351, 6463, 7005, 7039, 7049, 7075, 7178, 7475

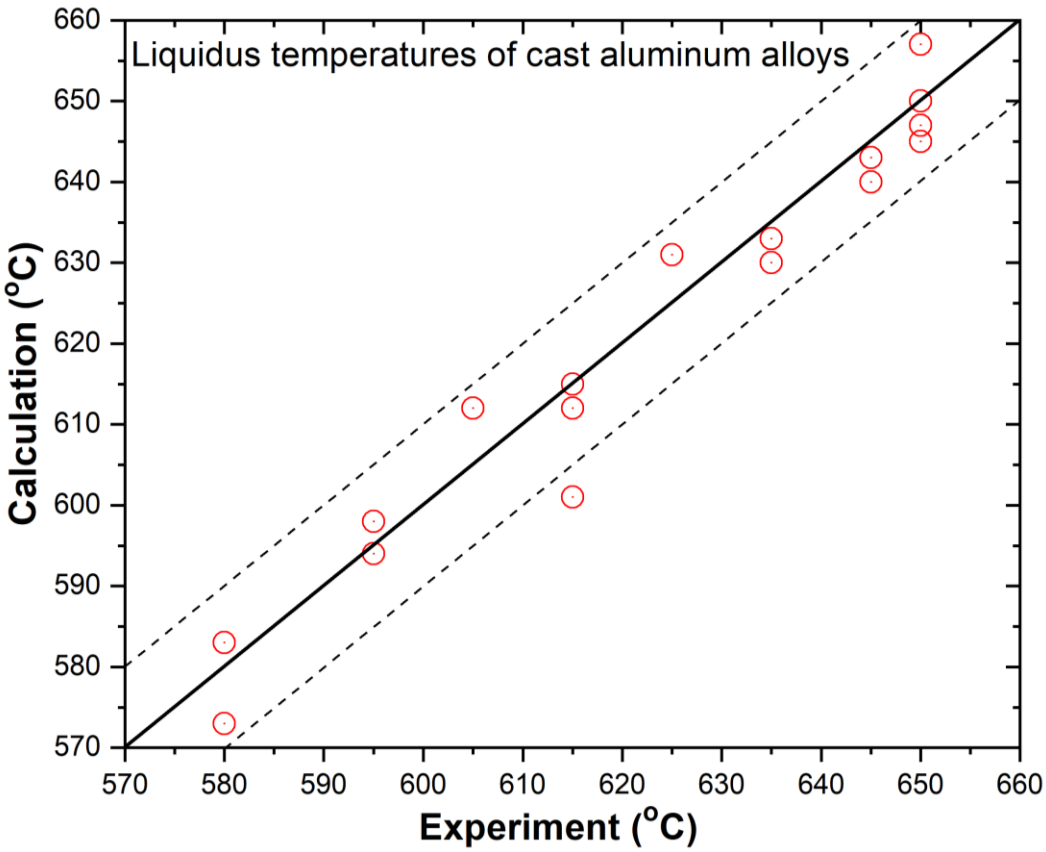


Figure 1.3: Comparison between calculated and experimentally measured liquidus temperatures of cast aluminum alloys

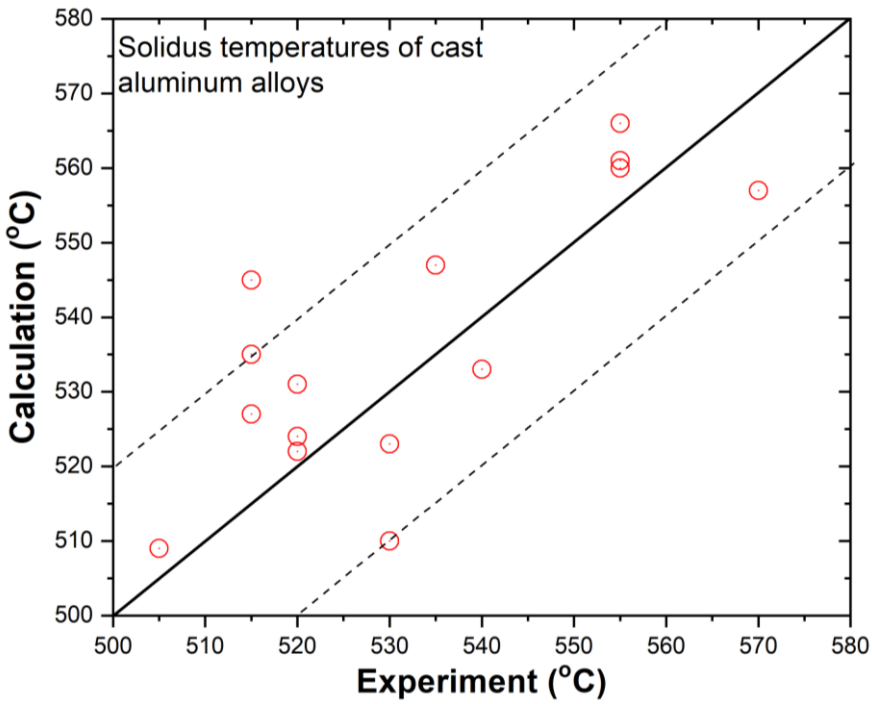


Figure 1.4: Comparison between calculated and experimentally measured solidus temperatures of cast aluminum alloys

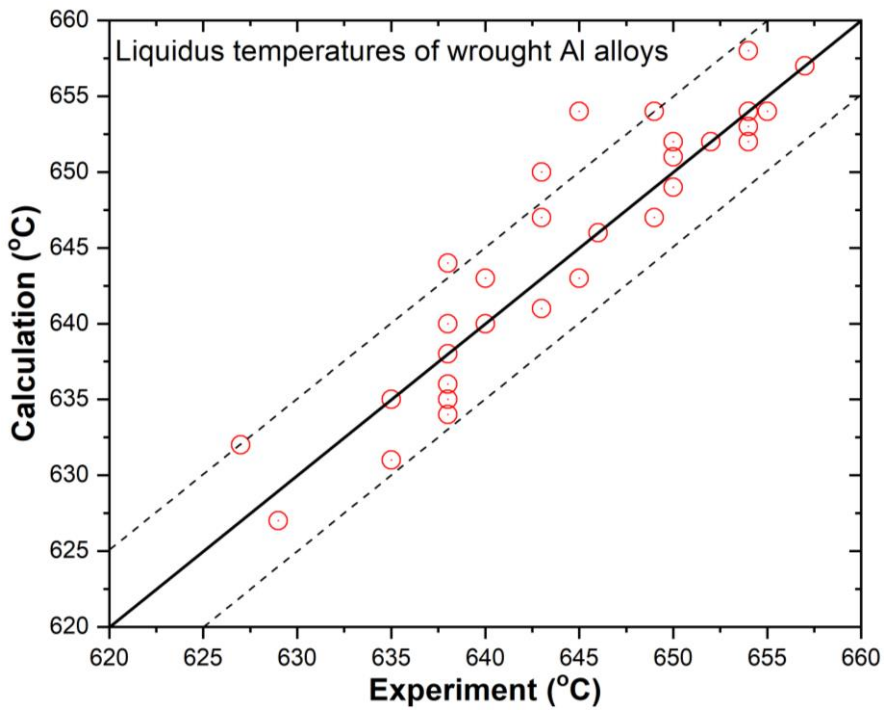


Figure 1.5: Comparison between calculated and experimentally measured liquidus temperatures of wrought aluminum alloys

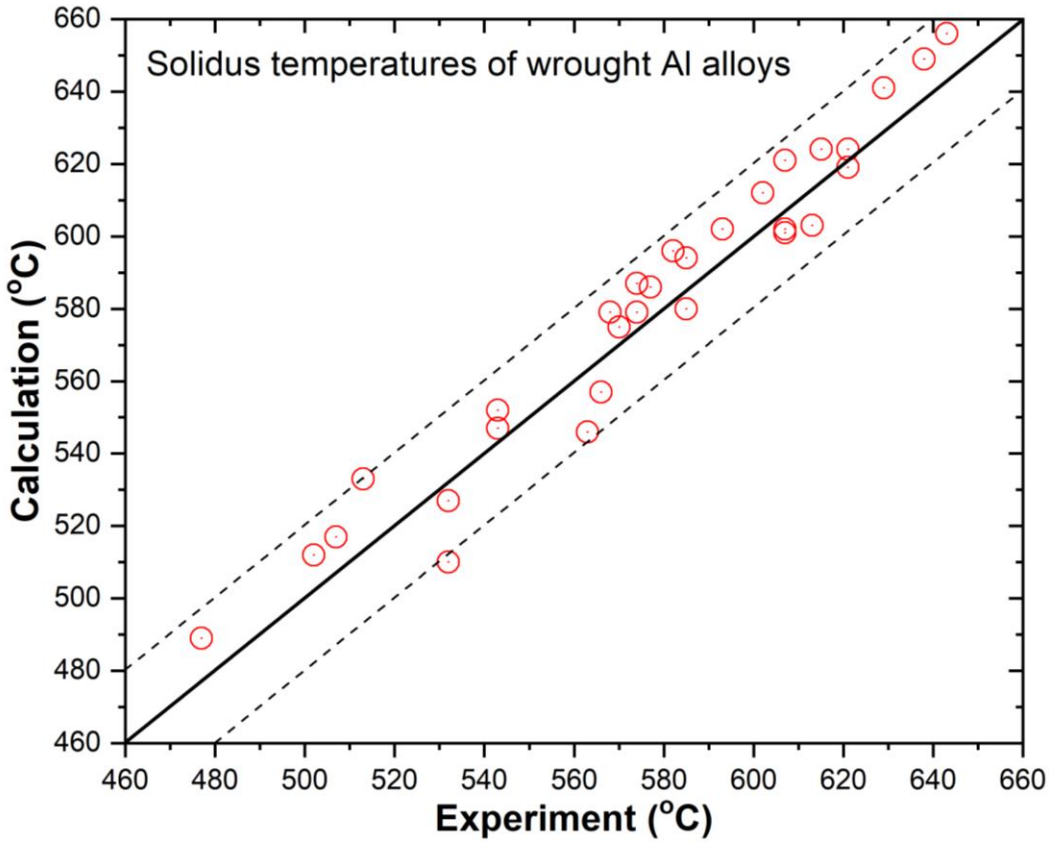

Figure 1.6: Comparison between calculated and experimentally measured solidus temperatures of wrought aluminum alloys

The solidification paths of several commercial aluminum alloys were experimentally investigated by Backerud et al [1986Bac]. The simulated solidification paths using both Scheil model and lever rule for four of these alloys (319.1, A357.2, A6351, A7075) are shown in Figure 1.7 ~ Figure 1.10 with the experimental data of Backerud et al [1986Bac].

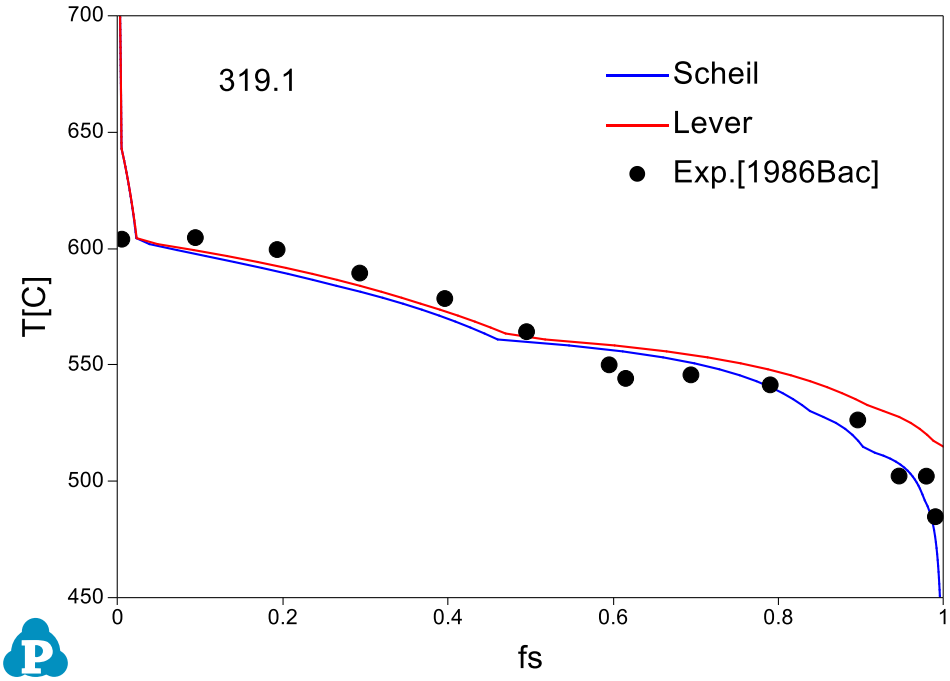


Figure 1.7: Comparison between calculated and experimentally measured solidification paths of 319.1 aluminum alloy

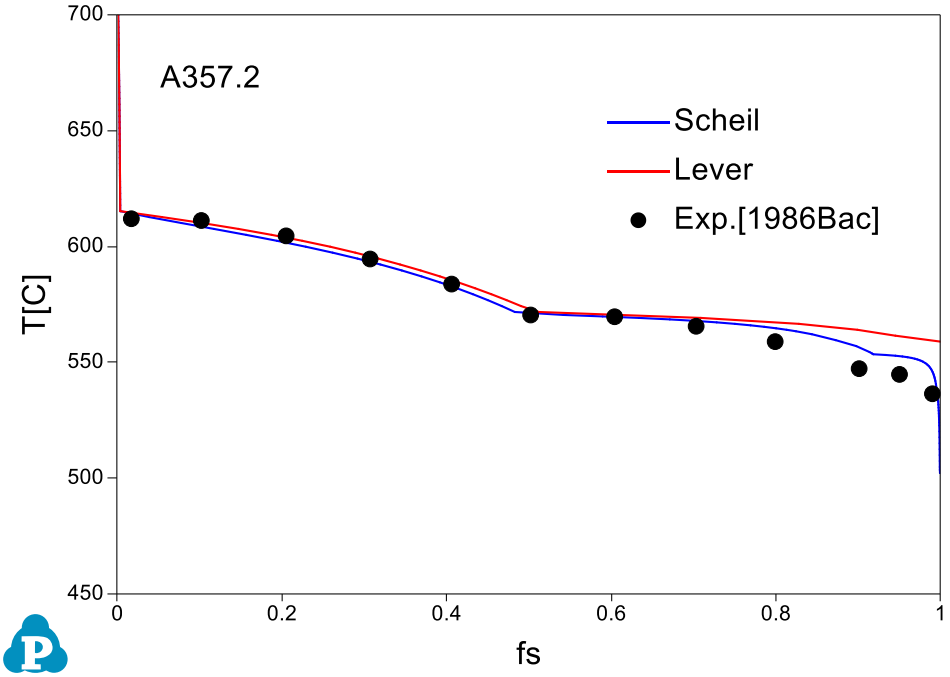


Figure 1.8: Comparison between calculated and experimentally measured solidification paths of A357.2 aluminum alloy

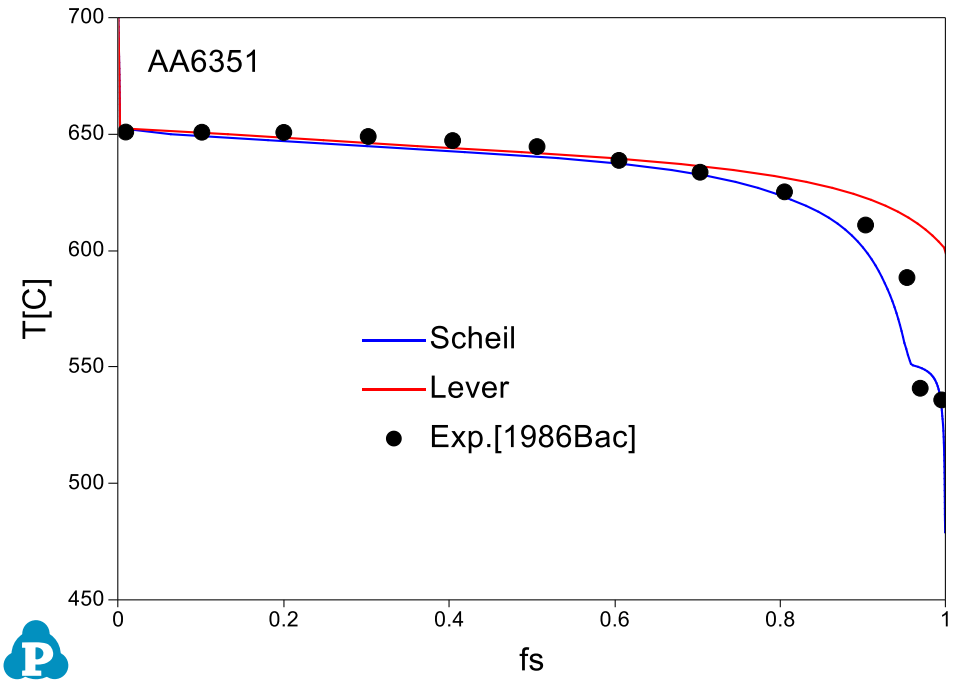


Figure 1.9: Comparison between calculated and experimentally measured solidification paths of AA6351 aluminum alloy

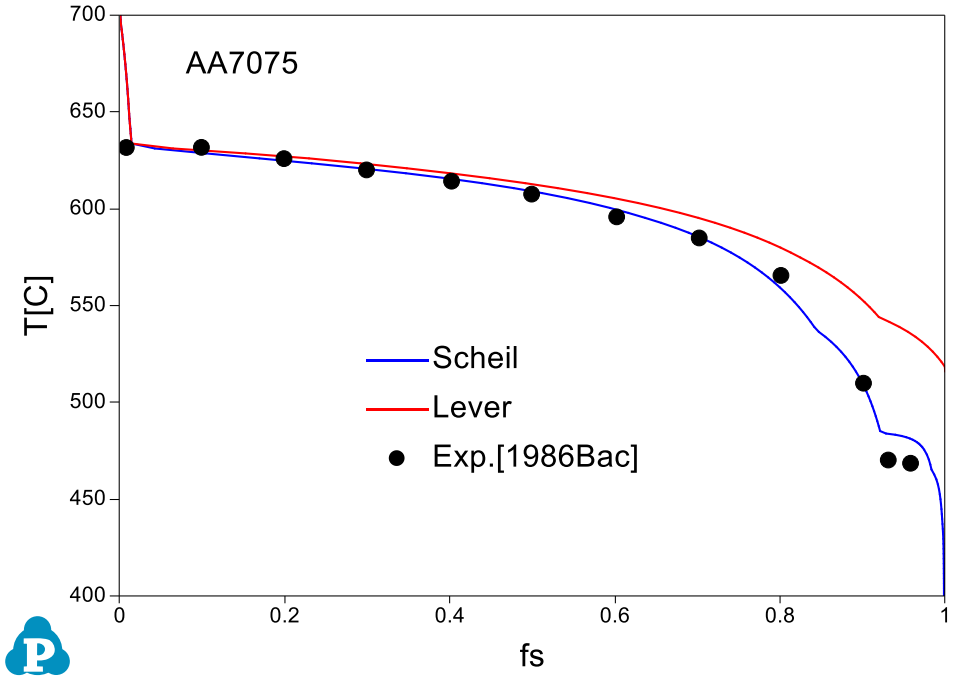


Figure 1.10: Comparison between calculated and experimentally measured solidification paths of AA7075 aluminum alloy

This database can also supply important parameters for processing simulation. One of these parameters is partition coefficient. The calculated partition coefficients have also been extensively validated. Examples for two Al-Cu-Mg-Zn quaternary alloys are given below. Figure 1.11 and Figure 1.12 show comparisons between calculated and measured partition coefficient for Al-4Cu-0.9Mg-2.6Zn (wt%) and Al-2.5Cu-1.3Mg-2.63Zn (wt%), respectively. The good agreement between the experimental and calculated results, as shown in these figures, indicates the reliability of the current PanAl thermodynamic database in providing thermodynamic input for processing simulation.

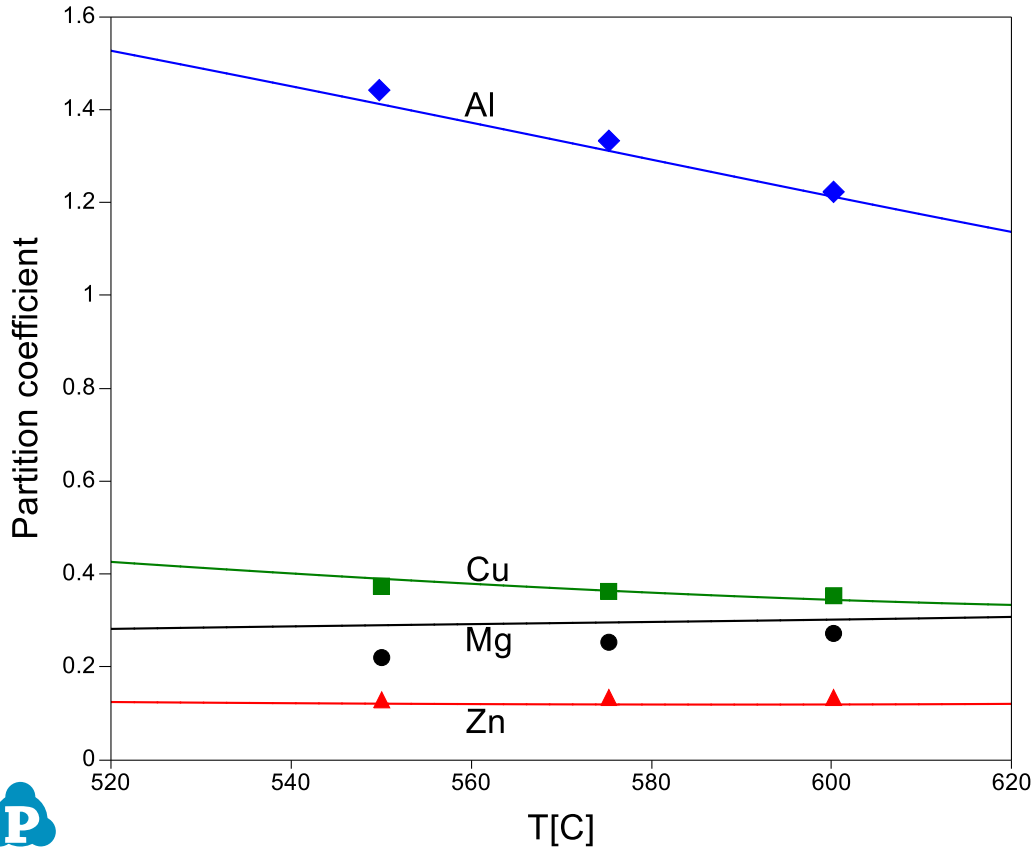


Figure 1.11: Calculated and experimentally determined [1998Lia] partition coefficients of Al-4Cu-0.9Mg-2.6Zn (wt%) alloy

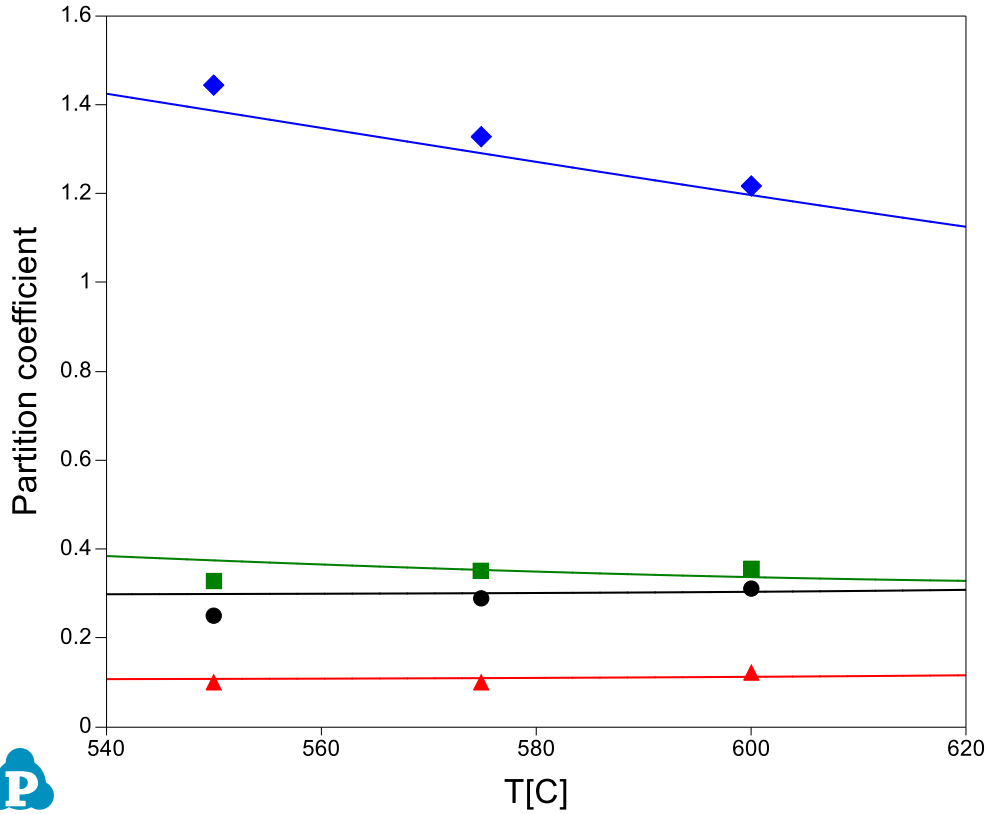


Figure 1.12: Calculated and experimentally determined [1998Lia] partition coefficients of Al-2.5Cu-1.3Mg-2.63Zn (wt%) alloy

# 1.7 References


[1962Smi] D.P. Smith, Metallurgia, 1(1962): 223-229.

[1961Phi] H.W.L. Phillips, "Equilibrium diagrams of aluminum alloy systems", The aluminum development association, Information Bulletin 25, London, 1961: 105-108.

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[1998Lia] P. Liang, T. Tarfa,J.A. Robinson, S.Wagner, P.Ochin, M.G. Harmelin, H.J. Seifert, H.L. Lukas,F. Aldinger, "Experimental investigation and thermodynamic calculation of the Al-Mg-Zn system", Thermochim. Acta, 314 (1998): 87-110.